Scientific Computing
Lecture 2

Introduction

Nikolay Koshev

October 4, 2021

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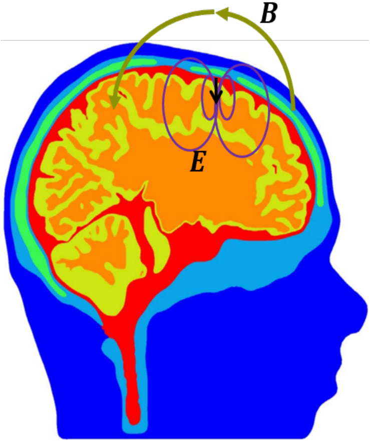
Structure of the lecture

- This intro: example of simulation problem (EEG) and occurring questions.
- Spaces.
- SLAE.
- Discretization.
- Finite Differences.
- Finite Elements.
- Overall pipeline for solving the Scientific Computing problem, and application of this pipeline to EEG simulation problem.



- Neuronal currents occur inside the cortex.
- **Computational domain:** $\Omega \in \mathbb{R}^3$
- **Phenomenon:** generation of the electric potential by cortical currents.
- **Input:**
  - $\mathbf{J}(\mathbf{x})$ - current density
  - $\sigma(\mathbf{x}), \mathbf{x} \in$ Head - electric properties
- **Mathematical model:**

$$-div(\sigma \nabla U) = div\mathbf{J};$$

- **OUTPUT:** electric potential: $U(\mathbf{x})$.

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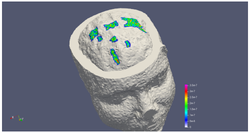
Problem 1: Infinite number of points

- How much points contains the complete number scale $\mathbb{R}$?
- How much points contains the interval $[0, 1] \subset \mathbb{R}$?
- How much points includes the head (computational domain)?
- Computers do not understand infinity.
- How can we use computers for calculations?

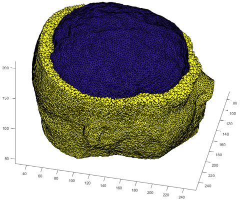
Answer: Divide et impera (lat).

Problem 2: Different properties of data

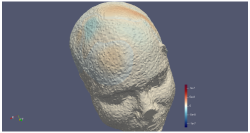
$\mathbf{J}(\mathbf{x})$ - current density inside the cortex:
Discontinuous.



$\sigma(\mathbf{x})$ - the conductivity of the tissues:
Discontinuous, piecewise-constant.



$u(\mathbf{x})$ - the electric potential:
Continuous, smooth function



Answer: Classify data by properties in order to formulate the final mathematical problem.

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Part 1: functional spaces

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Space - a set of something with some added structure

- The simplest space: real number scale $\mathbb{R}$. Elements of this space: real numbers $x \in (-\infty, \infty)$.
- We are living at space consisting of 3D vectors $\mathbb{R}^3$. Each area of this space is a volume.
- All integers form the space $\mathbb{Z}$.
- All rational numbers $\frac{p}{q}, p, q \in \mathbb{Z}$ form the space $\mathbb{Q}$.
- Consider the interval $[a, b] \subset \mathbb{R}$ for certain a and b. All functions $f(x), x \in [a, b]$ form a space.

The space X is called **linear** if:

- **Sum of elements** of X belongs to X.
- **Multiplication** of an element with an appropriate number maps to the same space.
- **Commutative property:** $x + y = y + x, \quad \forall x, y \in X$.
- **Zero element:** $\exists \theta \in X : x + \theta = x, \forall x \in X$.
- **Negative element:** $\forall x \in X, \exists (-x) \in X : x + (-x) = \theta$.
- **Linearity:**

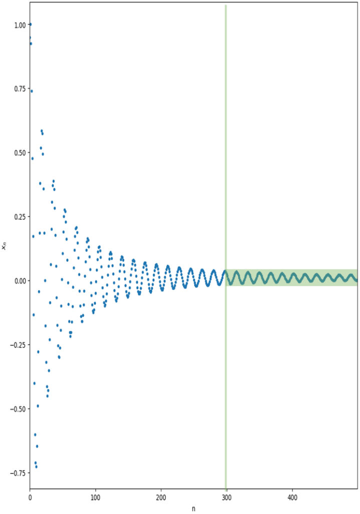
$$
\begin{gathered}
1 \cdot x = x, \quad \lambda(\mu x) = (\lambda\mu)x, \quad \forall \lambda, \mu \in \mathbb{R} \\
(\lambda + \mu)x = \lambda x + \mu x, \quad \forall \lambda, \mu \in \mathbb{R}, \quad \forall x \in X \\
\lambda(x + y) = \lambda x + \lambda y, \quad \forall x, y \in X, \forall \lambda \in \mathbb{R}
\end{gathered}
$$

- Thus, all properties of **Linear space** are **linear** :)

Space X is called **metric space** if there is a distance between two elements defined. The distance $\rho(x, y)$ is the functional mapping $X \to \mathbb{R}$, defined for $\forall x, y \in X$, and having the following properties:

- **Non-negativity:**
  $\rho(x, y) \geq 0$, and
  $\rho(x, y) = 0 \Rightarrow x \equiv y$.
- **Commutative property:**
  $\rho(x, y) = \rho(y, x)$.
- **Triangle inequality:**
  $\rho(x, y) + \rho(y, z) \geq \rho(x, z), \quad \forall x, y, z \in X$
- Metric space X with distance ρ sometimes being denoted with a pair (X, ρ).

