Chapter 1

Introduction

1.1 Examples

- **Chemical reactions** (see [8], pages 115 - 116)

  Brusselator: Six substances (species) A, B, D, E, X, Y undergo the following reactions:

$$\begin{aligned} A &\xrightarrow{k_1} X \\ B + X &\xrightarrow{k_2} Y + D \\ 2X + Y &\xrightarrow{k_3} 3X \\ X &\xrightarrow{k_4} E \end{aligned}$$

  Here, k_i are the rate constants.

  Using the law of mass action (Massenwirkungsgesetz) we obtain the following differential equations for the concentrations c_A, c_B, c_D, c_X, c_Y:

$$\begin{aligned} c_A'(t) &= -k_1\, c_A(t), \\ c_B'(t) &= -k_2\, c_B(t) c_X(t), \\ c_D'(t) &= k_2\, c_B(t) c_X(t), \\ c_E'(t) &= k_4\, c_X(t), \\ c_X'(t) &= k_1\, c_A(t) - k_2\, c_B(t) c_X(t) + k_3\, c_X(t)^2 c_Y(t) - k_4\, c_X(t), \\ c_Y'(t) &= k_2\, c_B(t) c_X(t) - k_3\, c_X(t)^2 c_Y(t). \end{aligned}$$

  Initial conditions: $c_A(0)$, $c_B(0)$, $c_D(0)$, $c_E(0)$, $c_X(0)$, $c_Y(0)$ are given

- **Mechanical systems** (see [8], pages 8, 30, 31)

  m: mass of the point mass.
  $x(t)$, $y(t)$: position of the point mass at time t.

– Elastic pendulum in 1D: $x(t) = 0$,
Newton's second law:

$$m\,\ddot{y}(t) = -m\,g - k\,\left(y(t) - (-\ell)\right)$$

with the acceleration of gravity g, the length of the spring at rest ℓ and the spring constant k (Hooke's law).
Initial conditions:

$$y(0) = y_0, \quad \dot{y}(0) = v_0.$$

Rewriting in Lagrangian mechanics: Euler-Lagrange equation

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}} = \frac{\partial \mathcal{L}}{\partial y}$$

with the Lagrangian

$$\mathcal{L} = T - U$$

with the kinetic energy T and the potential energy U. Here:

$$T = \frac{m}{2}\,\dot{y}^2, \quad U = mgy + \frac{k}{2}\,(y+\ell)^2.$$

– Elastic pendulum in 2D:

$$\mathcal{L} = \frac{m}{2}\,\left(\dot{x}^2 + \dot{y}^2\right) - mgy - \frac{k}{2}\left(\sqrt{x^2+y^2} - \ell\right)^2.$$

Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} = \frac{\partial \mathcal{L}}{\partial x}, \quad \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}} = \frac{\partial \mathcal{L}}{\partial y}.$$

Here:

$$m\,\ddot{x} = -k\,\left(\sqrt{x^2+y^2} - \ell\right)\frac{x}{\sqrt{x^2+y^2}},$$
$$m\,\ddot{y} = -mg - k\,\left(\sqrt{x^2+y^2} - \ell\right)\frac{y}{\sqrt{x^2+y^2}},$$

or, equivalently

$$m\,\ddot{x} = -2\,\lambda\,x,$$
$$m\,\ddot{y} = -mg - 2\,\lambda\,y$$

with

$$\lambda = \frac{k}{2}\,\frac{\sqrt{x^2+y^2} - \ell}{\sqrt{x^2+y^2}} = \frac{k}{2}\,\left(1 - \frac{\ell}{\sqrt{x^2+y^2}}\right). \quad \text{i.e.} \quad x^2 + y^2 = \frac{\ell^2}{\left(1 - \frac{2\lambda}{k}\right)^2}.$$

In the limit case $k \to \infty$ (pendulum with fixed length) we obtain a system of differential algebraic equations (DAE):

$$\begin{aligned} m\,\ddot{x} &= -2\,\lambda\,x \\ m\,\ddot{y} &= -mg - 2\,\lambda\,y \\ 0 &= x^2 + y^2 - \ell^2. \end{aligned}$$

Initial conditions: $x(0)$, $\dot{x}(0)$, $y(0)$, $\dot{y}(0)$,

Extension of the Lagrangian mechanics to mechanical systems with constraints: Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} = \frac{\partial \mathcal{L}}{\partial x}, \quad \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{y}} = \frac{\partial \mathcal{L}}{\partial y}$$

with

$$\mathcal{L} = T - U - \lambda\left(x^2 + y^2 - \ell^2\right),$$

where λ is called a Lagrangian multiplier.

