# Scientific Computing

## Part 4: Complex Dynamic Systems
## Introduction to Partial Differential Equations

22nd November 2022

# Contents

# Outline of this chapter



- Our aim of this part is to perform computational fluid dynamic (CFD) simulations.
- For this purpose, some understanding of partial differential equations (PDE) and their solutions is required.
- We thus start with an introduction in PDE before we turn to a special set of PDE, the Navier-Stokes equations, which we will then try to solve using the simulation tool OpenFOAM.

**Outline of this chapter:**

- Recap of partial derivatives
- Recap of Fourier Series
- What is a Partial Differential Equation?
- Classifying PDE's: Order, Linear vs. Nonlinear
- Analytical solutions of some PDEs

# Recap of Partial Derivatives

# Scalar & Vector Functions

# Scalar & Vector Functions

- The definition of a one-dimensional function

$$\begin{aligned} f : \mathbb{R} &\longrightarrow \mathbb{R} \\ x &\mapsto y = f(x) \end{aligned}$$

with the dependent variable $y$ and the independent variable $x$ is extended to functions in multiple dimensions

**Definition 1.1:**

- A function with $n$ independent variables $x_1, \ldots, x_n$ and one dependent variable $y$ maps a set of arguments $(x_1, x_2, \ldots, x_n)$ from a domain $D \subset \mathbb{R}^n$ to exactly one value $y$ from the codomain $W \subset \mathbb{R}$. Symbolically:

$$\begin{array}{rcl} f: \ D \subset \mathbb{R}^n & \longrightarrow & W \subset \mathbb{R} \\ (x_1, x_2, \ldots, x_n) & \mapsto & y = f(x_1, x_2, \ldots, x_n) \end{array}$$

Since the result $y \in \mathbb{R}$ is a scalar (a number), $f$ is a scalar-valued function.

# Scalar & Vector Functions

**Definition 1.1 (continued):**

- A vector-valued function, also referred to a vector function, is then defined as

$$\begin{aligned} \boldsymbol{f}: \quad D \subset \mathbb{R}^n \quad &\longrightarrow \quad W \subset \mathbb{R}^m \\ (x_1, x_2, \dots, x_n) \quad &\mapsto \quad \boldsymbol{y} = \boldsymbol{f}(x_1, x_2, \dots, x_n) = \begin{pmatrix} y_1 = f_1(x_1, x_2, \dots, x_n) \\ y_2 = f_2(x_1, x_2, \dots, x_n) \\ \vdots \\ y_m = f_m(x_1, x_2, \dots, x_n) \end{pmatrix} \end{aligned}$$

  where each component $f_i : \mathbb{R}^n \longrightarrow \mathbb{R}$ $(i = 1, \dots, m)$ is again a scalar-valued function.

# Scalar & Vector Functions

**Remarks:**

- Vectors $\boldsymbol{x}$ and vector-valued functions $\boldsymbol{f}$ are in bold face throughout this script, in contrast to scalars $x$ and scalar-valued functions $f$.

**Examples 1.1**:

1. Scalar-valued function: $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$ with

$$f(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2$$

2. Vector-valued function: $\boldsymbol{f} : \mathbb{R}^3 \longrightarrow \mathbb{R}^4$ with

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1^2 + x_2^2 \\ x_1^2 + x_3^2 \\ x_2^2 + x_3^2 \\ x_1^2 + x_2^2 + x_3^2 \end{pmatrix}$$

**Task 1.1:**

- Plot the scalar-valued functions $z_1 = f_1(x, y) = x^2 - y^2$ and $z_2 = f_2(x, y) = xy^2 \cdot (\sin x + \sin y)$ for $x \in [-\pi, \pi]$ and $y \in [-\pi, \pi]$ using the MATLAB functions meshgrid() and surf() or the Python functions numpy.meshgrid() and plt.plot_surface().

**Task 1.1:** Solution

**Task 1.1:** Solution

# Partial derivatives of first order

# Partial derivatives of first order

- In one dimension, the derivative of a scalar-valued function $f : \mathbb{R} \longrightarrow \mathbb{R}$ with respect to the independent variable $x$ is defined as

$$f'(x_0) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x},$$

and it gives the **slope** or **gradient** of the tangent line to the function $f$ at $x_0$.

- This Definition can be extended to functions of several independent variables.

# Partial derivatives of first order

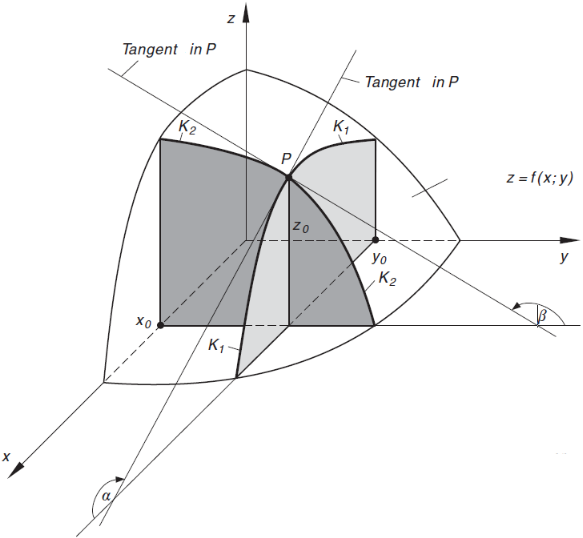


- For simplicity, let us first consider a scalar-valued function $z = f(x, y)$ of two independent variables $x$ and $y$, which defines a plane in the three dimensional space ($z$ can be considered as the heigth coordinate) .
- The point$P$ is located on this plane and has the coordinates $(x_0, y_0, z_0)$, where $z_0 = f(x_0, y_0)$. The intersection curves $K_1$ und $K_2$ parallel to the $(x, z)$ plane and $(y, z)$ plane through $P$ are depicted in the next figure.
- They can be defined as

$$
\begin{aligned}
K_1 : g(x) : &= f(x, y_0) \\
K_2 : h(y) : &= f(x_0, y)
\end{aligned}
$$

# Partial derivatives of first order





# Partial derivatives of first order

$$\begin{aligned} K_1 : g(x) : &= f(x, y_0) \\ K_2 : h(y) : &= f(x_0, y) \end{aligned}$$

- Note that $g(x)$ is a function only of $x$, while $h(y)$ is a function only of $y$.
- The derivative $g'(x_0)$ gives the slope of the tangent line to the the plane $z = f(x, y)$ at point $P$ in $x-$direction, $h'(y_0)$ in $y-$direction.
- We can write the derivatives as

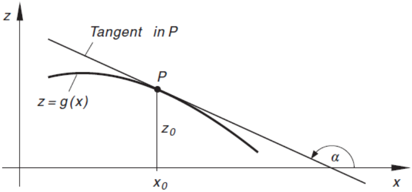
$$\begin{aligned} g'(x_0) &= \lim_{\Delta x \to 0} \frac{g(x_0 + \Delta x) - g(x_0)}{\Delta x} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x, y_0) - f(x_0, y_0)}{\Delta x} =: \frac{\partial f}{\partial x}(x_0, y_0) \\ h'(y_0) &= \lim_{\Delta y \to 0} \frac{h(y_0 + \Delta y) - h(y_0)}{\Delta y} = \lim_{\Delta y \to 0} \frac{f(x_0, y_0 + \Delta y) - f(x_0, y_0)}{\Delta y} =: \frac{\partial f}{\partial y}(x_0, y_0). \end{aligned}$$

- We call these limits **first-order partial derivatives** of $f$ at $(x_0, y_0)$.

