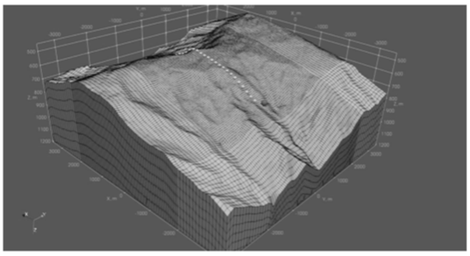
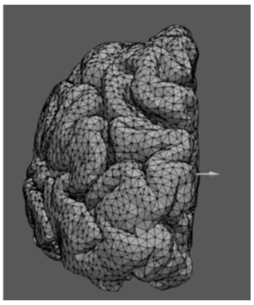
Advanced Solvers for Numerical Partial Differential Equations (PDEs)





Lecture 1

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Course Grades

Attendance	5
Homework Assignments • Python code using a finite-element (FE) package • Short written report	4 x 15
Presentation • Review of a publication relevant to the course, 10 min presentation	15
Final Exam • knowledge of major algorithms, FE discretizations, and computational effort estimates	20

Please, work individually!

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Prerequisites

The course is fairly self-sufficient, yet

- Basic knowledge of Python programming is required.
- Preferably the student have passed Scientific Computing and Numerical Modeling.

TA

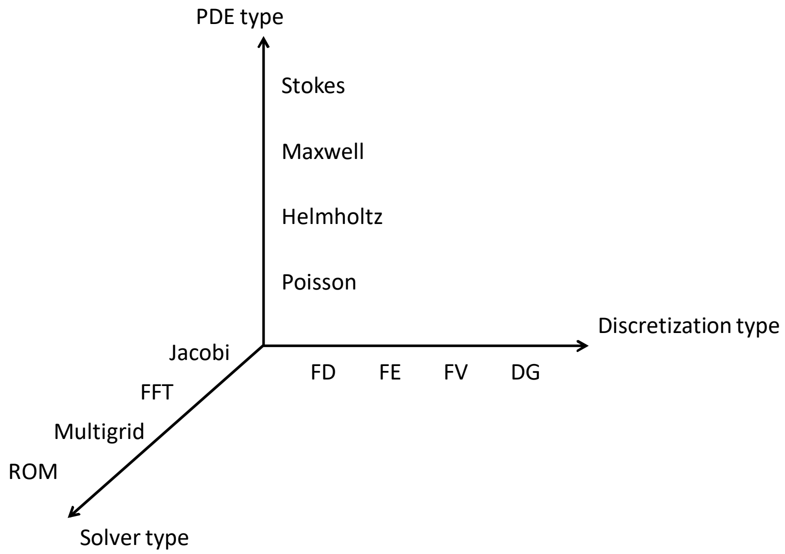
Iurii Minin

Textbooks

- P. Solin, *Partial Differential Equations and the Finite Element Method*, Wiley & Sons, 2006
- Y. Saad, *Iterative Methods for Sparse Linear Systems*, SIAM, 2003
- A. Greenbaum*, Iterative Methods for Solving Linear Systems*, SIAM, 1997.
- U. Trottenberg, C. Oosterlee, A. Schuller, *Multigrid*, 2000

Part 1
Introduction and Workflow in Numerical solution of the PDEs

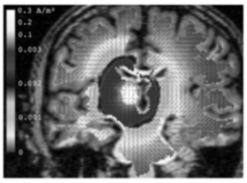
Major topics



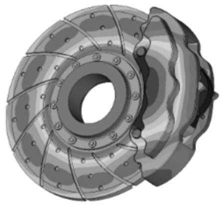
PDEs discussed

1. Diffusion equation

$$-\mathrm{div}\,(K\,\nabla u) + c\,u = f \quad \text{in } V$$
$$K\nabla u \cdot n = 0 \quad \text{on } \Gamma$$



