Mathematical modelling in science and engineering

Lecture 1
Preliminaries

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Notation and notational conventions

- $\Omega \subset \boldsymbol{R}^N$, N=$1,2$ or 3 – domain in 1D, 2D or 3D space
  - all domains are assumed to have smooth boundaries $\partial\Omega$
- standard font - scalar, bold - vector
  - $\boldsymbol{x} = [x, y, z] = [x_1, x_2, x_3]$ - point in 3D space
  - t - time instant
  - $f(\mathbf{x}, t)[\mathbf{f}(\mathbf{x}, t)]$ – scalar [vector] function of space and time
    - the function will usually denote some **description of state** of domain points
    - the dependence on space and time is often omitted in notation
- when indices i, j, k, l refer to cartesian space coordinates the summation convention for repeated indices is used
  - $u_i n_i = \sum_i u_i n_i$
- "," denotes differentiation (for indices i, j, k, l of cartesian space coordinates and partial derivatives with respect to time)
  - $u_{i,i} = \frac{\partial u_i}{\partial x_i} = \nabla \cdot \mathbf{u} = \mathrm{div}\mathbf{u} \qquad u_{,t} = \frac{\partial u}{\partial t}$
- standard mathematical notation, operators, etc.
  - e.g. indices of matrix entries: A_{ij} element i, j of matrix $\mathbf{A}$

Description of state

Examples of state description:

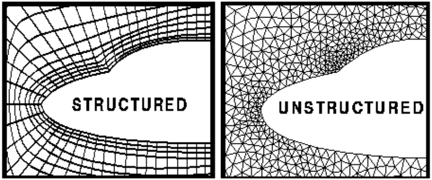
- material point
  - position (spatial coordinates)
    - **Cartesian** – $\boldsymbol{x}$, polar, spherical, cylindrical
  - velocity
    - $\boldsymbol{v} = \frac{d\boldsymbol{x}}{dt}$ (a single component: $v_i = \frac{dx_i}{dt} = x_{i,t}$)
  - acceleration
    - $\boldsymbol{a} = \frac{d\boldsymbol{v}}{dt}$ (a single component: $a_i = \frac{dv_i}{dt} = v_{i,t}$)
  - displacement
    - $\boldsymbol{l} = \boldsymbol{x} - \boldsymbol{x}_0 \quad (\frac{d\boldsymbol{l}}{dt} = \frac{d\boldsymbol{x}}{dt} = \boldsymbol{v})$
- continuous object (1D, 2D and 3D domains)
  - scalar fields: energy – $e(\boldsymbol{x}, t))$, temperature – $T(\boldsymbol{x}, t)$
  - vector fields: displacement – $\boldsymbol{l}(\boldsymbol{x}, t))$, velocity – $\boldsymbol{v}(\boldsymbol{x}, t)$
  - tensor fields: strain – $\boldsymbol{\epsilon}(\boldsymbol{x}, t)$ ($\epsilon_{ij} = l_{i,j} + l_{j,i}$), stress – $\boldsymbol{\sigma}(\boldsymbol{x}, t)$
- discretization – a process of transferring a description in terms of infinite number of values into a description that uses only a finite number of values

Discretization

- We will consider several types of discretization
  - domain discretization – using a finite number of points and parameters, instead of infinite number of points to describe geometric domains
  - function discretization – describing a function (usually continuous) using a finite number of parameters and values at a finite number of points
  - equation discretization – transforming a differential equation for a function (usually continuous) into an equation for a discretized function
- Discretization usually introduces an error – the original domain, original function and the solution to the original equation differ at certain points from their discretized counterparts
  - the discretization error can be measured in a number of different ways
  - with the increasing number of parameters and points the discretized domains, discretized functions and solutions to discretized equations usually tend to their original counterparts (the discretization error goes to 0)
  - discretization is a form of approximation, we will often use the two terms interchangeably
- Only discretized equations, functions and domains are amenable to computer processing

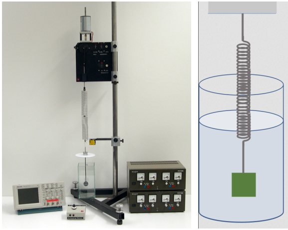
Domain discretization

- Computational domain
  - $\Omega \subset \boldsymbol{R}^N$, N=*1,2 or 3* – domain in 1D, 2D or 3D space
- Domain discretization – using a finite number of points and parameters, instead of infinite number of points to describe the domain
  - the simplest discretization uses a finite number of points and straight line segments to join them
  - more complex discretizations employ a finite number of points and curvilinear segments that join them
  - in 2D the most popular are linear or curvilinear triangles and quadrilaterals
  - in 3D the most popular are linear or curvilinear tetrahedra and hexahedra, as well as prisms and pyramids
- The set of points and segments joining them is called a grid (or mesh)
- There are two basic types of grids (with different neighbourhood relations)
  - structured (regular) grids
  - unstructured grids