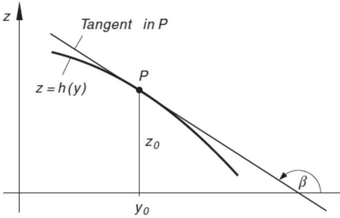
# Partial derivatives of first order



$$K_1\colon\; z = f(x; y_0) = g(x)$$




$$K_2\colon\; z = f(x_0; y) = h(y)$$



**Definition 1.2: Partial Derivatives of first order**

Consider a scalar-valued function $y = f(x,y)$:

- First-order partial derivative of $f$ with respect to $x$

$$\frac{\partial f}{\partial x}(x,y) = f_x = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, y) - f(x,y)}{\Delta x}$$

- First-order partial derivative of $f$ with respect to $y$

$$\frac{\partial f}{\partial y}(x,y) = f_y = \lim_{\Delta y \to 0} \frac{f(x, y+\Delta y) - f(x,y)}{\Delta y}$$

- The gradient of the function $f$ is defined as

$$\mathrm{grad}(f) = \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix}$$

wehre $\nabla$ is the so-called **Nabla** (or **del**) operator.

# Partial derivatives of first order



## Remarks (1):

- The above definitions can be easily extended $n$ independent variables, e.g.:

$$
\begin{aligned}
y &= f(x_1, x_2, \ldots, x_n) \\
\frac{\partial f}{\partial x_k}(x_1, \ldots, x_k, \ldots, x_n) = f_{x_k} &= \lim_{\Delta x_k \to 0} \frac{f(x_1, \ldots, x_k + \Delta x_k, \ldots, x_n) - f(x_1, \ldots, x_k, \ldots, x_n)}{\Delta x_k} \quad (k = 1, \ldots, n) \\
\nabla f &= \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}
\end{aligned}
$$

whith the Nabla-operator $\nabla = \left( \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_n} \right)^T$

# Partial derivatives of first order

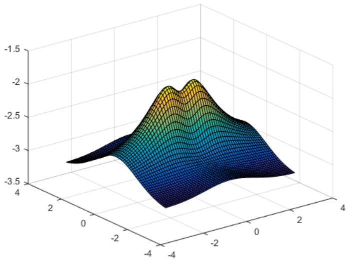


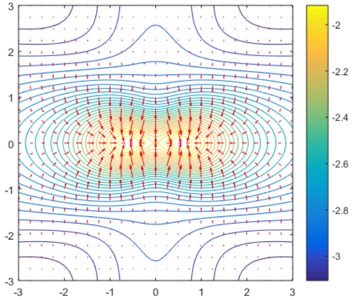
**Remarks (2):**

- The gradient $\nabla f(x_1, x_2, ..., x_n)$ is a vector that points in the direction of the greatest rate of increase of the function $f$ at point $(x_1, x_2, ..., x_n)$ , and its length is the slope of the graph in that direction. An example is given in the figure on the next slide for the function

$$z = f(x, y) = \frac{(x^2 - 1) + (y^2 - 4) + (x^2 - 1) \cdot (y^2 - 4)}{(x^2 + y^2 + 1)^2}$$

# Partial derivatives of first order



# Partial derivatives of first order



**Remarks (3):**

- Geometric interpretation of the partial derivatives of $z = f(x, y)$ at $(x_0, y_0)$:
  1. $\frac{\partial f}{\partial x}(x_0, y_0)$ is the slope of the tangent line at $P = (x_0, y_0, z_0)$ in positive $x-$direction
  2. $\frac{\partial f}{\partial y}(x_0, y_0)$ is the slope of the tangent line at $P = (x_0, y_0, z_0)$ in positive $y-$direction

# Partial derivatives of first order



**Remarks (4):**

- We can calculate the partial derivative $f_x$, if we treat $y$ as constant and differentiate $z = f(x,y)$ with respect to $x$:
  - Example:

$$\begin{aligned} z &= f(x,y) = 3xy^3 + 10x^2y + 5y + 3y \cdot \sin(5xy) \\ \frac{\partial f}{\partial x}(x,y) &= f_x = 3 \cdot 1 \cdot y^3 + 10 \cdot 2x \cdot y + 0 + 3y \cdot \cos(5xy) \cdot 5 \cdot 1 \cdot y \end{aligned}$$

# Partial derivatives of first order



**Remarks (5):**

- Accordingly, we can calculate the partial derivative $f_y$, if we treat $x$ as constant and differentiate $z = f(x,y)$ with respect to $y$:
  - Example:

$$\begin{aligned} z &= f(x,y) = 3xy^3 + 10x^2 y + 5y + 3y \cdot \sin(5xy) \\ \frac{\partial f}{\partial y}(x,y) &= f_y(x,y) = 3x \cdot 3y^2 + 10x^2 \cdot 1 + 5 \cdot 1 + (3 \cdot 1 \cdot \sin(5xy) + 3y \cdot \cos(5xy) \cdot 5x \cdot 1) \end{aligned}$$

**Task 1.2:**

- Calculate the first order partial derivatives of the following functions and specify the gradient $\nabla f(x_0, y_0)$ for $(x_0, y_0) = (0, 0)$:
  1. $z = f(x, y) = x^2 y^4 + e^x \cdot \cos y + 10x - 2y^2 + 3$
  2. $z = f(x, y) = xy^2 \cdot (\sin x + \sin y)$
  3. $z = f(x, y) = \ln(x + y^2) - e^{2xy} + 3x$

**Task 1.2: Solution**

## Task 1.3:

- Consider the function

$$z = f(x,y) = \frac{(x^2-1)+(y^2-4)+(x^2-1)\cdot(y^2-4)}{(x^2+y^2+1)^2}$$

Write a MATLAB/Python script that plots the surface and the vectors

$$\left(\frac{\partial f(x,y)}{\partial x}, \frac{\partial f(x,y)}{\partial y}, \left(\left(\frac{\partial f(x,y)}{\partial x}\right)^2 + \left(\frac{\partial f(x,y)}{\partial y}\right)^2\right)\right)$$

of the tangents plotted over it. Use the following:

  - symbolic toolbox and jacobian() in MATLAB or sympy and jacobian() in Python to calculate the partial derivatives
  - functions matlabFunction(), meshgrid(), surf(), quiver3() in MATLAB or lambdify(), meshgrid(), plt.plot_surface(), plt.quiver() in Python to plot

**Task 1.3: Solution**

# Partial derivatives of higher order

# Partial derivatives of higher order



- Partial derivatives of higher order are obtained when a function of mutliple independent variables is partially differentiated several times.
- For instance, for $z = f(x, y)$, one derives two partial derivatives of first order

$$f_x = \frac{\partial f}{\partial x}, \ f_x = \frac{\partial f}{\partial y},$$

four partial derivatives of second order

$$f_{xx} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial^2 f}{\partial x^2}, \ f_{yy} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial^2 f}{\partial y^2}$$

$$f_{xy} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial^2 f}{\partial x \partial y}, \ f_{yx} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial^2 f}{\partial y \partial x}$$