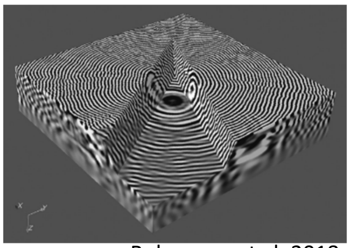
C.H. Wolters et al. 2006



www.theseus-fe.com

2. Indefinite Helmholtz equation

$$-\Delta u - \frac{\omega^2}{c^2} u = f$$
+ b.c. at $|x| \to \infty$

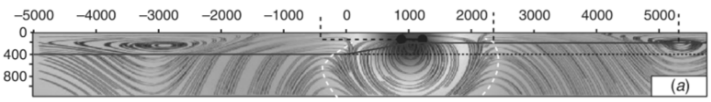


Belonosov et al, 2018

Major PDEs discussed

3. **Maxwell's equations**

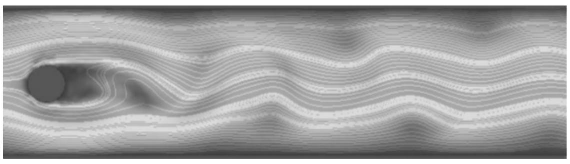
$$curl\ curl\ E + k^2\ E = F \ \text{ в } V$$
$$E \times n = 0 \quad \text{на } \Gamma$$



Pethick & Harris, 2014

4. Fluid dynamics

$$-\nu\Delta u + \nabla p = f$$
$$-div\,u = g$$
$$u = 0$$



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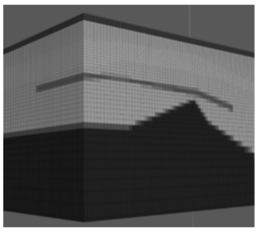
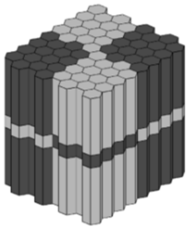
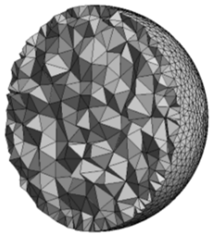
Major discretization methods

Finite-difference method | **Finite-volume method** | **Finite-element method**

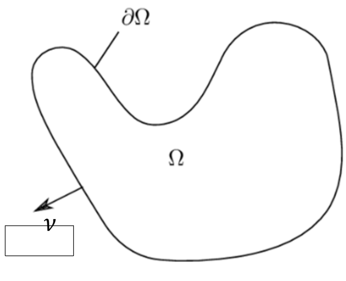






Commonly Used Notations

Ω modeling domain in $\mathbb{R}^n$, $n = 2{,}3$
$\Gamma = \partial\Omega$ domain boundary
ν unit outward normal vector to the boundary



$L_2(\Omega)$ space of square-integrable functions in Ω

$$\|u\|^2 = \int_\Omega u(x)^2\, dx$$

$\nabla u(x)$	gradient
div $\boldsymbol{F}(x)$	divergence
curl $\boldsymbol{F}(x)$	curl or rot

$\Delta u(x) = div\, \nabla u$ Laplacian

Integral Calculus Identities

Divergence/Gauss theorem

$$\int_{\Omega} div\, \boldsymbol{F} dx = \int_{\partial\Omega} \boldsymbol{F} \cdot \nu \, dS$$

$$div\, curl\, \boldsymbol{F} = 0$$
$$curl\, \nabla u = 0$$

Green's identity/integration by parts

$$\int_{\Omega} u\, div\, \boldsymbol{F} dx = \int_{\partial\Omega} u\, \boldsymbol{F} \cdot \nu \, dS - \int_{\Omega} \nabla u \cdot \boldsymbol{F} dx$$

$$\int_{\Omega} \boldsymbol{F} \cdot curl\, \boldsymbol{G} dx = \int_{\partial\Omega} \boldsymbol{F} \cdot (\nu \times \boldsymbol{G}) \, dS + \int_{\Omega} \boldsymbol{G} \cdot curl\, \boldsymbol{F} dx$$

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Matrix/Vector Notations

(u, v) vector dot product

A, A^T matrix and its transpose
$A > 0$ positive-definite matrix

$diag(A)$ matrix of diagonal entries

$Au = \lambda u$ eigenvalue problem, $\lambda(A)$ eigenvalue of a matrix

$\|g\|, \|A\|$ vector or matrix norm

$\rho(A) = |\lambda_{max}(A)|$ matrix spectral radius/largest eigenvalues

$cond\ A = \|A\| \|A^{-1}\|$ (and $\frac{\lambda_{max}}{\lambda_{min}}$ for $A = A^{\mathrm{T}} > 0$)
matrix condition number

I the identity matrix

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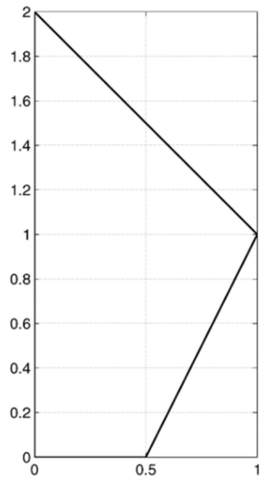
Workflow