Complete space



- *Fundamental sequence:* sequence $\{x_n\}_{n=1}^{\infty} \in X$ is fundamental if $\forall \varepsilon, \exists N$: $\rho(x_n, x_m) < \varepsilon, \forall n, m > N$
- Picture on the left: fundamental sequence $x_n = \frac{sin(\alpha n)}{n^2} \to 0$
- X is a **complete** space if for *every* fundamental sequence $x_n \in X$, the element $x = \lim_{n\to\infty} \in X$.
- Example: space $(\mathbb{Q}, d(x,y) = |x - y|)$ is not complete.

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Linear space X is a normed space if $\forall x \in X$ there is the functional $||x|| : X \to \mathbb{R}$ defined:

- **Non-negativity:** $||x|| \geq 0, \quad ||x|| = 0 \Rightarrow x = \theta.$
- **Triangle inequality:** $||x + y|| \leq ||x|| + ||y||, \quad \forall x, y \in X.$
- **Multiplication with a number:** $||\lambda x|| = |\lambda| \cdot ||x||, \quad \forall x \in X, \forall \lambda \in \mathbb{R}.$

Some properties:

- Each normed space is a metric space with $\rho(x, y) = ||x - y||$.
- If $y = \theta$, then $\rho(x, \theta) = ||x - \theta|| = ||x||$. Thus, a norm can be considered a distance to origin.
- Normed and complete space X is called **Banach space**
- **Cauchy-Schwartz inequality:** $||x \cdot y|| \leq ||x|| \cdot ||y||$

Hilbert space

Banach space H is called a **Hilbert space**, if for $\forall x, y \in H$ is defined a functional $H \to \mathbb{R}$ (**Scalar product**), satisfying the following points:

- **Non-negativity:** $(x, x) > 0, \quad \forall x \neq \theta.$
- **Commutative property:** $(x, y) = (y, x).$
- **Linearity:** $(x + y, z) = (x, z) + (y, z), \quad \forall x, y, z \in H.$
- **Linearity:** $(\lambda x, y) = \lambda(x, y), \quad \forall x, y \in H$ and $\forall \lambda \in \mathbb{R}.$
- **Norm is formed with inner product:** $||x||^2 \equiv ||x||_H^2 = (x, x), \quad \forall x \in H.$
- Every inner product defined within a Banach space forms a Hilbert space and thus, connected to a concrete space. Notation: $(x, y)_H$.

Reminder

- **Linear Space:** linear properties.
- **Metric Space:** space with distance between elements.
- **Normed Space:** space with norm of element.
- **Full Space:** Fundamental sequence converges to element of the space.
- **Banach Space:** Normed complete space.
- **Hilbert Space:** Banach space with scalar product.
- **Each Hilbert Space is:**
  - Normed
  - Metric
  - Complete

Examples of concrete spaces

- $\mathbb{R}^n: \quad x = (x_1, ..., x_n)^T, \quad (x, y) = \sum_{k=1}^{n} x_k y_k,$
  $||x|| = \Big(\sum_{k=1}^{n} x_k^2 \Big)^{\frac{1}{2}}.$
- $C[a, b]$ space. Consists of continuous real-valued functions $x(t), t \in [a, b]$. $||x||_C = max(|x(t)|), t \in [a, b]$. This space is Banach space.
- $C^m[a, b]$ space. Consists of m-times continuously differentiable functions $x(t), t \in [a, b]$.

$$||x||_{C^m} = ||x||_C + \sum_{k=1}^{m} ||x^{(k)}||_C.$$

- $L_p[a, b]$: The Lebesgue space:
  $x(t), \quad t \in [a, b]$.

$$||x||_{L_p} = \left(\int_a^b |x(t)|^p dt \right)^{1/p}$$

- $L_2[a, b]$ (Hilbert space) $\leftarrow$

$$(x, y)_{L_2} = \int_a^b x(t)y(t)dt, \quad x, y \in L_2[a, b].$$

- n-dimensional case: let $T \in \mathbb{R}^n$ be a closed bounded set.

$$(x, y)_{L_2(T)} = \int_T x(t)y(t), \quad t \in T.$$

Henri Lebesgue
(1875-1941)