# Partial derivatives of higher order



- eight partial derivatives of third order

$$f_{xxx} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)\right) = \frac{\partial^3 f}{\partial x^3}, \quad f_{yyy} = \frac{\partial}{\partial y}\left(\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right)\right) = \frac{\partial^3 f}{\partial y^3}$$

$$f_{xxy} = \frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)\right) = \frac{\partial^3 f}{\partial x \partial x \partial y}, \quad f_{xyx} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)\right) = \frac{\partial^3 f}{\partial x \partial y \partial x}, \quad f_{xyy} = \frac{\partial}{\partial y}\left(\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)\right) = \frac{\partial^3 f}{\partial x \partial y \partial y}$$

$$f_{yxx} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)\right) = \frac{\partial^3 f}{\partial y \partial x \partial y}, \quad f_{yxy} = \frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)\right) = \frac{\partial^3 f}{\partial y \partial x \partial y}, \quad f_{yyx} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right)\right) = \frac{\partial^3 f}{\partial y \partial y \partial x}$$

and so on

# Partial derivatives of higher order



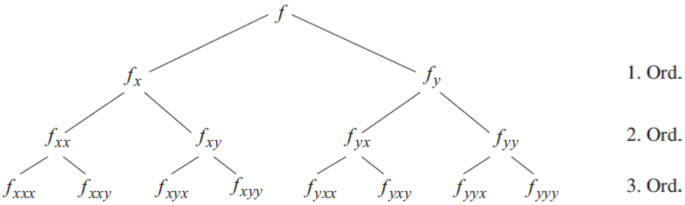


- The corresponding schematic is given in the figure on the next slide.
- The indices are read from left to right, i.e. $f_{xy}$ means that the function is first partially differentiated with respect to $x$ and after that with respect to $y$.
- A partial derivative of second or greater order with respect to two or more different variables, for example

$$f_{xy} = \frac{\partial^2 f}{\partial x \partial y}$$

is called a **mixed partial derivative**.

# Partial derivatives of higher order



# Partial derivatives of higher order



**Schwartz' Theorem:**

- Consider the function $f : \mathbb{R}^n \to \mathbb{R}$. If the mixed partial derivatives exist and are continuous at a point $\boldsymbol{x}_0 \in \mathbb{R}^n$, then they are equal at $\boldsymbol{x}_0$ regardless of the order in which they are taken.

- Schwartz' Theorem basically states that for $z = f(x, y)$ we have
$$f_{xy}(\boldsymbol{x}_0) = f_{yx}(\boldsymbol{x}_0)$$
and
$$f_{xxy}(\boldsymbol{x}_0) = f_{xyx}(\boldsymbol{x}_0) = f_{yxx}(\boldsymbol{x}_0)$$
and
$$f_{yyx}(\boldsymbol{x}_0) = f_{yxy}(\boldsymbol{x}_0) = f_{xyy}(\boldsymbol{x}_0)$$
if all these partial derivatives are continuous at $\boldsymbol{x}_0$.

# Partial derivatives of higher order



- For partial derivatives of second order, the Laplacian operator plays a major role.

**Definition 1.3: Laplacian**

Consider a scalar-valued function $f : \mathbb{R}^n \to \mathbb{R}$, $y = f(x_1, \dots, x_n)$:

- The Laplacian operator $\Delta$ is defined as

$$\Delta = \nabla \cdot \nabla = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} = \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \dots + \frac{\partial^2}{\partial x_n^2} \right)$$

i.e.

$$\Delta f = f_{x_1 x_1} + f_{x_2 x_2} + \dots + f_{x_n x_n} = \left( \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \dots + \frac{\partial^2 f}{\partial x_n^2} \right)$$

# Recap of Fourier Series

# Recap of Fourier Series



## Definition 1.4: Fourier Series/ Fourier Coefficients

- Let $f:\mathbb{R}\longrightarrow\mathbb{R}$ be a periodic continous function with angular frequency $\omega_0$ and period $T=\frac{2\pi}{\omega_0}$. The Fourier series of $f(x)$ is defined as

$$f(x)=\frac{A_0}{2}+\sum_{k=1}^{\infty}\left[A_k\cos\left(k\cdot\omega_0\cdot x\right)+B_k\sin\left(k\cdot\omega_0\cdot x\right)\right]$$

  where:
  - $\omega_0=\frac{2\pi}{T}$: angular frequency of the first harmonic oscillation
  - $k\cdot\omega_0$ : angular frequency of the $k-$th harmonic oscillation

- The Fourier coefficients of $f$ can be calculated according to

$$\begin{aligned}A_0 &= \frac{2}{T}\int_{(T)} f(x)dx\\ A_k &= \frac{2}{T}\int_{(T)} f(x)\cos(k\omega_0 x)dx\\ B_k &= \frac{2}{T}\int_{(T)} f(x)\sin(k\omega_0 x)dx\end{aligned}$$

# Recap of Fourier Series

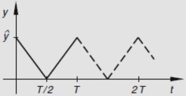
- Some Fourier series:

**(1) Rechteckkurve**


$$y(t) = \begin{cases} \hat{y} & \text{für} \quad 0 \le t \le \frac{T}{2} \\ 0 & \quad\quad \frac{T}{2} < t < T \end{cases}$$

$$y(t) = \frac{\hat{y}}{2} + \frac{2\hat{y}}{\pi}\left[\sin(\omega_0 t) + \frac{1}{3}\cdot\sin(3\omega_0 t) + \frac{1}{5}\cdot\sin(5\omega_0 t) + \ldots\right]$$

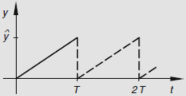
**(2) Dreieckskurve**




$$y(t) = \begin{cases} -\frac{2\hat{y}}{T}t + \hat{y} & \text{für} \quad 0 \le t \le \frac{T}{2} \\ \frac{2\hat{y}}{T}t - \hat{y} & \quad\quad \frac{T}{2} \le t \le T \end{cases}$$

$$y(t) = \frac{\hat{y}}{2} + \frac{4\hat{y}}{\pi^2}\left[\frac{1}{1^2}\cdot\cos(\omega_0 t) + \frac{1}{3^2}\cdot\cos(3\omega_0 t) + \frac{1}{5^2}\cdot\cos(5\omega_0 t) + \ldots\right]$$

**(3) Kippschwingung (Sägezahnimpuls)**




$$y(t) = \frac{\hat{y}}{T}t \quad (0 \le t < T)$$

$$y(t) = \frac{\hat{y}}{2} - \frac{\hat{y}}{\pi}\left[\sin(\omega_0 t) + \frac{1}{2}\cdot\sin(2\omega_0 t) + \frac{1}{3}\cdot\sin(3\omega_0 t) + \ldots\right]$$

# What is a partial differential equation (PDE)?

# PDE



- You have all seen an ordinary differential equation (ODE); for example the pendulum equation,

$$\frac{d^2\Theta}{dt^2} + \frac{g}{L}\sin\Theta = 0$$

describes the angle, $\Theta$, a pendulum makes with the vertical as a function of time, $t$.

- Here $g$ and $L$ are constants (the acceleration due to gravity and length of the pendulum respectively), $t$ is the independent variable and $\Theta = \Theta(t)$ is the dependent variable.
- This is an ODE because there is only one independent variable, here $t$, which represents time.

# PDE



- In contrast, a partial differential equation (PDE) such as the two-dimensional Laplace equation for $\Phi(x, y)$

$$\Delta\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0 \tag{1}$$

includes the partial derivatives of the function $\Phi(x, y)$ for multiple independent variables ($x$ and $y$ in this case).