Consider Poisson equation

$$-\Delta u = f \quad \text{in } \Omega$$
$$u = \varphi \quad \text{on } \Gamma$$



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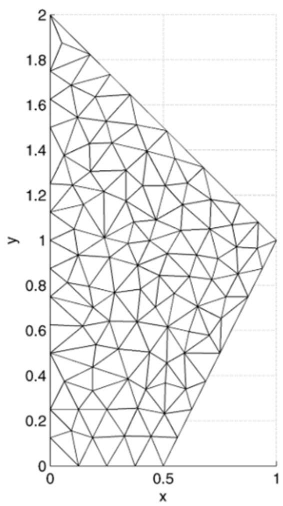
Workflow

$$-\Delta u = f \quad \text{in } \Omega$$
$$u = \varphi \quad \text{on } \Gamma$$

1. Cover the domain with a grid.



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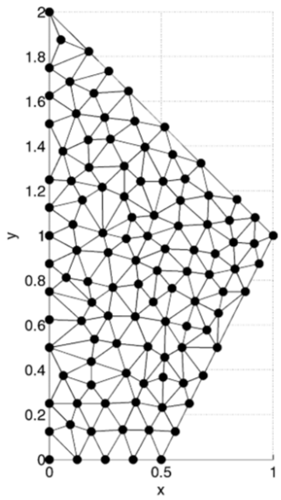
Workflow

$$-\Delta u = f \quad in\ \Omega$$
$$u = \varphi \quad on\ \Gamma$$

1. Cover the domain with a grid

2. Choose locations for discrete unknowns



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Workflow

$$-\Delta u = f \quad in\ \Omega$$
$$u = \varphi \quad on\ \Gamma$$

1. Cover the domain with a grid
2. Choose locations for discrete unknowns

3. Prepare the equation system

$$A\, u_h = f_h$$

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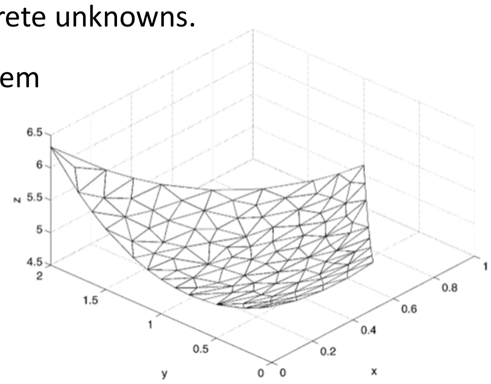
Workflow

$$-\Delta u = f \quad in\,\Omega$$
$$u = \varphi \quad on\;\Gamma$$

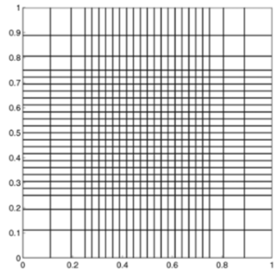
1. Cover the domain with a grid
2. Choose locations for discrete unknowns.

3. Prepare the equation system

4. Solve the system
   $u_h = A^{-1} f_h$



Part 2
Recall of the finite-difference method



Finite Difference Method

The idea goes back to L. Euler.

$$u_x\Big|_{x_i} = \frac{u_i - u_{i-1}}{h} + O(h) = \frac{u_{i+1} - u_i}{h} + O(h) = \frac{u_{i+1} - u_{i-1}}{2h} + O(h^2)$$

$$u_{xx}\Big|_{x_i} = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} + O(h^2)$$

Finite Difference Method

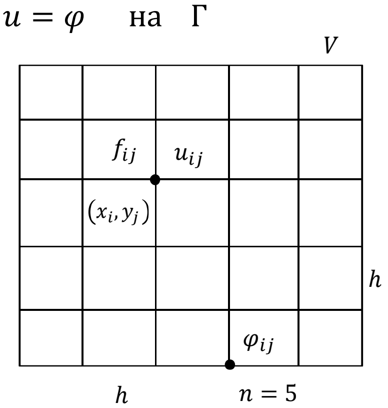
The model problem

$$-\Delta u = f \quad \text{в } V$$
$$u = \varphi \quad \text{на } \Gamma$$

$V = (0,1)^2$ with boundary Γ,

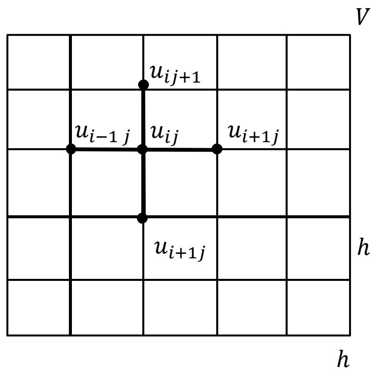
$x_i = i\,h, \quad i = 0..n,$
$y_j = j\,h, \quad j = 0..n.$