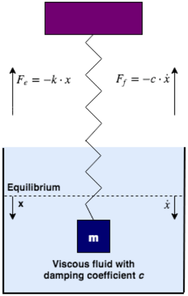


Example of modelling – mass-spring system with damping

- Reality (experiment)



- Physical model



Balance of forces:

$ma = \Sigma_i F_i$ - Newton's second law of mechanics

- Mathematical model

Ordinary differential equation

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0$$

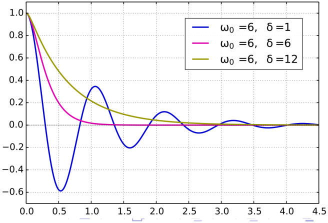
+ Initial conditions

$$x(0) = x_0 \qquad \frac{dx}{dt}(0) = v_0$$

= Initial value problem

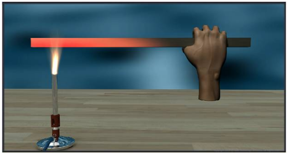
→ **existence and uniqueness of results**

- Result: oscillations
  - Predicted by the mathematical model
  - Compared with experimental results
  - Validation of the physical and mathematical model (quantitative!)



Example of modelling – heated 1D rod

- Reality (experiment)



- Physical model

Energy conservation - the rate of change of heat flux is equal to heat source

$$dq/dx = s(x)$$

Fourier's law - heat flux is proportional to the temperature gradient

$$q = -k \cdot dT/dx$$

- k - heat conduction coefficient

- Mathematical model

Ordinary differential equation

$$-\frac{d}{dx}\left(k\frac{dT}{dx}\right) = s(x)$$

+ Boundary conditions

(for both ends, possible types:

- temperature, e.g.

  $T(0) = T_0$

- heat flux, e.g.

  $q(L) = -k \cdot dT/dx = q_0$

- other (convection, radiation)

= Boundary value problem

$\rightarrow$ **existence and uniqueness of results**

Generalization of mathematical model derivation

Conservation principle(s)

- ”physics” – may be formulated as conservation principle(s)
  - for some flux q and source s
  - not necessarily related to energy conservation, i.e. heat problem
- general form for stationary 1D problems:
  - integral form (for any interval $(x, x+\Delta x)$):

$$q(x+\Delta x) - q(x) = \int_x^{x+\Delta x} s(\xi) d\xi$$

  - differential form (in the limit $\Delta x \rightarrow 0$) :

$$\frac{dq}{dx} = s(x)$$

Constitutive equation(s)

- often called material model
- connects different quantities used in process description

Generalization of mathematical model derivation

Conservation principle(s) (stationary form) + Constitutive equation(s)
= Differential equation(s)

- first or second order in space variables
- ordinary (ODE) or partial (PDE), depending on space dimension
- unknown u

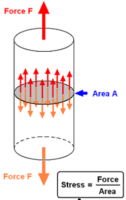
Boundary conditions:

- Dirichlet: $u = u_0$
- Neumann: $\dfrac{du}{dx} = \tilde{q}_0$
- Robin: $\dfrac{du}{dx} = \tilde{c}(u - u_0)$

Differential equation(s) + Boundary conditions
= Boundary value problem
$\rightarrow$ **existence and uniqueness of results**

One more 1D example – tensile test

- Stress - force intensity: $\sigma = F/A$

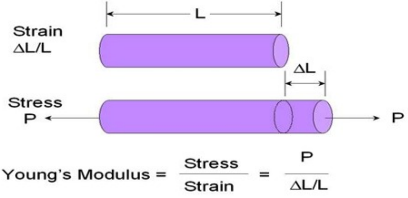


- Conservation principle – balance of forces

(from the conservation of momentum - Newton's second law of mechanics)

$$-\frac{d\sigma}{dx} = f(x)$$

- Strain: $\epsilon = \Delta L/L \to dl/dx$



- Constitutive equations – Hooke's law for linearly elastic material

$$\sigma = E\epsilon$$

Differential equation: $-E\frac{d^2 l}{dx^2} = f(x)$ (f - external force intensity)

+ Boundary conditions: displacements (l) or forces ($-E\frac{dl}{dx}$) at the ends