# PDE



**Definition 1.4: Partial Differential Equation**

- A **partial differential equation (PDE)** relates the partial derivatives of a function of two or more independent variables together.
- The order of the highest partial derivative is the order of the equation. For instance, the order of equation 1 is 2.
- We say a function is a **solution** to a PDE if it satisfies the equation and any side conditions given.

**Definition 1.5: Linear, homogenous PDE of first order**

- If the coefficients $a = a(x,y)$ , $b = b(x,y)$ are continuously differentiable functions $a : D \subset \mathbb{R}^2 \to \mathbb{R}$ and $b : D \subset \mathbb{R}^2 \to \mathbb{R}$, then the PDE for $u = u(x,y)$

  $$a(x,y) \cdot u_x + b(x,y) \cdot u_y = 0$$

  is a linear homogenous PDE of first order. Homogenous here means that the right-hand side of the PDE vanishes.
- Superposition-principle: any superpostion of

# PDE

**Remarks:**

1. The superposition principle states that any superposition (i.e. linear sum) of solutions to a given linear, homogenous PDE is again a solution. For example, if $u_1(x,y)$ and $u_2(x,y)$ are solutions to a linear homogenous PDE, then $u(x,y) = c_1 u_1(x,y) + c_2 u_2(x,y)$ is also a solution (for any constants $c_1, c_2 \in \mathbb{R}$).

# PDE



**Remarks:**

1. The superposition principle states that any superposition (i.e. linear sum) of solutions to a given linear, homogenous PDE is again a solution. For example, if $u_1(x,y)$ and $u_2(x,y)$ are solutions to a linear homogenous PDE, then $u(x,y) = c_1 u_1(x,y) + c_2 u_2(x,y)$ is also a solution (for any constants $c_1, c_2 \in \mathbb{R}$).

## Task 1.4:

- Show that the linear, homogenous PDE of first order

$$\frac{1}{x}\frac{\partial u}{\partial x} + y^3 \frac{\partial u}{\partial y} = 0$$

  has solutions of the form

$$u(x,y) = \bar{u}\left(x^2 + \frac{1}{y^2}\right)$$

  where $\bar{u} = \bar{u}(s)$ is any function that is conintuously differentiable twice with respect to $s = x^2 + \frac{1}{y^2}$.

- Use the chain rule for that:

$$\begin{aligned} \frac{\partial u(x,y)}{\partial x} &= \frac{d\bar{u}(s)}{ds} \cdot \frac{\partial s(x,y)}{\partial x} \\ \frac{\partial u(x,y)}{\partial y} &= \frac{d\bar{u}(s)}{ds} \cdot \frac{\partial s(x,y)}{\partial y} \end{aligned}$$

- Prove it then for the specific cases $\bar{u}_1(s) = \cos(s) = \cos\left(x^2 + \frac{1}{y^2}\right) = u_1(x,y)$ and $\bar{u}_2(s) == \left(x^2 + \frac{1}{y^2}\right)^2 = u_2(x,y)$ Plot these solutions for $x \in [-3,3]$ and $y \in [1,5]$.

## Task 1.4: Solution

- General proof:

$$\begin{aligned} \frac{\partial u(x,y)}{\partial x} &= \dots \\ \frac{\partial u(x,y)}{\partial y} &= \dots \\ \frac{1}{x}\frac{\partial u}{\partial x} + y^3 \frac{\partial u}{\partial y} &= \dots \\ &= \dots \\ &= 0 \text{ q.e.d.} \end{aligned}$$

## Task 1.4: Solution

- Specific case $u_{:1}(x,y) = \cos\left(x^2 + \frac{1}{y^2}\right)$:

$$\begin{aligned}
\frac{\partial u_1(x,y)}{\partial x} &= \ldots \\
\frac{\partial u_1(x,y)}{\partial y} &= \ldots \\
\frac{1}{x}\frac{\partial u_1}{\partial x} + y^3 \frac{\partial u_1}{\partial y} &= \ldots \\
&= \ldots \\
&= \mathbf{0 \text{ q.e.d.}}
\end{aligned}$$

## Task 1.4: Solution

- Specific case $u_{:2}(x,y) = \left(x^2 + \frac{1}{y^2}\right)^2$:

$$\begin{aligned} \frac{\partial u_1(x,y)}{\partial x} &= \ldots \\ \frac{\partial u_1(x,y)}{\partial y} &= \ldots \\ \frac{1}{x}\frac{\partial u_2}{\partial x} + y^3 \frac{\partial u_2}{\partial y} &= \ldots \\ &= \ldots \\ &= 0 \text{ q.e.d.} \end{aligned}$$

**Task 1.4: Solution**

**Task 1.4: Solution**

# PDE





- In science and engineering applications, many common applications inolve linear, second-order PDEs. We will hence focus on this type of PDE:

**Definition 1.6: Linear PDE of second order and their classification**

- Consider the continuously differentiable functions $a, b, c, d, e, f, g : D \subset \mathbb{R}^2 \to \mathbb{R}$. The PDE for $u = u(x, y)$

$$a(x,y) \cdot u_{xx} + 2b(x,y) \cdot u_{xy} + c(x,y) \cdot u_{yy} =$$

$$d(x,y) \cdot u_x + e(x,y) \cdot u_y + f(x,y) \cdot u + g(x,y)$$

is a linear (non-homogenous) PDE of second order (assuming $u_{xy} = u_{yx}$).

# PDE

**Definition 1.6 (continued): Linear PDE of second order and their classification**

- The above linear PDE of second order is said to be
  - parabolic, if $b^2 - ac = 0$, e.g. heat flow and diffusion-type problems
  - hyperbolic, if $b^2 - ac > 0$, e.g. vibrating problems and wave motion problems
  - elliptic, if $b^2 - ac < 0$, e.g. steady-state, potential-type problems

# PDE

**Examples 1.3:** Well known examples are the following equations of mathematical physics:

- The **heat transfer equation** (also diffusion equation) is a parabolic PDE that describes the temperature variation $u$ as a function of time and spacial coordinates ($k$ is a constant describing thermal diffusivity):
  - in one spacial dimension $u = u(x,t)$

    $$u_t = k u_{xx}$$

  - in three spacial dimensions $u = u(x,y,z,t)$

    $$u_t = k(u_{xx} + u_{yy} + u_{zz})$$

    or using the Laplacian

    $$u_t = k \Delta u$$

**Examples 1.3 (continued):**

- The **wave equation** is a hyperbolic PDE that describes the amplitude/displacement $u$ of a wave, e.g. electromagnetic waves, sound waves, or water waves with constant velocity $c$:
  - in one spacial dimension $u = u(x,t)$

    $$u_{tt} = c^2 u_{xx}$$

  - in three spacial dimensions $u = u(x,y,z,t)$

    $$u_{tt} = c^2 (u_{xx} + u_{yy} + u_{zz})$$

    or using the Laplacian

    $$u_{tt} = c^2 \Delta u$$

**Examples 1.3 (continued):**

- The **Poisson equation** is an elliptic PDE that describes the time-independent potential field caused by a charge or mass densitiy distribution, with which it is then possible to calculate the associated electrostatic or gravitational field:
  - in one spacial dimension $u = u(x)$

    $$u_{xx} = f(x)$$

  - in three spacial dimensions $u = u(x, y, z)$

    $$u_{xx} + u_{yy} + u_{zz} = f(x, y, z)$$

    or using the Laplacian

    $$\Delta u = f(x, y, z)$$

**Examples 1.3 (continued):**

- if $f = 0$ we obtain from the Poisson equation

$$\Delta u = f(x, y, z)$$

the special case of Laplace's equation

$$\Delta u = 0$$

which, for instance, describes the steady-state solution of the heat equation

$$u_t = k\Delta u = 0$$

i.e. when $u$ does not vary with time.