$$u(x_i, y_j) \approx u_{ij}$$
$$f(x_i, y_j) = f_{ij},$$
$$\varphi(x_i, y_j) = \varphi_{ij},$$



Overall number of unknowns $N = (n+1)^2$

Finite Difference Method



$$-u_{xx}\Big|_{(x_i,y_j)} \approx \frac{-u_{i-1j} + 2u_{ij} - u_{i+1\,j}}{h^2}$$

$$-u_{yy}\Big|_{(x_i,y_j)} \approx \frac{-u_{ij-1} + 2u_{ij} - u_{i\,j+1}}{h^2}$$

- Discrete equation

$$\frac{-u_{i-1j} + 2u_{ij} - u_{i+1\,j}}{h^2} + \frac{-u_{ij-1} + 2u_{ij} - u_{i\,j+1}}{h^2} = f_{ij}$$

- Boundary data

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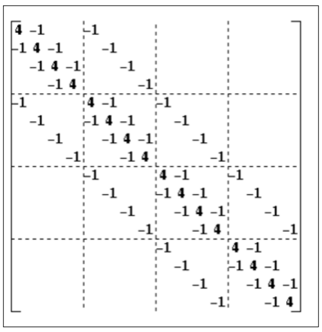
Equation System

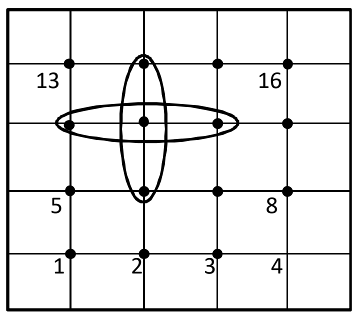
We receive a large equation system

$$A\,u_h = f_h$$

Its size

$$N = (n_x - 1)(n_y - 1)$$





$$n_x = n_y = 5$$
$$N = 16$$

$$A = \begin{pmatrix} C & -I & \\ -I & C & \ddots \\ & \ddots & \ddots \end{pmatrix}$$

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Spectral Properties of the Matrix

Eigenvalue problem:

$$A\,u_h = \lambda\,u_h,$$
$$A = L_x + L_y$$
$$u_h = (0 \cdots 0\; u_{11}\; \mathrm{u}_{12} \cdots u_{1n} u_{21} \cdots 0)$$
$$\lambda_{km} = \frac{4}{h^2}\sin\left(\frac{\pi k h}{2}\right)^2 + \frac{4}{h^2}\sin\left(\frac{\pi m h}{2}\right)^2$$
$$u_{km,ij} = \sin(\pi i k h)\sin(\pi j m h)\,.$$

The smallest and largest eigenvalues

$$\lambda_{min} = \lambda_{11} \approx 2\pi^2$$
$$\lambda_{max} = \lambda_{(n-1)(n-1)} \approx \frac{8}{h^2}$$
$$\mathrm{cond}\,A = \frac{\lambda_{max}}{\lambda_{min}} \approx \frac{4}{\pi^2 h^2}$$

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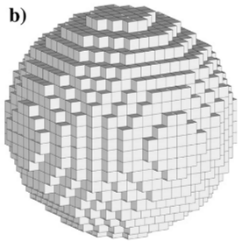
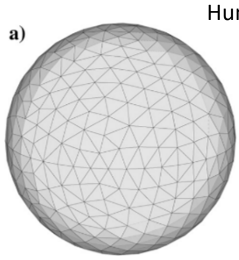
Limitation of the FD method

b)



Hun et al, 2011

a)



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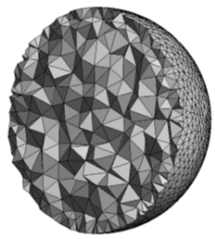
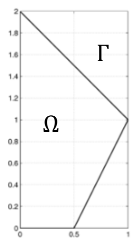
Part 3
Basics of the finite-element method



