# Outline

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# Method of lines for time dependent PDEs

Idea:

- use a semi-discretization and transform the PDE into an ODE system
- solve the ODE, by an ODE solver to compute the solution layer-by-layer

Advantages of MoL:

- applying of high order (implicit) methods with step size control (instead of Euler or Crank-Nicolson)
- use already implemented and tested routines

Discretization in space:

$$u_t = D^{(2)}u + f(t,u), \quad u \in \mathbb{R}^n$$

ODE system:

$$\begin{aligned} U' &= D^{(2)}U + f(t,U), \quad t > 0 \\ U(0) &= u_0(X) \qquad \text{with } X = (x_1, \ldots, x_n)^T \end{aligned}$$

## Example

*Consider once again the parabolic initial boundary value problem*

$$u_t = u_{xx} + 0.1\sin(0.5\pi x) \quad \textit{in } \Omega = (0,2),\ t > 0,$$
$$u(x,0) = \max(1 - 5|1-x|, 0), \quad u(0,t) = u(2,t) = 0.$$

*We can write the problem in form of an ODE system as*

$$U'(t) = D^{(2)}U + 0.1\sin(0.5\pi X)$$

*with* $X = (x_1, \ldots, x_n)^T$ *and the initial condition*

$$U(0) = \max(1 - 5|1-x|, 0).$$

# Method of lines for parabolic problems

## Example

*Consider once again the parabolic initial boundary value problem*

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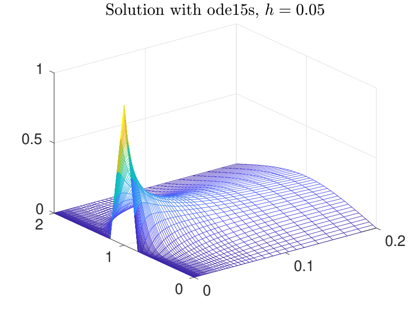
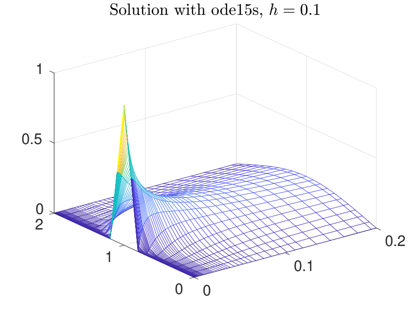
*The ode15s solver in matlab using BDF-formulas (multistep methods).*



Application of MoL for hyperbolic problems:

- transformed system is in $\mathbb{R}^n$ and the ODE is of second order
- to apply an ODE-solver one has to transform it a second time
- thus the final 1st order ODE system is in $\mathbb{R}^{2n}$

ODE system of 2nd order:

$$\begin{aligned} U'' &= AU + f(t, U) \\ U(0) &= u_0(X) \end{aligned}$$

With $V = (U,\ U')^T \in \mathbb{R}^{2n}$ the 1st order system is

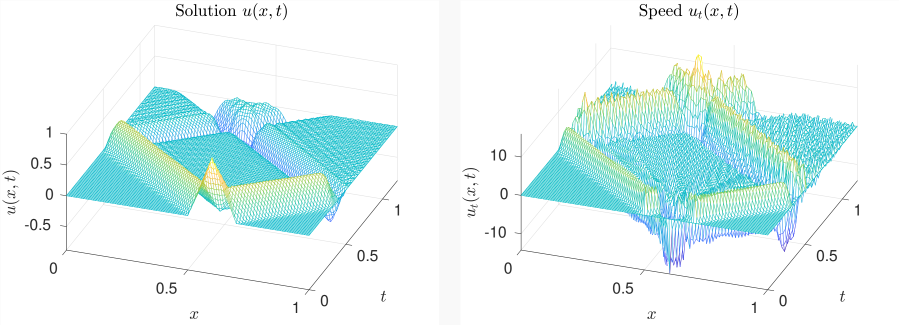
$$V' = \begin{pmatrix} 0 & I_{n\times n} \\ A & 0 \end{pmatrix} V + f(t, V(1:n)), \qquad V(0) = \begin{pmatrix} u_0(X) \\ u_t(X) \end{pmatrix}$$

Take care on the boundary conditions at $x_0$ and $x_N$.