# Analytical Solutions

- There are a variety of methods for obtaining symbolic, or closed-form, solutions to differential equations.
- The method of separation of variables can be used to obtain analytical solutions for some simple PDEs.
- The method consists in writing the general solution as the product of functions of a single variable, then replacing the resulting function into the PDE, and separating the PDE into ODEs of a single variable each.
- The ODEs are solved separately and their solutions combined into the solution of the PDE.

# The heat equation in 1 dimension

# The Heat Equation in 1d

- The flow of heat in a thin, laterally insulated homogeneous rod of length $L$ is modeled by

$$u_t = k u_{xx}$$

  where $u$ is the temperature and $k$ is a parameter resulting from combining thermal conductivity and density.
- For the PDE to have a uniqe solution, an initial condition for $t = 0$ and boundary conditions at $x = 0$ and $x = L$ are required.

**Definition 1.7: Initial Value Boundary Problem for the Heat Transfer Equation**

- We search for a twice continuously differentiable function $u = u(x,t)$ which solves the heat transfer equation

$$u_t = ku_{xx}$$

subject to the initial condition

$$u(x,0) = f(x)$$

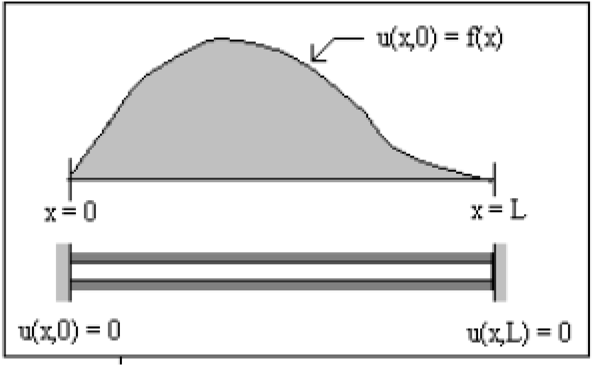
and the constant-value boundary conditions

$$u(0,t) = 0, \text{ and } u(L,t) = 0$$

for $x \in [0,L]$ and $t \geq 0$.

# The Heat Equation in 1d

- The physical phenomenon described by this PDE and its initial and boundary conditions is illustrated in the figure below (from [4]) with $u_0 = u_L = 0$.



# The Heat Equation in 1d



- We will try to find a solution by the method of separation of variables.
- This method assumes that the solution, $u(x,t)$, can be expressed as the product of two functions, $X(x)$ and $T(t)$:

$$u(x,t) = X(x)T(t).$$

# The Heat Equation in 1d

- With this substitution, the initial condition

$$u(x,0) = f(x) = X(x)T(0),$$

yields the set of conditions:

$$X(x) = f(x) \text{ when } t = 0 \text{ (i.e. we have set } T(0) = 1\text{)},$$

Also, from the boundary conditions follows

$$\begin{aligned} u(0,t) &= X(0)T(t) = 0 \Rightarrow X(0) = 0 \text{ (since } T(t) \neq 0\text{)} \\ u(L,t) &= X(L)T(t) = 0 \Rightarrow X(L) = 0 \text{ (since } T(t) \neq 0\text{)} \end{aligned}$$

- The partial derivatives are

$$\begin{aligned} u_t &= X \cdot T_t \\ u_{xx} &= X_{xx} \cdot T \end{aligned}$$

- For convenience, we have dropped the variables $x$ and $t$, but remember that $u(x,t) = X(x)T(t)$. The heat transfer equation then turns into

$$X \cdot T_t = k \cdot X_{xx} \cdot T.$$

Dividing by $u = X \cdot T$ yields

$$\frac{T_t}{T} = \frac{kX_{xx}}{X}.$$

# The Heat Equation in 1d



- Since the left-hand side $T_t/T$ is only a function of $t$ and the right-hand side $kX_{xx}/X$ is only a function of $x$, equality can only occur if both sides are equal to a constant, say $-\alpha$ $(\alpha > 0)$, which is independet of $x$ and $t$, i.e.

$$\frac{T_t}{T} = \frac{kX_{xx}}{X} = -\alpha$$

- The lef-thand side of the heat equation produces an ordinary differential equation (ODE) with independent variable $t$:

$$\frac{T_t}{T} = -\alpha$$

whose solution is

$$T(t) = e^{-\alpha t}$$

- Now we have to find the solution for $X(x)$. The right-hand side of the heat equation produces an ordinary differential equation (ODE) with independent variable $x$:

$$\frac{kX_{xx}}{X} = -\alpha$$

or

$$X_{xx} = -\frac{\alpha}{k} X$$

whose general solution is linear combination of the Sine and Cosine functions:

$$X(x) = a_n \cos\left(\sqrt{\frac{\alpha}{k}} \cdot x\right) + b_n \sin\left(\sqrt{\frac{\alpha}{k}} \cdot x\right)$$

- From the first boundary condition $X(0)=0$ we obtain

$$\begin{aligned} X(0) &= \underbrace{a_n \cos\left(\sqrt{\frac{\alpha}{k}}\cdot 0\right)}_{=1} + \underbrace{b_n \sin\left(\sqrt{\frac{\alpha}{k}}\cdot 0\right)}_{=0} = a_n \overset{!}{=} 0 \\ \Rightarrow X(x) &= b_n \sin\left(\sqrt{\frac{\alpha}{k}}\cdot x\right). \end{aligned}$$

- From the second boundary condition $X(L)=0$ we subsequently obtain

$$X(L) = b_n \sin\left(\sqrt{\frac{\alpha}{k}}\cdot L\right) = 0$$

- We need to find all possible values of $\alpha$ for which this equation is satisfied. Since we want $b_n \neq 0$, we set

$$\sin\left(\sqrt{\frac{\alpha}{k}} \cdot L\right) = 0.$$

- Since the roots of the Sine function are located at multiples of $\pi$, we have

$$\begin{aligned} \sqrt{\frac{\alpha}{k}} \cdot L &= n\pi \; (n \in \mathbb{N}_0) \\ \Rightarrow \alpha &= \alpha_n = \frac{n^2 \pi^2 k}{L^2} \end{aligned}$$

# The Heat Equation in 1d



- Thus we obtain

$$
\begin{aligned}
T(t) &= e^{-\alpha t} = e^{-\frac{n^2\pi^2 k}{L^2} t} \\
X(x) &= b_n \sin\left(\sqrt{\frac{n^2\pi^2 k}{L^2 k}} \cdot x\right) = b_n \sin\left(\frac{n\pi x}{L}\right)
\end{aligned}
$$

# The Heat Equation in 1d



- There will be a different expression for $u(x,t) = X(t)T(t)$ for each value of $n = 1, 2, 3, \ldots$. Therefore, we will call $u_n(x,t)$ the solution corresponding to a particular value of $n$ and write:

$$u_n(x,t) = b_n \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{n^2\pi^2 k}{L^2} t}$$