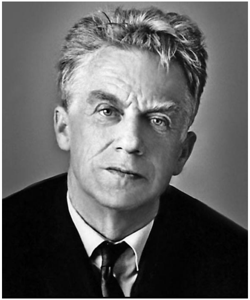
- $T \in \mathbb{R}^n$ is a bounded closed domain.
- If function $x(t) \in L_p(T)$, and all its derivatives up to l^{th} order also belong to $L_p(t)$, then function belongs to Sobolev space W_p^l.
- $W_2^l \equiv H^l$.

$$(x, y)_{H^l(T)} = (x, y)_{L_2(T)} +$$
$$+ \sum_{1 \le k \le l} \int_T \frac{\partial^k x}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} \frac{\partial^k y}{\partial t_1^{k_1} \dots \partial t_n^{k_n}} dt,$$

$k = k_1 + \dots + k_n$.

- H^1 case: $\leftarrow$

$$||x||^2_{H^1} = ||x||^2_{L_2(T)} + \sum_{r=1}^{n} ||\frac{\partial x}{\partial t_r}||^2_{L_2(T)}.$$



Sergei Sobolev (1908-1989)

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Part 2: SLAE

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Systems of linear equations

$$Au = f$$

- A is a matrix of the system
- u is a vector to be found
- f is the right-hand side (vector)

Properties of the matrix

- Condition number $\kappa(A)$ defines the system to be well- or ill-conditioned.
- Dense or sparse
- Symmetric or not
- Positively or negatively definite

Methods of SLAE solution

- Direct methods:
  - Gauss methods
  - Tridiagonal matrix algorithm
  - LU-decomposition
  - And many other methods...
- Iterative methods:
  - Jacobi method
  - Seidel method
  - Multigrid method
  - Successive over-relaxation
  - Conjugate and biconjugate gradients
  - And many other methods...

Performance of some methods

Method	**Computational complexity**
Gauss method	$O(N^3)$
Tridiagonal method	$O(N^{2.5})$
Jacobi's and Seidel's method	$O(N^2 log\frac{1}{\varepsilon})$
Successive over-relaxation	$O(N^{\frac{3}{2}} log\frac{1}{\varepsilon})$
Lower-bound estimate	$O(N)$.

'Bad' systems

$$Au = f.$$

- **Ill-conditioned** systems. The solution is unstable with respect to errors in the right-hand-side f.
- **Overdetermined systems**. The system may be inconsistent (do not have solutions).
- **Underdetermined systems**. Such systems have more than one solution.

The regularization:

$u_\alpha = argmin\big(||Au - f||^2 + \alpha||u||^2_?\big)$ - the approximate solution.

The space "?" should be chosen using reasoning!

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Part 3: Mesh approximation

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Why do we need to descretize the problem?

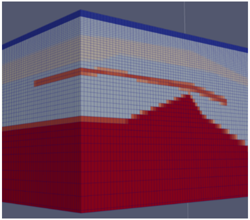
- Generally, the solution of complex problem could be rarely found analytically; and, if if could, you don't need a computer...
- The continuous function $f(x)$ is defined for the infinite number of points
- From the point of view of computer, it seems an infinite-dimensional vector
- Having only two states of the bit, computers do not understand infinity.

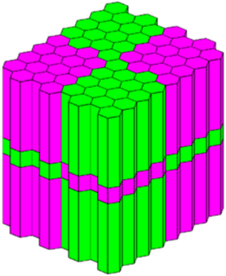
Three main approaches for macroscopic problems:

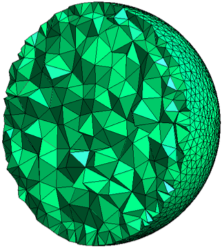
Finite Difference Method (FDM)

Finite Volume Method (FVM)

Finite Element Method (FEM)





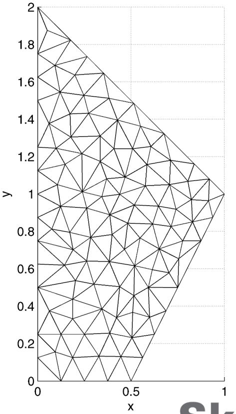


Poisson equation 2D example: solution steps

The computational domain: $\Omega \subset \mathbb{R}^n, \quad n = 2$ or $n = 3$.
The boundary: $\partial\Omega$: the boundary of computational domain;

$$-\Delta u(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad , u|_{\partial\Omega} = \varphi(\mathbf{x}).$$

- Cover the computational domain with some mesh.



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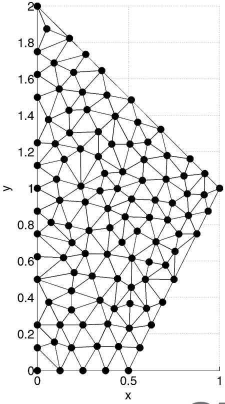
- Cover the computational domain with some mesh.
- Define the locations of known and unknown variables: nodes (vertices), cellular centers of mass, centers of links, sides etc.