## Example

*Consider the initial-boundary value problem for* $\Omega = (0,1)$, $t \in (0,1)$

$$\begin{aligned} u_{tt} &= c u_{xx}, \\ u(x,0) &= \max\big(0, \min(10x-5, -10x+7)\big), \\ u_t(x,0) &= 0, \\ u(0,t) &= u(1,t) = 0. \end{aligned}$$



# Outline

Finite differences (FD):

- problem for curved boundaries using a rectangular grid, less flexible in terms of a refinement
- analysis of difference methods needs strong assumptions on smoothness

Finite element method (FEM):

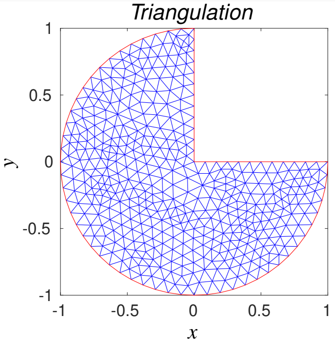
- state of the art for elliptic PDEs
- the PDE is transformed into a so-called weak formulation
- only so-called weak solutions are computed
- domain is (usually) decomposed into small triangles (triangulation)
- approximate solutions are determined using locally defined basis functions and Soboloev spaces

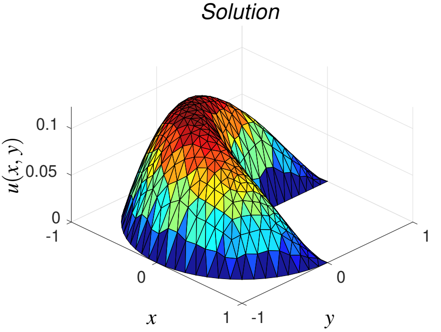
## Example

*Consider the boundary value problem*

$$-\Delta u(x,y) = 1 \; in \; \Omega, \qquad\qquad u(x,y) = 0 \; on \; \partial\Omega$$

*with $\Omega$ being a three-quarter circle. We solve this problem by the finite element method and use linear elements.*



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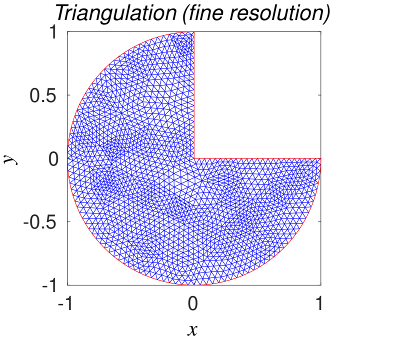
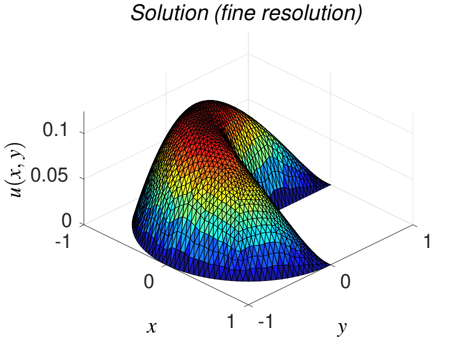


# Weak formulation in 1D

Consider $\Omega = (0,1)$ and with $a(x) \geq a_0 > 0$, $c(x) \geq 0$ the boundary value problem

$$-\frac{\mathrm{d}}{\mathrm{d}x}\big(a(x)u'(x)\big) + c(x)u(x) = f(x), \tag{17}$$
$$u(0) = u(1) = 0$$

