Mathematical modeling

and finite element method

### Principles of mathematical modeling

mathematical model = mathematical description of a physical process

How to build a mathematical model to a physical process?

- determine physical quantities that characterize this process (state variable, flow variable)
- describe relations between these quantities (simplification of physical rules)

#### Solution

- analytical
- numerical (approximate)
  - solved in finite precision arithmetic (inaccurate)

### State variable and flow variable in several physical processes

### Stationary heat conduction in 1 dimension

- physical process = heat conduction in a domain  $\Omega = (0, L)$ 
  - state variable = temperature u(x)
  - flow variable = temperature flow  $\tau(x)$
- input variables:
  - material properties = thermal conductivity k(x)
  - density of heat sources f(x)
- relationships:
  - from the conservation law:  $\tau'(x) = f(x)$
  - Fourier law:  $\tau(x) = -k(x)u'(x)$

### Flow in porous media (stationary)

- physical process = saturated flow of a fluid through porous media
  - state variable = pressure p(x)
  - flow variable = velocity v(x)
- input variables:
  - material properties = hydraulic conductivity k(x)
  - density of sources f(x)
- relationships:
  - from the mass conservation law: v'(x) = f(x)
  - Darcy law: v(x) = -k(x) p'(x)

### String deformation

- physical process:
  - state variable = deformation u(x)
  - flow variable = stress v(x)
- input variables:
  - material properties (including Young's elastic modulus) k(x)
  - density of forces f(x)
- relationships:
  - from the conservation law: v'(x) = f(x)
  - Hooke's law: v(x) = -k(x)u'(x)

### Conservation law

"Difference between the total amount of some physical variable in the domain at time  $t_1$  and at time  $t_2$ 

### equals

total inflow/outflow through boundary plus total sources in the domain."

- state function u(x,t)
- total amount of u in the domain at time  $t_1 \dots A$
- total amount of u in the domain at time  $t_2 \dots B$
- $\bullet$  total flow through the boundary ... C
- ullet total sources in the domain ... D

$$B - A = C + D$$

### Conservation law in 1 dimension

- domain in 1d:  $\langle a, b \rangle \subset \mathbb{R}$
- boundary in 1d:  $\{a, b\}$
- state function: u(x,t)
- flow function:  $\phi(x,t)$

### Derive:

- total amount of u in the domain at time  $t_1 \dots$ ?
- total amount of u in the domain at time  $t_2$  ... ?
- total flow through the boundary ... ?
- total sources in the domain ... ?

### Conservation law in 1 dimension

(integral formulation)

$$\int_{a}^{b} u\left(x,t_{2}\right) \mathrm{d}x - \int_{a}^{b} u\left(x,t_{1}\right) \mathrm{d}x = \int_{t_{1}}^{t_{2}} \left(\phi\left(a,t\right) - \phi\left(b,t\right)\right) \mathrm{d}t + \int_{t_{1}}^{t_{2}} \int_{a}^{b} f\left(x,t\right) \mathrm{d}x \mathrm{d}t$$

$$\downarrow$$
which requirements?
$$\downarrow$$

$$u_{t}\left(x,t\right) + \phi_{x}\left(x,t\right) = f\left(x,t\right)$$
(differential formulation)

Stationary problem:

$$\phi_x\left(x\right) = f\left(x\right)$$

# Analytical solution of several boundary value problems

- these problems will be used as model exaples in numerical experiments
- prepare their analytical solutions, we will compare them with numerical solutions

### Problem 1 (diffusion)

- constants: f, k, L, U, T
- boundary value problem:

$$\begin{cases}
-k \cdot u''(x) = f & \forall x \in (0, L) \\
u(0) = U \\
-k \cdot u'(L) = T
\end{cases}$$

### Problem 2 (material interface)

- constants:  $f, k_1, k_2, L, M, U, T$
- boundary value problem:

$$\begin{cases} -k_{1} \cdot u_{1}''(x) = f & \forall x \in (0, M) \\ -k_{2} \cdot u_{2}''(x) = f & \forall x \in (M, L) \\ u_{1}(0) = U & \\ -k_{2} \cdot u_{2}'(L) = T & \\ u_{1}(M) = u_{2}(M) & \\ k_{1} \cdot u_{1}'(M_{+}) = k_{2} \cdot u_{2}'(M_{-}) & \end{cases}$$

### Problem 3 (with reaction)

- constants:  $k, k_0, L, g, U, T$
- boundary value problem:

$$\begin{cases}
-k \cdot u''(x) + k_0 u(x) = g & \forall x \in (0, L) \\
u(0) = U \\
-k \cdot u'(L) = T
\end{cases}$$

### Problem 4 (with convection)

- constants: f, k, L, D, U, T
- boundary value problem:

$$\begin{cases} -k \cdot u''(x) + D \cdot u'(x) = f & \forall x \in (0, L) \\ u(0) = U \\ -k \cdot u'(L) = T \end{cases}$$

## Solution of several boundary value problems using finite differences method

• we will focus on numerical solutions using the finite elements method (FEM); however, numerical solution can also be obtained using a simpler method - finite differences method (FDM)

- constants: f, k, L, U, T
- boundary value problem:

$$\begin{cases}
-k \cdot u''(x) = f & \forall x \in (0, L) \\
u(0) = U \\
-k \cdot u'(L) = T
\end{cases}$$

Solve this boundary value problem using finite differences method (for arbitrary parameters f, k, L, U, T).

Compare the numerical solution and the analytical solution, using different lengths of discretization steps.

- constants:  $f, k_1, k_2, L, M, U, T$
- boundary value problem:

$$\begin{cases} -k_{1} \cdot u_{1}''(x) = f & \forall x \in (0, M) \\ -k_{2} \cdot u_{2}''(x) = f & \forall x \in (M, L) \\ u_{1}(0) = U & \\ -k_{2} \cdot u_{2}'(L) = T & \\ u_{1}(M) = u_{2}(M) & \\ k_{1} \cdot u_{1}'(M_{+}) = k_{2} \cdot u_{2}'(M_{-}) & \end{cases}$$

Solve this boundary value problem using finite differences method (for arbitrary parameters f,  $k_1$ ,  $k_2$ , L, M, U, T).

Compare the numerical solution and the analytical solution.

- constants:  $k, k_0, L, g, U, T$
- boundary value problem:

$$\begin{cases}
-k \cdot u''(x) + k_0 u(x) = g & \forall x \in (0, L) \\
u(0) = U \\
-k \cdot u'(L) = T
\end{cases}$$

Solve this boundary value problem using finite differences method (for arbitrary parameters k,  $k_0$ , L, g, U, T).

Compare the numerical solution and the analytical solution.

- constants: f, k, L, D, U, T
- boundary value problem:

$$\begin{cases}
-k \cdot u''(x) + D \cdot u'(x) = f & \forall x \in (0, L) \\
u(0) = U \\
-k \cdot u'(L) = T
\end{cases}$$

Solve this boundary value problem using finite differences method (for arbitrary boundary conditions and arbitrary parameters f, k, L, D, U, T):

- 1. using central differences
- 2. using up-wind (up-stream) differences
- 3. using down-wind (down-stream) differences