- Since the heat transfer equation is linear and homogenous, the superposition (i.e. linear combination) of the solutions $u_n(x,t)$ is again a solution. Therefore we can write the overall solution $u(x,t)$ as

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{n^2\pi^2 k}{L^2} t}.$$

- The last task is to calculate the coefficients $b_n$. From the inital condition $u(x,0) = f(x)$ we get

$$u(x,0) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \underbrace{e^{-\frac{n^2\pi^2 k}{L^2}\cdot 0}}_{=1} = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) = f(x)$$

- This is nothing else than the Fourier series of $f$, for which we know the coefficients already:

$$b_n = \frac{2}{L}\int_0^L f(x)\sin(\frac{n\pi x}{L})\,dx.$$

# The Heat Equation in 1d

- Thus the analytical solution to the IVBP of the heat transfer equation is

$$\boxed{\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{n^2\pi^2 k}{L^2}t} \\ b_n &= \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right) dx \end{aligned}}$$

**Task 1.5:**

- Determine the solution $u(x,t)$ for the one-dimensional heat equation for boundary conditions $u(0,t) = u(L,t) = 0$. The initial conditions are given by $u(x,0) = f(x) = 4(x/L)(1-x/L)$. Use values of $k=1$ and $L=1$. Plot $u(x,t)$ for $x \in [0,L]$ and $t \in [0,0.25]$ as surface in 3d.
- Hint: Use the MATLAB functions integral() or the Python function scipy.integrate.quad() to calculate $b_n$ for $n = 1,\ldots,40$

# The wave equation in 1 dimension

# The Wave Equation in 1d



- The wave equation in one dimension

$$u_{tt} = c^2 u_{xx}$$

can be used to model the displacement $u(x,t)$ of an elastic string or the vibration of a beam. For the case of an elastic string, it is

$$c^2 = \frac{T}{\mu},$$

where $T$ is the constant tension in the string and $\mu$ is the mass per unit length of the string. For the case of vibrations of a beam, it is

$$c^2 = \frac{gE}{\rho},$$

where $g$ is the acceleration of gravity, $E$ is the modulus of elasticity, and $\rho$ is the density of the beam.

# The Wave Equation in 1d

For the PDE to have a uniqe solution, an initial condition for $t = 0$ and boundary conditions at $x = 0$ and $x = L$ are required.

**Definition 1.7: Initial Value Boundary Problem for the Wave Equation**

- We search for a twice continuously differentiable function $u = u(x, t)$ which solves the heat transfer equation

$$u_{tt} = c^2 u_{xx}$$

subject to the **two** initial conditions

$$\begin{aligned} u(x,0) &= f(x) \\ u_t(x,0) &= g(x) \end{aligned}$$

and the constant-value boundary conditions

# The Wave Equation in 1d



- As in the case of the 1d heat transfer equation, the 1d wave equation can be solved by separating the variables

$$u(x,t) = X(x)T(t)$$

and repeating the same steps as above, which is omitted here.

- The analytical solution to the IVBP of the wave equation is

$$\boxed{\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right)\left(a_n \cos\left(\frac{n\pi ct}{L}\right) + b_n \sin\left(\frac{n\pi ct}{L}\right)\right) \\ a_n &= \frac{2}{L}\int_0^L f(x)\sin(\frac{n\pi x}{L})\,dx \\ b_n &= \frac{2}{n\pi c}\int_0^L g(x)\sin(\frac{n\pi x}{L})\,dx \end{aligned}}$$

# The Wave Equation in 1d

**Task 1.6 [4]:**

- Determine the solution $u(x,t)$ for the one-dimensional wave equation for a vibrating string. The boundary conditions are $u(0,t) = u(L,t) = 0$. The initial conditions are given by $u(x,0) = f(x) = (x/L)(1-x/L)$ and $u_t(x,0) = g(x) = (x/L)^2(1-x/L)$. Use values of $c = 1$ and $L = 1$. Plot $u(x,t)$ for $x \in [0,L]$ and $t \in [0,4]$ as surface in 3d.
- Hint: Use the MATLAB function integral() or the Python function scipy.integrate.quad() to calculate $a_n$ and $b_n$ for $n = 1, ..., 40$

# Numerical solutions to parabolic PDEs: heat transfer equation

# Numerical solution of the heat transfer



- Let us have a look at the heat transfer equation again

$$\frac{\partial u}{\partial t}(x,t) = k\frac{\partial^2 u}{\partial x^2}(x,t)$$

# Numerical solution of the heat transfer





- From the numerical analysis lecture ([5], chapter 6), we know that we can approximate partial derivatives of first order by finite differences such as

$$\begin{aligned}
D_1 : \frac{\partial u}{\partial x}(x_0, y_0) &\approx \frac{u(x_0 + h, y_0) - u(x_0, y_0)}{h} \text{ Forward Difference (first order)} \\
D_2 : \frac{\partial u}{\partial x}(x_0, y_0) &\approx \frac{u(x_0 + h, y_0) - u(x_0 - h, y_0)}{2h} \text{ Central Difference (first order)} \\
D_3 : \frac{\partial u}{\partial x}(x_0, y_0) &\approx \frac{u(x_0, y_0) - u(x_0 - h, y_0)}{h} \text{ Backward Difference (first order).}
\end{aligned}$$

- For the second order we have

$$D_4 : \frac{\partial^2 u}{\partial x^2}(x_0, y_0) \approx \frac{u(x_0 + 2h, y_0) - 2u(x_0 + h, y_0) + u(x_0, y_0)}{h^2}$$

Forward Difference (second order)

$$D_5 : \frac{\partial^2 u}{\partial x^2}(x_0, y_0) \approx \frac{u(x_0 + h, y_0) - 2u(x_0, y_0) + u(x_0 - h, y_0)}{h^2}$$

Central Difference (second order)

$$D_6 : \frac{\partial^2 u}{\partial x^2}(x_0, y_0) \approx \frac{u(x_0, y_0) - 2u(x_0 - h, y_0) + u(x_0 - 2h, y_0)}{h^2}$$

Backward Difference (second order)

# Numerical solution of the heat transfer

- The idea is to replace the partial derivatives $u_t$ and $u_{xx}$ with the corresponding finite differences. But first, as for ODE, we need to discrtise the independet varaiables $t$ and $x$ as

$$\begin{aligned} x_{i+1} &= x_i + \Delta x \, (i = 1, ..., n-1) \\ t_{j+1} &= t_j + \Delta t \, (j = 1, ..., m-1) \end{aligned}$$

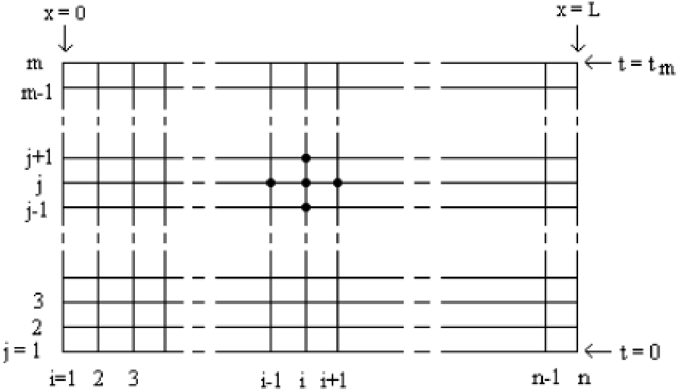
where

$$\begin{aligned} \Delta x &= x_{i+1} - x_i = \frac{x_{max} - x_{min}}{n-1} \\ \Delta t &= t_{i+1} - t_i = \frac{t_{max} - t_{min}}{m-1} \end{aligned}$$

and are the constant stepwidths for $x_i \in [x_{min}, x_{max}]$ and $t_j \in [t_{max}, t_{min}]$.