## Definition 4.1

*We call a function $v \in C_0^1$ a test function with*

$$C_0^1 = \{v \in C^1(\bar{\Omega}) : \; v(0) = v(1) = 0\}.$$

Multiplication of (17) with a test function as well as integration over $\Omega$:

$$\int_0^1 (au'v' + cuv)\,\mathrm{d}x = \int_0^1 fv\,\mathrm{d}x \qquad \forall v \in C_0^1(\bar{\Omega}). \tag{18}$$

**Definition 4.2**

*The formulation in (18) is the* *<u>weak formulation</u>* *of the PDE. Further, we call*

$$B(u,v) := \int_0^1 (au'v' + cuv)\,\mathrm{d}x$$

*a* *<u>bilinear form</u>* *on* $C_0^1(\bar{\Omega})$ *and*

$$I(v) := \int_0^1 fv\,\mathrm{d}x$$

*a* *<u>linear form</u>* *on* $C_0^1(\bar{\Omega})$.

Rayleigh-Ritz method:

- approximation of the solution $u$ with $B(u, v) = I(v)$ by $Pu$ as the best approximation in a finite subspace $\mathcal{S} \subset C_0^1(\bar{\Omega})$
- basis functions $\psi_1, \ldots, \psi_n$ of the $n$-dimensional subspace $\mathcal{S}$
- linear combination of the best approximation is

$$Pu(x) = \sum_{i=1}^{n} w_i \psi_i(x)$$

System of linear equations:

- evaluating the bilinear form and the linear form result in

$$\begin{aligned} A_{ij} &:= B(\psi_j, \psi_i), \quad i, j \in \{1, \ldots, n\}, \\ b_i &:= I(\psi_i), \end{aligned}$$

- the coefficients $w \in \mathbb{R}^n$ are the solution of

$$Aw = b,$$

- $A$ is symmetric and positive definite for $a(x) \geq a_0 > 0$, $c(x) \geq 0$

## Example

*Boundary value problem:*

$$-4u''(x) + u(x) = (1 - \sqrt{\mathbf{e}})x, \quad 0 \le x \le 1,$$
$$u(0) = u(1) = 0.$$

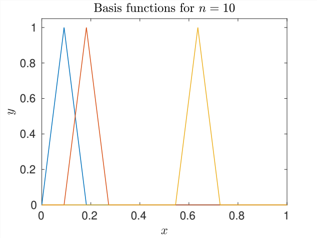
*Discretization:*

$$x_i = ih, \quad i = 0, 1, \ldots, n+1, \; h = \frac{1}{n+1}$$

*Basis functions:*

$$\psi_k(x) = \begin{cases} (x - x_{k-1})/h & \text{for } x_{k-1} \le x \le x_k, \\ (x_{k+1} - x)/h & \text{for } x_k \le x \le x_{k+1}, \\ 0 & \text{otherwise} \end{cases}$$

$$\psi_k'(x) = \begin{cases} h^{-1} & \text{for } x_{k-1} \le x \le x_k, \\ -h^{-1} & \text{for } x_k \le x \le x_{k+1}, \\ 0 & \text{otherwise} \end{cases}$$

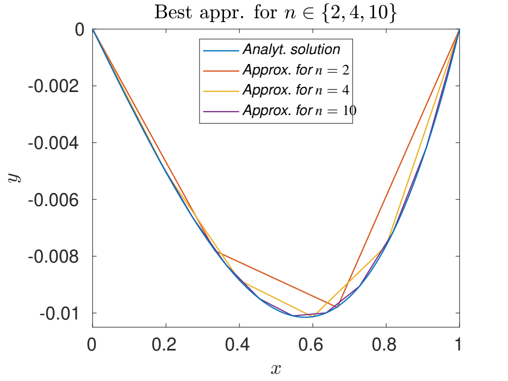


## Example (Continuation)

*System of linear equations:*

$$A_{ij} = \int_0^1 4\psi_i'(x)\psi_j'(x) + \psi_i(x)\psi_j(x)\,\mathrm{d}x, \qquad b_i = I(\psi_i) = \int_0^1 (1-\sqrt{\mathbf{e}})x\psi_i(x)\,\mathrm{d}x$$

$$A = \operatorname{tridiag}\left(-\frac{4}{h}+\frac{h}{6},\ \frac{8}{h}+\frac{2h}{3},\ -\frac{4}{h}+\frac{h}{6}\right), \qquad b = (1-\sqrt{\mathbf{e}})h^2(1,2,3,\dots,n)^T$$



# Weak formulation in 2D

Use Soboloev spaces and weak derivatives to extent the theory to $n$D.

