Numerical Simulation of Transport Processes in Porous Media

Spatial Discretisation Methods

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(Spatial) Discretisation Methods

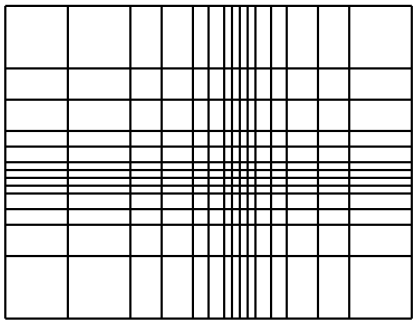
- Partial differential equations can only be solved analytically for very special cases with a very restricted choice of domain shapes, boundary conditions and parameter fields.
- Approximations can be calculated with numerical methods
- Numerical methods usually yield approximations of
  - the solution at certain points in space (e.g. Finite Differences)
  - the solution with a parameterised function (e.g. Finite Elements, Discontinuous Galerkin . . .)
  - certain mathematical properties (mass conservation, continuity of fluxes) of the equation (e.g. Finite Volumes, Mimetic Finite Differences)

Grids

- For most discretisation schemes it is necessary to partition the domain Ω into sub-domains (elements) e with a simple geometrical structure (triangulation).
- Typical element geometries are:
  - 1D line segments
  - 2D triangle, quadrilateral
  - 3D tetrahedron, cuboid, pyramid, prism, hexahedron
- All the elements together are called a grid.
- It is not always possible to fill the whole domain with elements of a simple geometry, but there should be no holes in the grid and $\bigcup_{i=1}^{n} e_i \approx \bar{\Omega}$

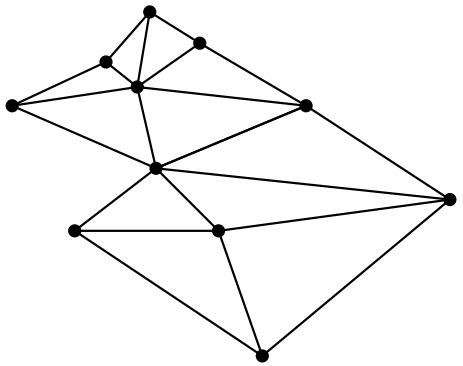
Characterisation of Grids

There are different varieties of grids depending on the purpose and the numerical scheme. Grids can be



structured is constructed with regular elements from a simple construction principle. Typical examples are grids with rectangular elements with a width which is

- **equidistant** element width is h_i in dimension $i \in \{x, y, z\}$
- **tensor product** element width is $h_i = f(x_i)$ in dimension $i \in \{x, y, z\}$



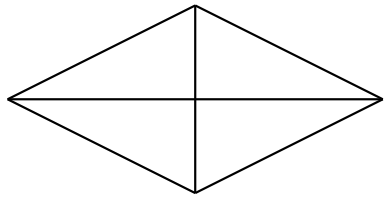
unstructured can be composed of elements with different geometries and shapes

Characterisation of Grids

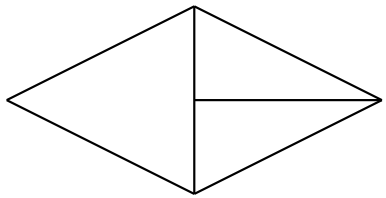
There are different varieties of grids depending on the purpose and the numerical scheme. Grids can be

conforming there are no hanging nodes, i.e. if the intersection $e_i \cap e_j$ between two elements e_i and e_j is a

- point they have a common node
- a line they have a common edge
- a surface they have a common face



non-conforming there are hanging nodes, i.e. nodes of one element, which are not nodes of an element with which an intersection exists



The Finite Difference Method

Basic Idea: Partial derivatives are replaced with difference quotients (Taylor series expansion)
Let us use the one-dimensional Poisson equation as example:

$$-\frac{\partial^2 u}{\partial x^2} = f(x) \qquad x \in (0,1)$$
$$u(0) = \varphi_0, \quad u(1) = \varphi_1.$$

We do a Taylor expansion of $u(x+h)$:

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(x+\vartheta^+ h) \qquad \vartheta^+ \in (0,1)$$
$$\iff u'(x) = \frac{u(x+h)-u(x)}{h} - \underbrace{\left(\frac{h}{2}u''(x+\vartheta^+ h)\right)}_{O(h)} \qquad \vartheta^+ \in (0,1)$$

This is a first order accurate approximation of the gradient of u.