• Partial differential equations

Initial boundary value problems

- **Heat equation**

  1D example:

  $$u_t - a\,u_{xx} = f \quad x \in (0,1),\ t > 0$$

  boundary conditions:

  $$u(0,t) = u(1,t) = 0 \quad t > 0$$

  initial conditions:

  $$u(x,0) = u_0(x) \quad x \in [0,1]$$

  The problem can also be seen as an initial value problem of an ODE (ordinary differential equation) in Banach space:

  $$\begin{aligned} u' + Au &= f, \\ u(0) &= u_0 \end{aligned}$$

  with $u : [0,T] \longrightarrow V \subset \mathbb{R}^\Omega$, $t \mapsto u(t) = u(.,t)$

  Semi-discretization in space: method of lines

  Finite difference method (FDM) on an equidistant mesh with nodes $x_i = i \cdot h$ for $i = 0, 1, \ldots, n+1$ and mesh size $h = 1/(n+1)$. The expression

  $$u_{xx}(x_i, t)$$

is replaced by

$$\frac{1}{h^2}\left[u(x_{i-1},t) - 2u(x_i,t) + u(x_{i+1},t)\right].$$

This leads to the following (ordinary) differential equations for approximate solutions $u_i(t)$ to $u(x_i,t)$:

For $i = 1$:

$$u_1'(t) - \frac{a}{h^2}\big[\underbrace{u_0(t)}_{=0} - 2u_1(t) + u_2(t)\big] = f(x_1,t)$$

For $i = 2,\ldots,n-1$:

$$u_i'(t) - \frac{a}{h^2}\big[u_{i-1}(t) - 2u_i(t) + u_{i+1}(t)\big] = f(x_i,t)$$

For $i = n$:

$$u_n'(t) - \frac{a}{h^2}\big[u_{n-1}(t) - 2u_n(t) + \underbrace{u_{n+1}(t)}_{=0}\big] = f(x_n,t)$$

In matrix-vector notation:

$$\underline{u}_h'(t) + K_h\underline{u}_h(t) = \underline{f}_h(t)$$

with

$$K_h = \frac{a}{h^2}\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix}, \quad \underline{u}_h(t) = \begin{bmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_n(t) \end{bmatrix}, \quad \underline{f}_h(t) = \begin{bmatrix} f(x_1,t) \\ f(x_2,t) \\ \vdots \\ f(x_n,t) \end{bmatrix}$$

Initial conditions

$$\underline{u}_h(0) = \underline{u}_{h0} \quad \text{with} \quad \underline{u}_{h0} = \begin{bmatrix} u_0(x_1) \\ u_0(x_2) \\ \vdots \\ u_0(x_n) \end{bmatrix}.$$

The finite element method (FEM) with continuous and piecewise linear elements leads to similar problems:

$$\begin{aligned} M_h\underline{u}_h'(t) + K_h\underline{u}_h(t) &= \underline{f}_h(t) \\ M_h\underline{u}_h(0) &= \underline{g}_h \end{aligned}$$

where M_h is the so-called mass matrix.

Both systems of differential equations are special cases of linear systems with constant coefficients:

$$u'(t) = Ju(t) + f(t)$$

Here: $J = -K_h$ or $J = -M_h^{-1} K_h$. The eigenvalues of J are real and negative. The problem is an example of a stiff problem.
MultiD: replace u_{xx} by Δu with

$$\Delta u = \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}.$$

- **Wave equation**

  1D example:

  $$u_{tt} - c^2\, u_{xx} = f \quad x \in (0,1),\ t > 0$$

  boundary conditions:

  $$u(0,t) = u(1,t) = 0 \quad t > 0$$

  initial conditions:

  $$\begin{aligned} u(x,0) &= u_0(x) \quad x \in [0,1], \\ u_t(x,0) &= v_0(x) \quad x \in [0,1] \end{aligned}$$

  The problem can also be seen as an initial value problem of an ODE (ordinary differential equation) in Banach space:

  $$\begin{aligned} u'' + Au &= f, \\ u(0) &= u_0, \\ u'(0) &= v_0 \end{aligned}$$

  with $u : [0,T] \longrightarrow V \subset \mathbb{R}^{\Omega}$, $t \mapsto u(t) = u(.,t)$
  Semi-discretization in space by a FDM:

  $$\begin{aligned} \underline{u}_h''(t) + K_h \underline{u}_h(t) &= \underline{f}_h(t), \\ \underline{u}_h(0) &= \underline{u}_{h0}, \\ \underline{u}_h'(0) &= \underline{v}_{h0}. \end{aligned}$$