## Definition 4.3

*Let $\Omega \subset \mathbb{R}^n$ be a domain. The set $L_2(\Omega)$ includes all functions $u : \Omega \to \mathbb{R}$ with $|u(x)|^2$ being Lebesgue integrable. We use the inner product and the norm*

$$(u, v) = \int_\Omega u(x)v(x)\,\mathrm{d}x, \quad \|u\|_\Omega = \left(\int_\Omega |u(x)|^2\,\mathrm{d}x\right)^{1/2}.$$

## Definition 4.4

*Let $\Omega \subset \mathbb{R}^n$ be a domain, $u \in L_2(\Omega)$, and $z \in \mathbb{N}^n$ be a multi index with $|z| = z_1 + \ldots + z_n$. A function $v \in L_2(\Omega)$ is a <u>weak derivation of order $z$</u>, if*

$$\int_\Omega v\varphi\,\mathrm{d}x = (-1)^{|z|}\int_\Omega uD^z\varphi'\,\mathrm{d}x, \qquad \varphi \in C_0^\infty(\Omega).$$

## Remark 11

*If the weak derivative exists, then it is unique.*

## Definition 4.5

*The* <u>*Sobolev space*</u> $H^m(\Omega)$ *of* $m$*th order includes all functions* $u \in L_2(\Omega)$ *with* $D^z u \in L_2(\Omega)$ *for all* $z$ *with* $|z| \leq m$, *thus*

$$H^m(\Omega) = \left\{u : \; D^m u \in L_2(\Omega) \text{ for } |z| \leq m\right\}.$$

*for* $H^m(\Omega)$ *we defines the inner product*

$$(u, v) := \sum_{|z| \leq m} \int_\Omega (D^z u)(x)(D^z v)(x) \, \mathrm{d}x$$

*and the norm*

$$\|u\|_m := (u, u)^{1/2}.$$

# Weak formulation in 2D

Operator:

$$(Lu)(x) = -\nabla \cdot (A\nabla u) + b^T \nabla u + cu = f(x) \tag{19}$$

Domain:

$$\Omega \subset \mathbb{R}^2$$

Theorem of Gauss and integration by parts:

$$\int_\Omega (A\nabla u) \cdot \nabla v + b^T \nabla uv + cuv \,\mathrm{dx}\,\mathrm{dy} = \int_\Omega fv \,\mathrm{dx}\,\mathrm{dy}, \quad \forall v \in H_0^1(\bar{\Omega}) \tag{20}$$

## Definition 4.6

*We call (20) the weak formulation of the PDE from (19).*

# Weak formulation in 2D

## Example

*The weak formulation of the boundary value problem*

$$
\begin{aligned}
-\Delta u &= x + y \quad \textit{in}\ \Omega = (0,1)^2, \\
u &= 0 \quad \textit{on}\ \partial\Omega
\end{aligned}
$$

*reads*

$$
\begin{aligned}
\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x\,\mathrm{d}y &= \int_\Omega (x+y) v \,\mathrm{d}x\,\mathrm{d}y \quad \forall v \in H_0^1(\Omega), \\
\int_\Omega u_x v_x + u_y v_y \,\mathrm{d}x\,\mathrm{d}y &= \int_\Omega (x+y) v \,\mathrm{d}x\,\mathrm{d}y \quad \forall v \in H_0^1(\Omega).
\end{aligned}
$$