# Numerical solution of the heat transfer

- Thus we get a two dimensional grid in the $(x, t)$ plane as shown below (from [4]):




$$0 \leq x_i \leq L, \Delta x = \frac{L}{n-1} \text{ and } 0 \leq t_j \leq L, \Delta t = \frac{t_m}{m-1}.$$

# Numerical solution of the heat transfer



- Let us now replace $\frac{\partial u}{\partial t}(x,t)$ in the heat transfer equation with the forward difference $D_1$ of first order and $\frac{\partial^2 u}{\partial x^2}(x,t)$ with the central difference $D_5$ of second order.
- Using the discretised coordinates $(x_i, t_j)$ and the abbreviation

$$u(x_i, t_j) = u_{i,j}$$

(note the the indices $i$ and $j$ here indicate the position in the grid and not partial derivatives) we get

$$\frac{\partial u}{\partial t}(x_i,t_j) \approx \frac{u(x_i,t_j+\Delta t)-u(x_i,t_j)}{\Delta t} = \frac{u(x_i,t_{j+1})-u(x_i,t_j)}{\Delta t} = \frac{u_{i,j+1}-u_{ij}}{\Delta t} \quad (2)$$

$$\frac{\partial^2 u}{\partial x^2}(x_i,t_j) \approx \frac{u(x_i+\Delta x,t_j)-2u(x_i,t_j)+u(x_i-\Delta x,t_j)}{(\Delta x)^2} = \frac{u(x_{i+1},t_j)-2u(x_i,t_j)+u(x_{i-1},t_j)}{(\Delta x)^2}$$

$$= \frac{u_{i+1,j}-2u_{ij}+u_{i-1,j}}{(\Delta x)^2} \quad (3)$$

# Numerical solution of the heat transfer

- The heat transfer equation

$$\frac{\partial u}{\partial t}(x_i, t_j) = k\frac{\partial^2 u}{\partial x^2}(x_i, t_j)$$

turns into

$$\frac{u_{i,j+1} - u_{ij}}{\Delta t} \approx k\frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{(\Delta x)^2}$$

which can be solved for $u_{i,j+1}$ :

$$u_{i,j+1} = u_{i,j} + \alpha\left(u_{i+1,j} - 2u_{ij} + u_{i-1,j}\right) \; (i = 2, ..., n-1, \; j = 1, ..., m-1) \quad (4)$$

Here we have set $\alpha = k\frac{\Delta t}{(\Delta x)^2}$ .Note that $2 \le i \le n-1$, since $u_{1j}$ and $u_{nj}$ are defined by the two boundary conditions.

# Numerical solution of the heat transfer



- This discretisation based on finite differences thus allows for the the calculation of $u(x_i, t_j)$ when the initial condition

$$u(x,0) = f(x)$$

and the boundary conditions

$$\begin{aligned} u(0,t) &= u_0(t) \\ u(L,t) &= u_L(t) \end{aligned}$$

are included as

$$\begin{aligned} u_{i1} &= f(x_i)\,(i = 1, ..., n) \\ u_{1j} &= u_0(t_j)\,(j = 1, ..., m) \\ u_{nj} &= u_L(t_j)\,(j = 1, ..., m). \end{aligned}$$

Stability conditions for this explicit solution requires that $\alpha < 0.5$.

## Numerical Solution to the Heat Transfer Equation:

- The numerical solution $u(x_i, t_j) = u_{ij}$ of the IVBP

$$\begin{aligned}
\frac{\partial u}{\partial t}(x,t) &= k\frac{\partial^2 u}{\partial x^2}(x,t) \\
u(x,0) &= f(x) \\
u(0,t) &= u_0(t) \\
u(L,t) &= u_L(t)
\end{aligned}$$

in a domain $D$ defined by $x \in [0,L]$ and $t \in [0,T]$ can be calculated for stepwidths $\Delta x = \frac{L}{n-1}$ and $\Delta t = \frac{T}{m-1}$ as:

$$\begin{aligned}
x_{i+1} &= x_i + \Delta x \, (i = 1, ..., n-1) \\
t_{j+1} &= t_j + \Delta t \, (j = 1, ..., m-1) \\
u_{i1} &= f(x_i) \, (i = 1, ..., n) \\
u_{1j} &= g_1(t_j) \, (j = 1, ..., m) \\
u_{nj} &= u_L(t_j) \, (j = 1, ..., m). \\
u_{i,j+1} &= u_{i,j} + \alpha \left(u_{i+1,j} - 2u_{ij} + u_{i-1,,j}\right) \; (i = 2, ..., n-1, \, j = 1, ..., m-1)
\end{aligned}$$

if $\alpha = k\frac{\Delta t}{(\Delta x)^2} < 0.5$.

# Task 1.7



1. Write a MATLAB/Python function

[u] = Heat_PDE_Task1_7(xrange, trange, u_inital, u0_boundary, uL_boundary, $k$)

where

| | | |
|---|---|---|
| xrange | : | a vector of lengt $n$ with equally spaced values $x_1, \ldots, x_n$ |
| trange | : | a vector of lengt $m$ with equally spaced values $t_1, \ldots, t_m$ |
| u_initial | : | a vector of lengt $n$ with the initial conditions $f(x_1), \ldots, f(x_n)$ |
| u0_boundary | : | a vector of lengt $m$ with the boundary conditions $u_0(t_1), \ldots, u_0(t_m)$ |
| uL_boundary | : | a vector of lengt $m$ with the boundary conditions $u_L(t_1), \ldots, u_L(t_m)$ |
| $k$ | : | constant from the heat equation |

The function returns the matrix $u$ of size $n \times m$, which represents the solution $u(x,t)$ of the heat equation according to Eqn. 4. Hint: the loop over $j$ is the outer loop, the loop over $i$ is the inner loop.

# Task 1.7 (continued)



2. Write a MATLAB script that solves the heat transfer equation using your above function

- for the same parameters as in Task 1.5 (adjust the stepsize so that $\alpha < 0.5$);
- for new parameters: $x = [0 : 0.1 : 2]$, $t = [0 : 0.005 : 1.5]$, $u(x,0) = 0$, $u(0,t) = e^{-2t}\sin(50t)$, $u(2,t) = e^{-3t}\cos(50t)$, $k = 1$
- Plot $u(x,t)$.