Second Order Approximation

If we do an expansion up to the fourth order terms of $u(x+h)$ and $u(x-h)$

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u''''(x+\vartheta^+ h)$$
$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u''''(x-\vartheta^- h)$$

we get the second order accurate formula for gradient u

$$u(x+h) - u(x-h) = 2hu'(x) + \frac{h^3}{6}\left\{u'''(x+\vartheta^+ h) + u'''(x-\vartheta^- h)\right\}$$
$$\iff u'(x) = \frac{u(x+h) - u(x-h)}{2h} \quad \underbrace{- \left(\frac{h^2}{12}\left\{u'''(x+\vartheta^+ h) + u'''(x-\vartheta^- h)\right\}\right)}_{O(h^2)}$$

Second Derivative

and the second order accurate approximation of the second derivative of u:

$$u(x+h) + u(x-h) = 2u(x) + h^2 u''(x) + \frac{h^4}{24}\left\{u''''(x+\vartheta^+ h) + u''''(x-\vartheta^- h)\right\}$$

$$\Longleftrightarrow \quad u''(x) = \frac{u(x-h) - 2u(x) + u(x+h)}{h^2} \quad \underbrace{- \left(\frac{h^2}{24}\{\ldots\}\right)}_{O(h^2)}$$

Application to one-dimensional Poisson Equation

If we insert this in our partial differential equation we get for $x_i = i \cdot h$

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

one equation per grid point. Dirichlet boundary conditions can be easily incorporated by setting $u_0 = \varphi_0$ and $u_n = \varphi_1$ and bringing the corresponding terms to the right hand side.

Application to two-dimensional Poisson Equation

In 2D the Poisson equation is

$$-\Delta u(x) = f(x)$$

and we get for $x_i = i \cdot h$ and $y_j = j \cdot h$ with

$$\Delta u(x_i, y_j) \approx \frac{u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j)}{h^2} + \frac{u(x_i, y_{j-1}) - 2u(x_i, y_j) + u(x_i, y_{j+1})}{h^2}$$

for each grid point the linear equation

$$\frac{4u(x_i, y_j) - u(x_{i-1}, y_j) - u(x_{i+1}, y_j) - u(x_i, y_{j-1}) - u(x_i, y_{j+1})}{h^2} = f(x_i, y_j)$$

Boundary Conditions

- Dirichlet boundary conditions can easily be integrated by rearranging the equation systems and bringing them to the right side of the equation.
- Neumann boundary conditions are integrated by either replacing them with a forward difference formula or by introduction of ghost nodes

Rate of Convergence

The approximation error $e = ||u - u_h||$ of the approximated solution u_h on a grid with element width h is proportional to the size of the grid cells.

- We get a *linear grid convergence* if

$$\lim_{h \to 0} \frac{e_{i+1}}{e_i} = \lim_{h \to 0} \frac{||u - u_{h_{i+1}}||}{||u - u_{h_i}||} \leq C \cdot \frac{h_{i+1}}{h_i}$$

- We get a *grid convergence of order q* if

$$\lim_{h \to 0} \frac{e_{i+1}}{e_i} = \lim_{h \to 0} \frac{||u - u_{h_{i+1}}||}{||u - u_{h_i}||} \leq C \cdot \left(\frac{h_{i+1}}{h_i} \right)^q$$

- It can be proved that the Finite Difference Method is second-order accurate on an equidistant grid if the solution is regular enough

Properties of the Finite Difference Method

- Advantages:
  - easy to formulate and implement
  - well suited for structured grids
- Problems:
  - Only linear convergence rate on non-equidistant grids
  - What's the value between two points?
  - Representation of complex domains difficult
  - In general not (locally) mass-conservative.

The Finite Element Method

- A parameterised trial function $y(x)$ is inserted in the partial differential equation, resulting in a residual.
- The trial function is build as a sum over products of base functions times parameters $y(x) = \sum_{i=1}^{n} c_i \cdot \psi_i(x)$
- We would like to choose the parameters c_i of the trial function to minimise the error between the approximation and the correct solution. As the latter is unknown this is not possible
- For the correct solution the partial differential equation is zero:

$$F\left(\frac{\partial^m u}{\partial x_1^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_1^{m-1}}(\vec{x}), \ldots, \frac{\partial^m u}{\partial x_1^{m-1}\partial x_2}(\vec{x}), \ldots, \frac{\partial^m u}{\partial x_n^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_n^{m-1}}(\vec{x}), \ldots, u(\vec{x}), \vec{x}\right) = 0 \quad \forall \vec{x} \in \Omega \tag{1}$$