PDEs and Sobolev Spaces

Poisson equation

$$-\Delta u + u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \Gamma$$



$V = H_0^1(\Omega)$ Sobolev space
Square-integrable functions with square-integrable gradients and zero values on the boundary

$$= \{v \in L_2(\Omega) \text{ such that } \nabla v \in L_2(\Omega) \text{ and } v = 0 \text{ on } \Gamma\}$$

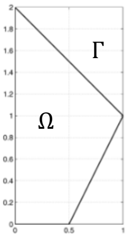
$$\|v\|_1^2 = \int_\Omega v^2\,dx + \int_\Omega |\nabla v|^2\,dx$$

That is
$$\|v\|_1^2 = \|v\|^2 + \|\nabla v\|^2$$

PDE, weak and variational formulations

Poisson equation

$$-\Delta u + u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \Gamma$$



Exercise Weak formulation

$$\int_\Omega \nabla u \cdot \nabla v dx + \int_\Omega uv\, dx = \int_\Omega v\, f dx \quad \forall v \in V$$

$$V = H_0^1(\Omega)$$

Variational formulation

$$\min_{v \in V} \frac{1}{2} \int_\Omega |\nabla v|^2\, dx + \int_\Omega v^2\, dx - \int_\Omega f \cdot v\, dx$$

- Under regularity assumptions, all three problems have the same solution

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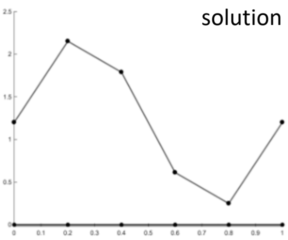
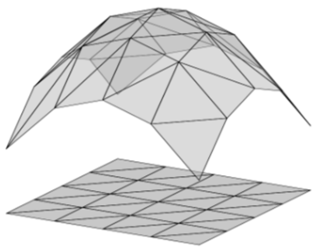
Finite Element Interpolation

solution

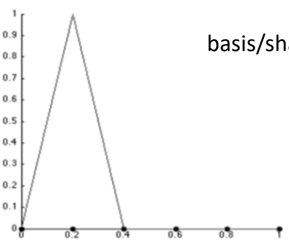




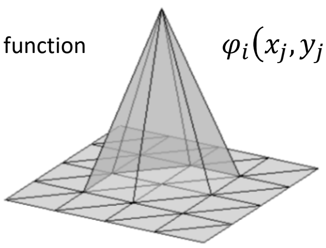
L.Chen, UCI

1D

2D



basis/shape function



$$\varphi_i(x_j, y_j) = \begin{cases} 1 & if\ i = j \\ 0 & else \end{cases}$$

1D

2D

- Note, basis functions produce some subspace V_h

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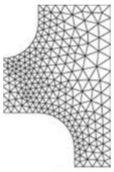
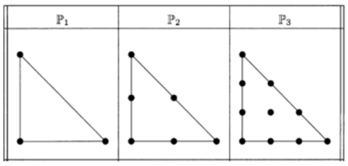
Finite Element Interpolation in 2D

Lagrange finite elements

Triangular grid



P_k

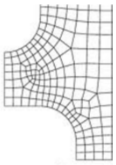


$v_h = a + bx + cy$

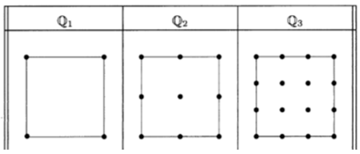
$v_h = \cdots + dx^2 + exy + fy^2$

$v_h = \cdots + \cdots + gx^3 + hx^2y + ixy^2 + jy^3$

Quadrilateral grid



Q_k



$v_h = a + bx + cy + dxy$

Each of these interpolation types produce a subspace $V_h \subset V$

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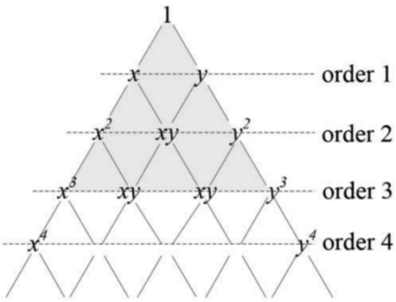
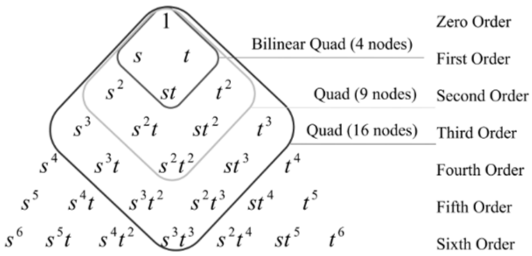
Pascal Triangle