# Weak formulation in 2D

## Example

*Consider the PDE*

$$Lu = -xu_{xx} - u_{xy} - yu_{yy} - u_x + u = 1$$

*Formulation as*

$$-\nabla(A\nabla u) + b^T\nabla u + cu = 1$$

*with*

$$A = \begin{pmatrix} x & 0.5 \\ 0.5 & y \end{pmatrix}, \qquad b = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \qquad c = 1$$

*Weak formulation:*

$$\int_\Omega (xu_x + 0.5u_y)v_x + (yu_y + 0.5u_x)v_y + (u - u_y)v \,\mathrm{d}x\,\mathrm{d}y = \int_\Omega v \,\mathrm{d}x\,\mathrm{d}y.$$

Triangulation in $\mathbb{R}^2$:

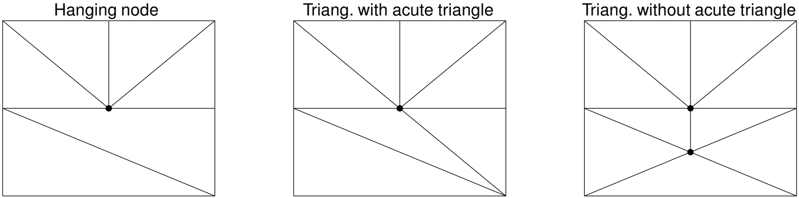
- decomposition of $\Omega$ into triangles $T_i$, $i = 1, \ldots, M$
- a triangulation is valid if
  (i) $\overline{\Omega} = \bigcup_{i=1}^{M} T_i$
  (ii) the intersection of two different triangles is empty, a complete edge or only a vertex

Triangulation in FEM:

- consequently, only functions for adjacent elements contribute to the discretization matrix
- refinement of a triangulation by <u>uniform</u> (homogeneous) and <u>adaptive</u> refinements (green and red edges in hierarchical approach)

Problem of hanging nodes:

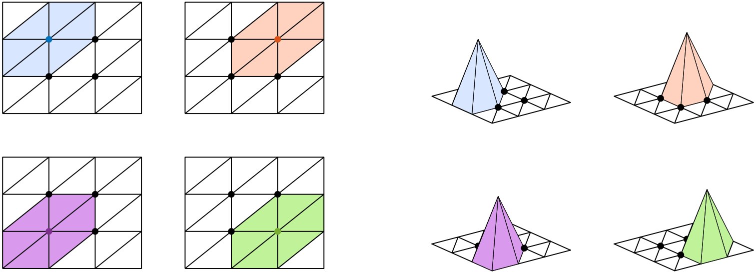
- no hat function can be defined
- a hanging node would have always the value 0 for a continuous function
- additional edge to avoid hanging a node



Basis functions: (typically with $n = 1$ or $n = 2$)

$$\mathcal{S} = \{u : \Omega \to \mathbb{R} \mid u|_T = \text{Polynom with } \deg(u|_T) \leq n,\ \forall T \in \mathcal{T}\}$$

Finite elements:

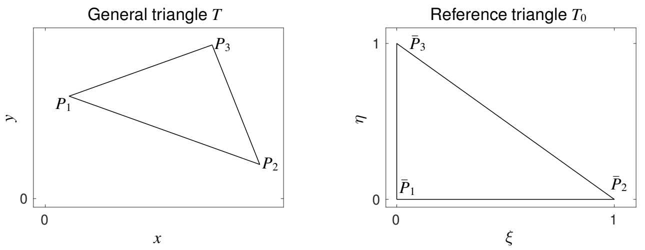


Procedure:

- computation of the system matrix by evaluating the bilinear form $B(\psi_i, \psi_j)$ (2 options: nodes oriented strategy or element-wise oriented strategy)
- computations only for a triangle of reference with the edges $(0,0)$, $(1,0)$ and $(0,1)$
- transformation to an arbitrary triangle
- use numerical integration (cubature formulas)

### Definition 4.7

*The triangle with the vertices $(0,0)$, $(1,0)$ and $(0,1)$ is called reference triangle $T_0$.*