Weak Solution

- We demand that the partial differential equation F should only be fulfilled in the integral over Ω. For generality we multiply F with a weighting function w:

$$\iiint_{\Omega} F\left(\frac{\partial^m u}{\partial x_1^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_1^{m-1}}(\vec{x}), \ldots, \frac{\partial^m u}{\partial x_1^{m-1}\partial x_2}(\vec{x}), \ldots, \frac{\partial^m u}{\partial x_n^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_n^{m-1}}(\vec{x}), \ldots, u(\vec{x}), \vec{x}\right) \cdot w(\vec{x})\, dV = 0 \tag{2}$$

As the partial differential equation is only fulfilled "on an average" we call this a *weak formulation*.

Trial and Weighting Functions

- To reduce the computational costs and increase the flexibility, the base functions are defined element wise, i.e. for each element there is a set of base functions, which is different from zero on this element, but zero on all other elements. We get:

$$y(x) = \sum_{e_i} \sum_{j=1}^{n_{e_i}} c_{e_i,j} \cdot \psi_{e_i,j}(x)$$

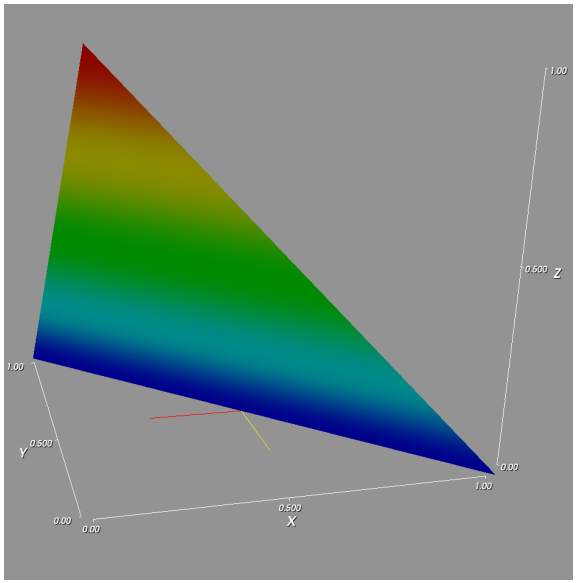
$$w(x) = \sum_{e_i} \sum_{j=1}^{n_{e_i}} \phi_{e_i,j}(x)$$

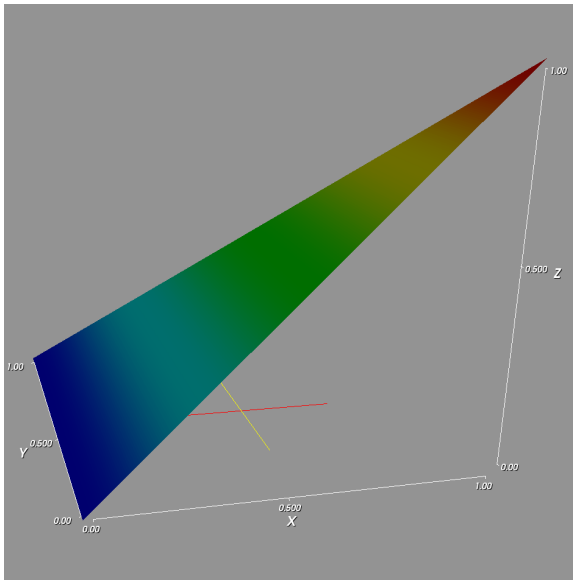
- This allows the integral over the whole domain to be replaced with a sum over integrals over each of the elements
- Different Finite Element methods differ in the choice of the trial and weight functions.