# Task 1.7 Solution

# Task 1.7 Solution

# Numerical solutions to hyperbolic PDEs: wave equation

# Numerical solution of the wave equation

- Let us now have a look at the wave equation again

$$\frac{\partial^2 u}{\partial t^2}(x,t) = c^2 \frac{\partial^2 u}{\partial x^2}(x,t)$$

where $c$ is the velocity of propagation of one-dimensional waves in a medium along the $x-$direction, with $0 \leq x \leq L$ and $t > 0$. The equation requires for its solution **two initial conditions**, typically

$$\begin{aligned} u(x,0) &= f(x) \\ \frac{\partial u}{\partial t}(x,0) &= g(x) \end{aligned}$$

and **two boundary conditions**

$$\begin{aligned} u(0,t) &= u_0(t) \\ u(L,t) &= u_L(t) \end{aligned}$$

# Numerical solution of the wave equation

- For the numerical solution of the wave equation we use a grid similar to that used in the solution of the heat equation, with $x$ increment $\Delta x$ and time increment $\Delta t$.
- As in the heat transfer equation, the numerical solution seeks to find the values

$$u_{ij} = u(x_i, t_j)$$

for each grid point. Note again that indices $i$ and $j$ here indicate the position in the grid and not partial derivatives.
- Replacing the partial derivatives with the central difference $D_5$ of second order yields (cf. Eqn. 3):

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2}(x_i, t_j) &\approx \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{(\Delta t)^2} \\ \frac{\partial^2 u}{\partial x^2}(x_i, t_j) &\approx \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{(\Delta x)^2}. \end{aligned}$$

# Numerical solution of the wave equation



- Defining the parameter

$$\alpha^2 = c^2 \frac{(\Delta t)^2}{(\Delta x)^2}$$

and substituting the above terms in the wave equation we get

$$u_{i,j+1} = \alpha^2 (u_{i-1,j} + u_{i+1,j}) + 2(1 - \alpha^2) u_{ij} - u_{i,j-1}.$$

# Numerical solution of the wave equation

- However, when $j = 1$ (first time step) the above equation yields

$$u_{i,2} = \alpha^2(u_{i-1,1} + u_{i+1,1}) + 2(1-\alpha^2)u_{i1} - u_{i0},$$

which introduces a term $u_{i0}$ that is not defined and must be eliminated. We can achieve this with the second initial condition

$$\frac{\partial u}{\partial t}(x,0) = g(x)$$

and replace it with the first oder central difference $D_2$ :

$$\begin{aligned} \frac{\partial u}{\partial t}(x_i, t_1 = 0) &\approx \frac{u(x_i, t_2) - u(x_i, t_0)}{2\Delta t} = \frac{u_{i2} - u_{i0}}{2\Delta t} = g(x_i) \\ \Rightarrow u_{i0} &= u_{i2} - 2\Delta t \cdot g(x_i) \end{aligned}$$

- When $u_{i0}$ is replaced in the expression for $u_{i2}$ we get

$$\begin{aligned} u_{i,2} &= \alpha^2(u_{i-1,1} + u_{i+1,1}) + 2(1-\alpha^2)u_{i1} - u_{i0} \\ &= \alpha^2(u_{i-1,1} + u_{i+1,1}) + 2(1-\alpha^2)u_{i1} - u_{i2} + 2\Delta t \cdot g(x_i) \\ \Rightarrow u_{i,2} &= \frac{\alpha^2}{2}(u_{i-1,1} + u_{i+1,1}) + (1-\alpha^2)u_{i1} + \Delta t \cdot g(x_i) \end{aligned}$$

Thus, we can calculate $u(x_i, t_j) = u_{ij}$ now for all spacial coordinates $x_i\,(i = 1, ..., n)$ and time steps $t_j\,(j = 1, ..., m)$.

## Numerical Solution to the Wave Equation:

- The numerical solution $u(x_i,t_j) = u_{ij}$ of the IVBP

$$
\begin{aligned}
\frac{\partial^2 u}{\partial t^2}(x,t) &= c^2 \frac{\partial^2 u}{\partial x^2}(x,t) \\
u(x,0) &= f(x) \\
\frac{\partial u}{\partial t}(x,0) &= g(x) \\
u(0,t) &= u_0(t) \\
u(L,t) &= u_L(t)
\end{aligned}
$$

in a domain $D$ defined by $x \in [0,L]$ and $t \in [0,T]$ can be calculated for stepwidths $\Delta x = \frac{L}{n-1}$ and $\Delta t = \frac{T}{m-1}$ as:

$$
\begin{aligned}
x_{i+1} &= x_i + \Delta x \, (i = 1, ..., n-1) \\
t_{j+1} &= t_j + \Delta t \, (j = 1, ..., m-1) \\
u_{1j} &= u_0(t_j) \, (i = 1, j = 1, ..., m) \\
u_{nj} &= u_L(t_j) \, (i = n,, j = 1, ..., m) \\
u_{i,1} &= f(x_i) \, ((i = 1, ..., n,, j = 1) \\
u_{i,2} &= \frac{\alpha^2}{2}(u_{i-1,1} + u_{i+1,1}) + (1-\alpha^2)u_{i1} + \Delta t \cdot g(x_i) \, ((i = 2, ..., n-1,, j = 2) \\
u_{i,j+1} &= \alpha^2(u_{i-1,j} + u_{i+1,j}) + 2(1-\alpha^2)u_{ij} - u_{i,j-1} \, ((i = 2, ..., n-1,, j = 2, ..., m-1)
\end{aligned}
$$

if $\alpha^2 = c^2 \frac{(\Delta t)^2}{(\Delta x)^2} < 1$ (for stability reasons).

# Task 1.8

1. Write a MATLAB/Python function

[u] = Wave_PDE_Task1_8(xrange, trange, u_inital, du_inital, u0_boundary, uL_boundary, $c$)

where

| | | |
|---|---|---|
| xrange | : | a vector of lengt $n$ with equally spaced values $x_1, \ldots, x_n$ |
| trange | : | a vector of lengt $m$ with equally spaced values $t_1, \ldots, t_m$ |
| u_initial | : | a vector of lengt $n$ with the initial conditions $f(x_1), \ldots, f(x_n)$ |
| du_initial | : | a vector of lengt $n$ with the initial conditions $g(x_1), \ldots, g(x_n)$ |
| u0_boundary | : | a vector of lengt $m$ with the boundary conditions $u_0(t_1), \ldots, u_0(t_m)$ |
| uL_boundary | : | a vector of lengt $m$ with the boundary conditions $u_L(t_1), \ldots, u_L(t_m)$ |
| $c$ | : | constant velocity from the wave equation |

The function returns the matrix $u$ of size $n \times m$, which represents the solution $u(x, t)$ of the wave equation. Hint: the loop over $j$ is the outer loop, the loop over $i$ is the inner loop.

# Task 1.8 (continued)

2. Write a MATLAB script that solves the wave equation using your above function:
   - for the same parameters as in Task 1.6. Plot $u(x,t)$;
   - for the parameters: $x = [0:0.1:1]$, $t = [0:0.01:9]$, $u(x,0) = x(1-x)$, $\frac{\partial u}{\partial t}(x,0) = 0.2$, $u(0,t) = u(1,t) = 0$, $c = 1$. Plot $u(x,t)$.
   - Create a "movie" of 2d plots of $u(x,t)$ for increasing $t$ using a for-loop. Use pause(0.01) to display each plot before the loop continues.

# Task 1.8 Solution

# Task 1.8 Solution

# Sources




- [1] The series of lectures given by Andrew J. Bernoff and others, “An Introduction to Partial Differential Equations in the Undergraduate Curriculum”, available at https://www.math.hmc.edu/~ajb/PCMI/lecture_schedule.html
- [2] 'Mathematik für Ingenieure und Naturwissenschaftler: Band 2', L. Papula, Vieweg + Teubner Verlag (13. Auflage), 2012
- [3] 'Ausgewähle Kapitel der höheren Mathematik', W. Strampp, Springer, 2014
- [4] Introduction to Partial Differential Equations, G.E. Urroz, 2004
- [5] “Vorlesung Numerische Mathematik 1 & 2, Studiengang Informatik der ZHAW”, R. Knaack, 2015