# Transformation to the reference triangle

Transformation:

- general triangle $P_1 = (x_1, y_1)$, $P_2 = (x_2, y_2)$, $P_3 = (x_3, y_3)$
- transformation $T_0 \to T$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \underbrace{\begin{pmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{pmatrix}}_{=:B} \begin{pmatrix} \xi \\ \eta \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}$$

Integral:

- substitution

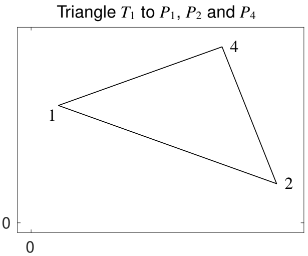
$$\mathrm{d}x\,\mathrm{d}y = J\,\mathrm{d}\xi\,\mathrm{d}\eta \quad \text{with} \quad J = |\det(\begin{pmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{pmatrix})| = |\det(B)|$$

- transformation of the integral using $B$, the Jacobean matrix of the transformation

$$\int_{T_0} v|\det(B)|\,\mathrm{d}\xi\,\mathrm{d}\eta = \int_T u\,\mathrm{d}x\,\mathrm{d}y$$

# Element-wise oriented strategy

Idea of the element-wise oriented strategy (1):




$e =$element $T_1$, index $i^*$ ($e$ for element)
$g =$triangulation $\mathcal{T}$, index $i$ ($g$ for global)
$\varphi_1$, $\varphi_2$, $\varphi_3$ linear basis functions to $T_1$

Idea of the element-wise oriented strategy (2):

$$
\begin{array}{ccccc|c|c}
e & \rightarrow & \rightarrow & & 1 & 2 & 3 \\
\downarrow & g & \rightarrow & & 1 & 2 & 4 \\
\downarrow & \downarrow & & & & & \\
1 & 1 & & & B(\varphi_1,\varphi_1) & B(\varphi_1,\varphi_2) & B(\varphi_1,\varphi_3) \\
\cline{5-7}
2 & 2 & & & B(\varphi_2,\varphi_1) & B(\varphi_2,\varphi_2) & B(\varphi_2,\varphi_3) \\
\cline{5-7}
3 & 4 & & & B(\varphi_3,\varphi_1) & B(\varphi_3,\varphi_2) & B(\varphi_3,\varphi_3)
\end{array}
$$

$$
(A|_{T_1})_{i^*j^*} = B(\varphi_{i^*}, \varphi_{j^*}) = \int \dots
$$

$$
A|_{T_1} = \left(\begin{array}{c|c|c|c}
\circ & \circ & & \circ \\ \hline
\circ & \circ & & \circ \\ \hline
 & & & \\ \hline
\circ & \circ & & \circ
\end{array}\right), \qquad
A|_{T_1} + A|_{T_2} = \left(\begin{array}{c|c|c|c}
\circ + \ast & \circ + \ast & \ast & \circ \\ \hline
\circ + \ast & \circ + \ast & \ast & \circ \\ \hline
\ast & \ast & \ast & \\ \hline
\circ & \circ & & \circ
\end{array}\right)
$$

# Cubature formulas

Problem:

$$u : S \to \mathbb{R},\ S \subset \mathbb{R}^2, \quad \iint_S u(x,y)\,\mathrm{d}\sigma = ?$$

Approximation for the reference triangle

$$I = \iint_{T_0} u(x,y)\,\mathrm{d}y\,\mathrm{d}x = \int_0^1 \int_0^{1-x} u(x,y)\,\mathrm{d}y\,\mathrm{d}x$$

## Example

*The following cubature formula is exact for all polynomials up to degree 1*

$$\frac{1}{6}\big(u(0,0) + u(1,0) + u(0,1)\big).$$

## Example

*The following cubature formula is exact for all polynomials up to degree 2*

$$\frac{1}{6}\big(u(0.5,0) + u(0,0.5) + u(0.5,0.5)\big).$$

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