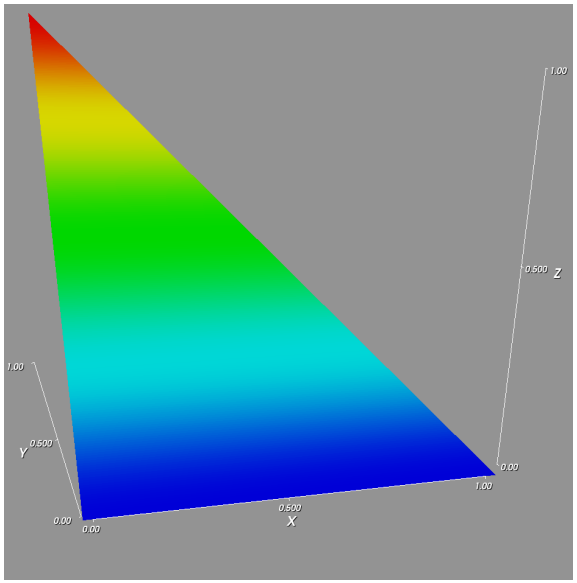
Element-wise Formulation

- Usually the trial function on an element is parameterised with the value of the trial function at certain positions (the nodes, additionally on edges or faces) and the base chosen to be one at one of these positions and zero at all others (similar to Lagrange interpolation). For a conforming grid this guarantees a solution which is steady over element boundaries.
- The base functions are defined on a reference element and scaled to the real geometry

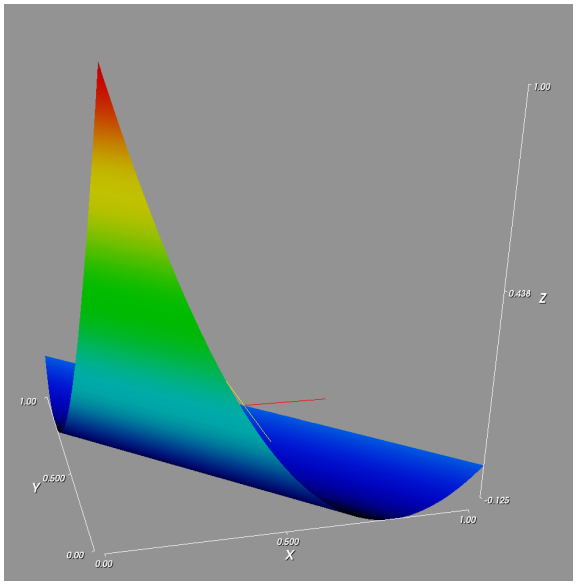
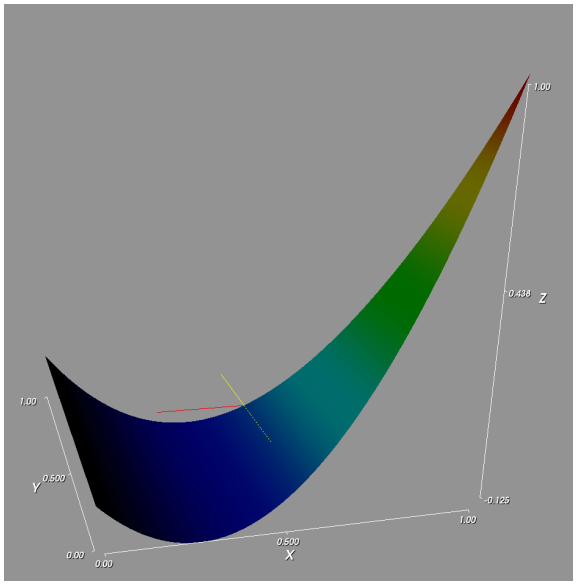
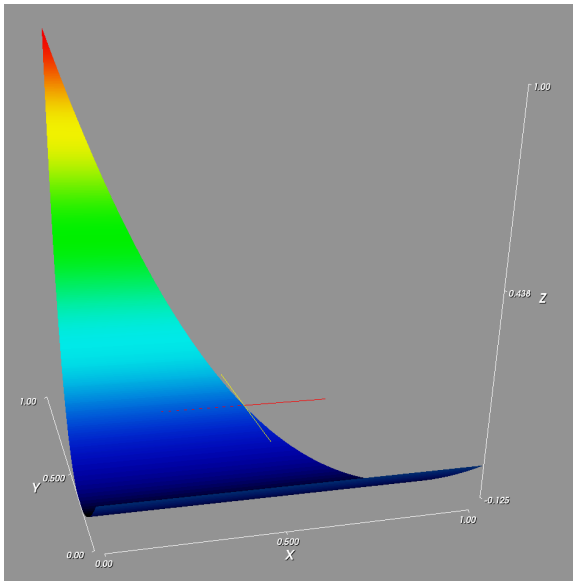
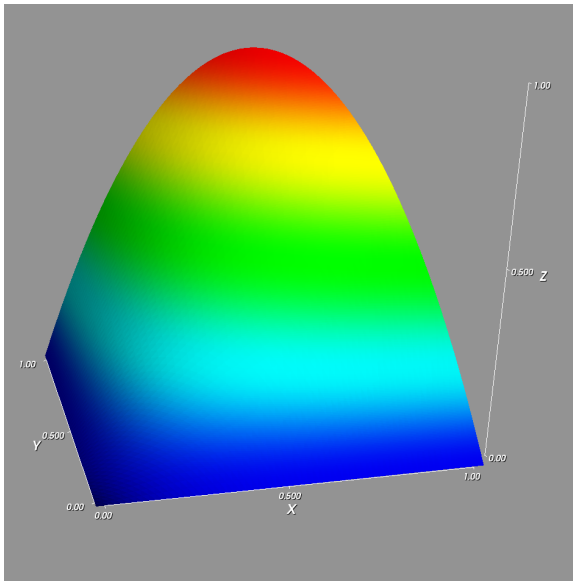
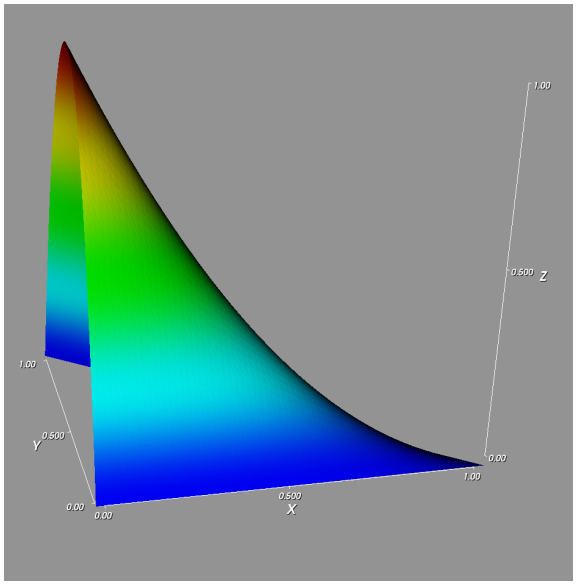
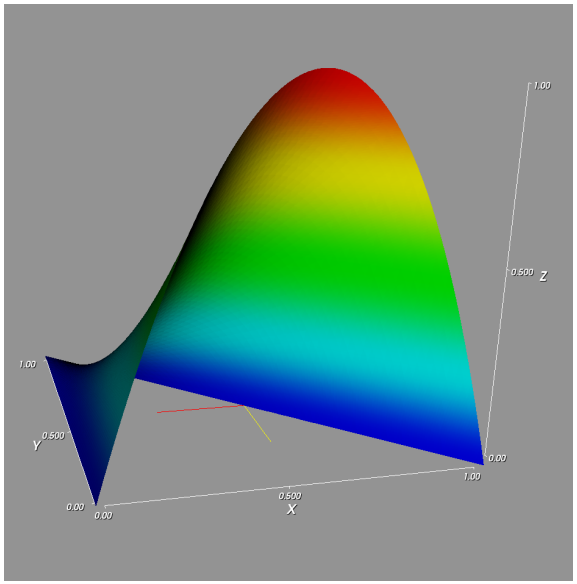
P1 Base Functions