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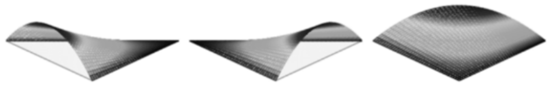
Finite Element Interpolation in 2D

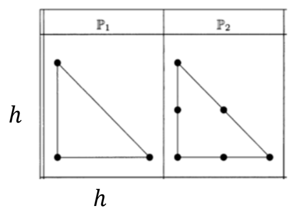
P_1 basis/shape functions

P_2 basis/shape functions (3 of 6)



Exercise ☺

Derive P_1 and P_2 finite-element basis functions for the rectangular triangle



Approach 1: Set 3x3 (P_1) and 6x6 (P_2) systems of linear equations up

Approach 2: Use area/barycentric coordinates

Galerkin Method

$$-\Delta u + u = f \quad \text{в } \Omega,$$
$$u = 0 \quad \text{на } \Gamma$$

Integral identity/weak formulation

$$\int_\Omega \nabla u \cdot \nabla v dx + \int_\Omega u \cdot v dx = \int_\Omega v\, f dx \qquad \forall v \in V$$

Galerkin method
Pick subspace $V_h \subset V$ and fine $u_h \in V_h$

$$\int_\Omega \nabla u_h \cdot \nabla v_h dx + \int_\Omega u_h \cdot v_h dx = \int_\Omega v_h f dx \qquad \forall v_h \in V_h$$

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FE System Matrix

$$\int_\Omega \nabla u_h \cdot \nabla v_h dx + \int_\Omega u_h \cdot v_h dx = \int_\Omega v_h f dx \qquad \forall v_h \in V_h$$

$$u^h(x,y) = \sum_{i=1}^{N} u_i \varphi_i(x,y) \qquad v^h(x,y) = \sum_{j=1}^{N} v_j \varphi_j(x,y)$$

$$A_{ij} = \int_V (\nabla\varphi_i \cdot \nabla\varphi_j + \varphi_i\varphi_j) dx \qquad b_j = \int_V \varphi_j\, f dx$$

$$A\, u = b \qquad A \in \mathbb{R}^{N\times N},\, b \in \mathbb{R}^N$$

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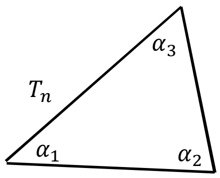
Local Matrices for P_1

$A = \mathrm{asm}\{S^n + M^n\}$



$S_{ij}^n = \int_{T_n} \nabla\varphi_j \cdot \nabla\varphi_j dx$ local stiffness matrix

$$S^n = \frac{1}{2}\begin{pmatrix} \operatorname{ctg}\alpha_2 + \operatorname{ctg}\alpha_3 & -\operatorname{ctg}\alpha_3 & -\operatorname{ctg}\alpha_2 \\ -\operatorname{ctg}\alpha_3 & \operatorname{ctg}\alpha_1 + \operatorname{ctg}\alpha_3 & -\operatorname{ctg}\alpha_1 \\ -\operatorname{ctg}\alpha_2 & -\operatorname{ctg}\alpha_1 & \operatorname{ctg}\alpha_1 + \operatorname{ctg}\alpha_2 \end{pmatrix}$$

$M_{ij}^n = \int_{T_n} \varphi_j\, \varphi_j dx$ $\qquad M^n = \frac{1}{12}|T_n|\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$

local mass matrix

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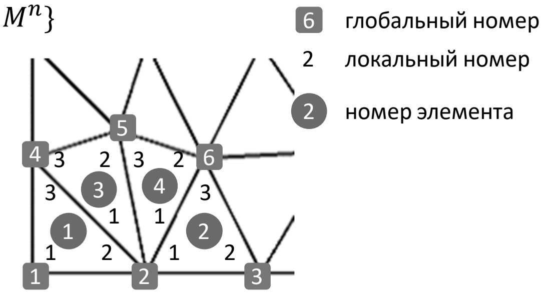
Matrix Assembly