  This leads to the following first order linear system:

  $$u'(t) = Ju(t) + f(t)$$

  with

  $$u(t) = \begin{bmatrix} \underline{u}_h(t) \\ \underline{u}_h'(t) \end{bmatrix}, \quad J = \begin{bmatrix} 0 & I \\ -K_h & 0 \end{bmatrix}.$$

  All eigenvalues of J are purely imaginary. This problem is also an example of a stiff problem.

– **Navier-Stokes equations**

The velocity u and the pressure p of a Newtonian fluid satisfy the following system of PDEs:

$$\begin{aligned} u_t - (u \cdot \nabla)u - \nu\,\Delta u + \nabla p = f \quad & x \in \Omega,\ t > 0, \\ \nabla \cdot u = 0 \quad & x \in \Omega,\ t > 0 \end{aligned}$$

with appropriate boundary and initial conditions.

Semi-discretization in space leads to a DAE:

$$\begin{aligned} M_h \underline{u}_h'(t) + A_h(\underline{u}_h(t))\,\underline{u}_h(t) + B_h^T \underline{p}_h(t) = \underline{f}_h(t) \quad & t > 0, \\ B_h \underline{u}_h = \underline{g}_h \qquad & x \in \Omega,\ t > 0. \end{aligned}$$

1.2 Standard Forms

- **explicit ODEs:**

Find $u : [0,T] \longrightarrow \mathbb{R}^n$ such that

$$\begin{aligned} u'(t) &= f(t, u(t)) \quad t \in (0,T), \\ u(0) &= u_0 \end{aligned}$$

with given right-hand side $f : D \times (0,T) \longrightarrow \mathbb{R}^n$, $D \subset \mathbb{R}^n$ and initial value $u_0 \in \mathbb{R}^n$.

Second (and higher) order initial value problems like

$$\begin{aligned} u''(t) &= f(t, u(t), u'(t)) \quad t \in (0,T), \\ u(0) &= u_0, \\ u'(0) &= v_0 \end{aligned}$$

can be transformed into this standard form: With

$$u_1(t) = u(t),\ u_2(t) = u'(t)$$

we have

$$u_1'(t) = u_2(t), \quad u_2'(t) = f(t, u_1(t), u_2(t))$$

with initial conditions:

$$u_1(0) = u_0, \quad u_2(0) = v_0.$$

Special cases:

– Linear ODEs with constant coefficients

$$u'(t) = Ju(t) + f(t)$$

– Right-hand side does not depend on u:

$$u'(t) = f(t)$$

Then

$$u(t) = u(0) + \int_0^t u'(s)\ ds = u_0 + \int_0^t f(s)\ ds.$$

(integration problem)

– autonomous ODEs:

$$u'(t) = f(u(t))$$

Each ODE of the form

$$u'(t) = f(t, u(t))$$

can be transformed into an equivalent autonomous problem: With

$$u_1(t) = t, \quad u_2(t) = u(t)$$

we obtain

$$u_1'(t) = 1, \quad u_2'(t) = f(u_1(t), u_2(t))$$

Initial conditions:

$$u_1(0) = 0, \quad u_2(0) = u_0.$$

Formulation as a Volterra integral equation:

$$u(t) = u_0 + \int_0^t f(s, u(s))\ ds$$

Formulation as an operator equation:

$$\mathcal{F}(u) = 0 \quad \text{with} \quad \mathcal{F}(u) = \begin{bmatrix} u'(t) - f(t, u(t)), \quad t \in (0, T) \\ u(0) - u_0 \end{bmatrix}$$

e.g.: $\mathcal{F} : C^1(0, T) \cap C[0, 1] \longrightarrow C(0, T) \times \mathbb{R}$.

- **(fully) implicit ODEs:**

$$F(t, u(t), u'(t)) = 0$$

- **semi-explicit DAEs:**

$$u(t) = \begin{bmatrix} y(t) \\ z(t) \end{bmatrix}$$

$$\begin{aligned} y'(t) &= f(t, y(t), z(t)), \\ 0 &= g(t, y(t), z(t)). \end{aligned}$$