P2 Base Functions

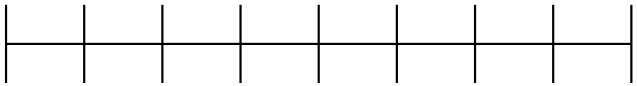







Example: One-dimensional Poisson Equation

$$-\frac{\partial^2 u(x)}{\partial x^2} = f(x) \qquad \text{in } (0,1)$$

with the boundary conditions $u(0) = 0$ and $u(1) = 0$

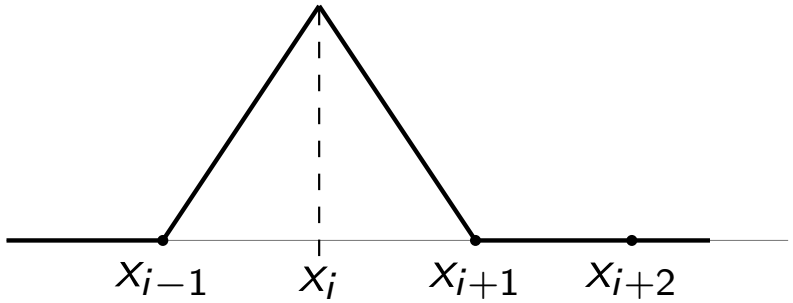
We use an equidistant grid



$$x_i = i \cdot h \quad i = 0, \ldots, n, \quad h = \frac{1}{n}$$

Example: One-dimensional Poisson Equation

As base functions we use the hat functions $\psi_i, \quad i = 1, ..., n-1$



$$\psi_i(x) = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}} & x \in (x_{i-1}, x_i) \\ \frac{x - x_{i+1}}{x_i - x_{i+1}} & x \in (x_i, x_{i+1}) \\ 0 & \text{else} \end{cases}$$