$A = \mathrm{asm}\{S^n + M^n\}$



Num =
1 2 4
2 3 6
2 5 4
2 6 5

$A = \mathrm{asm}\{A^n\}$

```
for n=1..N
    for i=1..3
        for j=1..3
          A(Num(n,i),Num(n,j))+= S^n(i,j)+M^n(i,j)
```

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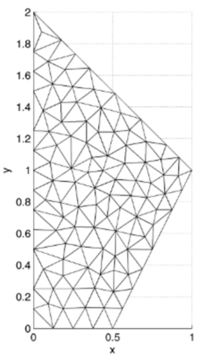
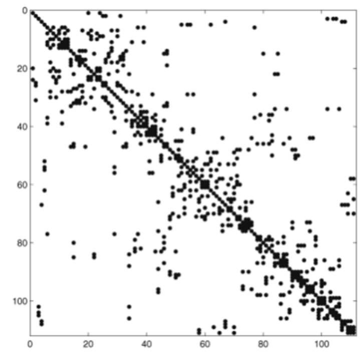
Matrix structure





Sparse symmetric positive-definite
Condition number

$$O\left(\frac{1}{h^2}\right)$$

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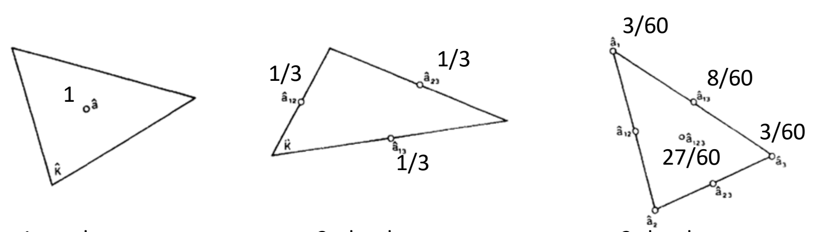
Numerical Integration

$$\int_{T_n} \nabla\varphi_j \cdot \nabla\varphi_j dx \qquad \int_{T_n} \varphi_j\ \varphi_j dx \qquad \int_{T_n} \varphi_j\ f dx$$

- How to compute those integrals?

x_i quadrature points
w_i weight

$$\int_{T_n} g(x)dx = |T_n| \sum w_i g(x_i)$$



1st order 2nd order 3rd order

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Convergence Results

Theorem. For P_k and Q_k elements on a sequence of grids

$$\begin{aligned} \|u-u_h\|_1 &\le Ch^k\|u\|_{k+1} \\ \|u-u_h\| &\le ch^{k+1}\|u\|_{k+1} \end{aligned} \qquad k \ge 1$$

For example, for the P_1 element,

$$\begin{aligned} \|u-u_h\|_1 &= O(h) \\ \|u-u_h\| &= O(h^2) \\ \|u-u_h\|_\infty &= O(h^2) \end{aligned}$$

- Solution converges faster than the gradient!
  What if we are more interested in the gradient/flux ?

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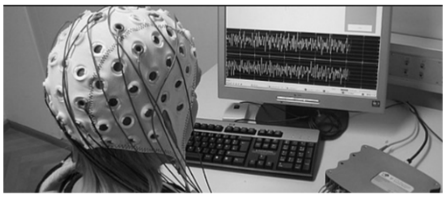
Example

Modeling neural currents
within the head / electroencephalography



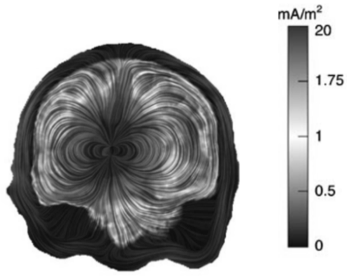
uni-graz.at

$$-div(\sigma\, \nabla u) = -div\, \boldsymbol{J} \text{ в } V$$

$$\boldsymbol{n}\cdot\sigma\nabla u = 0 \text{ на } \Gamma$$

$$\boldsymbol{J} = \boldsymbol{M}\,\delta(x-x_0)$$

Tran & Fang



C.H. Wolters et al. 2006

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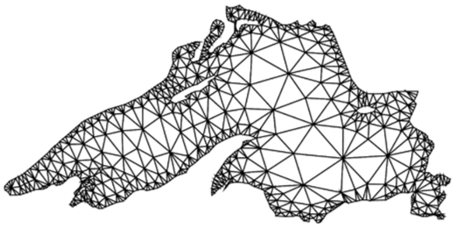
Grid Adaptation



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