with the special property:

$$\psi_i(x_j) = \begin{cases} 1 & i = j \\ 0 & \text{else} \end{cases}$$

$$-\int_0^1 \frac{\partial^2 y}{\partial x^2} \cdot w \, dx = \int_0^1 f \cdot w \, dx$$

with partial integration:

$$-\left[-\int_0^1 \frac{\partial y}{\partial x} \cdot \frac{\partial w}{\partial x} \, dx + \frac{\partial y}{\partial x}(1)w(1) - \frac{\partial y}{\partial x}(0)w(0)\right] = \int_0^1 f \cdot w \, dx$$

as $w(x)$ is zero at the boundary we get

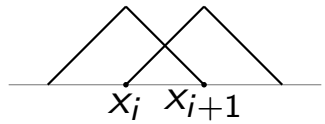
$$\int_0^1 \frac{\partial y}{\partial x} \cdot \frac{\partial w}{\partial x} \, dx = \int_0^1 f \cdot w \, dx$$

With $y(x) = \sum_i y_i \psi_i(x)$ and $w(x) = \sum_i \psi_i(x)$ we get on the interval for each base function of the weighting function one line of a linear equation system:

$$y_{i-1} \int_{x_{i-1}}^{x_i} \frac{\partial \psi_{i-1}}{\partial x} \cdot \frac{\partial \psi_i}{\partial x} dx + y_i \int_{x_{i-1}}^{x_{i+1}} \frac{\partial \psi_i}{\partial x} \cdot \frac{\partial \psi_i}{\partial x} dx + y_{i+1} \int_{x_i}^{x_{i+1}} \frac{\partial \psi_{i+1}}{\partial x} \cdot \frac{\partial \psi_i}{\partial x} dx = \int_{x_{i-1}}^{x_{i+1}} f \cdot \psi_i dx$$

The integrals can be evaluated to:

$$\int \psi_i \psi_k = \begin{cases} \int_{x_i-h}^{x_i} \frac{1}{h} \cdot \frac{1}{h} dx + \int_{x_i}^{x_i+h} (-\frac{1}{h}) \cdot (-\frac{1}{h}) dx = \frac{1}{h} + \frac{1}{h} = \frac{2}{h} & k = i \\ \int_{x_i}^{x_i+h} (-\frac{1}{h}) \cdot \frac{1}{h} dx = -\frac{1}{h} & k = i \pm 1 \\ 0 & \text{else} \end{cases}$$



If we integrate the right hand side with the trapezoidal rule we get

$$\int_{x_{i-1}}^{x_{i+1}} f \cdot \psi_i dx \approx h \cdot (\frac{1}{6} f_{i-1} + \frac{2}{3} f_i + \frac{1}{6} f_{i+1})$$

and finally the linear equation

$$\frac{1}{h}(-y_{i-1} + 2y_i - y_{i+1}) = h \cdot (\frac{1}{6} f_{i-1} + \frac{2}{3} f_i + \frac{1}{6} f_{i+1})$$

Boundary Conditions and Convergence Rate

- Dirichlet boundary conditions can be directly incorporated into the trial functions.
- Neumann boundary conditions are handled in the integrals.
- Convergence order depends on the choice of weight and trial functions.

Properties of the Finite Element Method

- Advantages:
  - can be used for domains with complicated shape
  - yields function values everywhere
  - well suited for unstructured grids
  - local adaptivity possible
- Problems:
  - grid generation can be complicated (must often fullfill certain conditions)
  - more computationally expensive for simple problems
  - not always (locally) mass-conservative

Comparison of one-dimensional Finite Differences and Finite Element Equation

$$
\begin{aligned}
-\frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2} &= f(x_i) \\
\frac{1}{h}(-y_{i-1} + 2y_i - y_{i+1}) &= h \cdot (\frac{1}{6} f_{i-1} + \frac{2}{3} f_i + \frac{1}{6} f_{i+1})
\end{aligned}
$$