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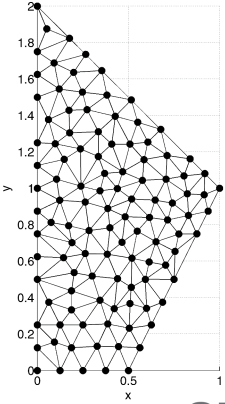
- Cover the computational domain with some mesh.
- Define the locations of known and unknown variables.
- Construct the system of equations to solve numerically:

$$Au_h = g.$$



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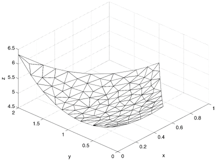
- Cover the computational domain with some mesh.
- Define the locations of known and unknown variables.
- Construct the system of equations to solve numerically.
- Solve the SLAE:

$$u_h = A^{-1} g$$



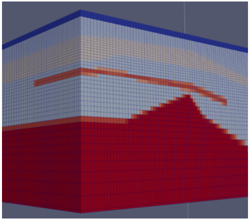
Macroscopic approaches

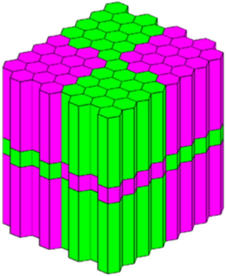
Three main approaches for macroscopic problems:

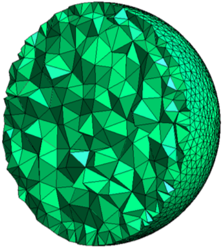
Finite Difference Method (FDM)

Finite Volume Method (FVM)

Finite Element Method (FEM)







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Part 4: Discretization. Finite differences.

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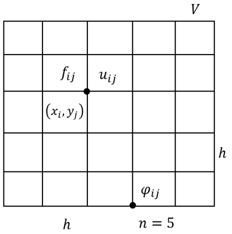
FDM: The mesh

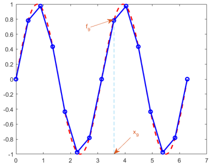
- Let the computational domain be $\Omega \subset \mathbb{R}^r$
- All $r-$dimensional points to be processed are therefore belong to this domain: $\mathbf{x} \in \Omega$
- **Nodes:** A finite set of points $\{x_n\}$ being considered in real computations. Here n is a multiindex.
- $x_n = (x^1_{n_1}, x^2_{n_2}, ..., x^r_{n_r})$; $n_i = 1, ..., N_i$, where N_i is a number of nodes at i-th dimension.
- For example, for $r = 3$, the nodes will be denoted as: $x_{ijk}, i = 1, ..., N_x, j = 1, ..., N_y, k = 1, ..., N_z$.
- The falue of some function depending on x will be denoted as: $f_n = f(x_n)$. For $r = 3$ it then will be f_{ijk}.

FDM: The uniform mesh

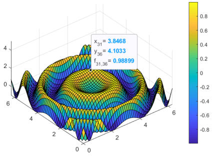
$$\textbf{Uniform mesh: } x_n = (n_1 h_1, n_2 h_2, ..., n_r h_r).$$



The structure of the mesh



The function $u(x) = sin(2x)$, approximated with a mesh $x_i = i/N$



The function $u(x, y) = sin((x - \pi)^2 + (y - \pi)^2)$, approximated with a mesh $x_i = i/N, y_j = j/N, N = 50$.

Approximation of the first derivatives. For short notations, consider the 2d case:

$$x_i = ih_x, \quad y_j = jh_y, \quad f_{ij} = u(x_i, y_j).$$

- Backward difference:

$$\frac{\partial u}{\partial x}(x_i, y_j) \equiv \left(\frac{\partial u}{\partial x}\right)_{ij} \approx \frac{u_{ij} - u_{i-1,j}}{h}.$$

- Forward difference:

$$\frac{\partial u}{\partial x}(x_i, y_j) \equiv \left(\frac{\partial u}{\partial x}\right)_{ij} \approx \frac{u_{i+1,j} - u_{ij}}{h}.$$

- Symmetric difference:

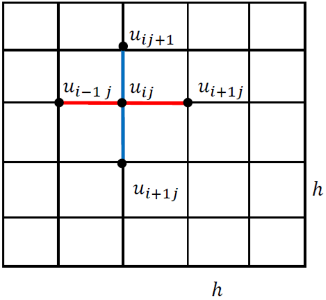
$$\frac{\partial u}{\partial x}(x_i, y_j) \equiv \left(\frac{\partial u}{\partial x}\right)_{ij} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2h}.$$

- The same is for other variables;

FDM: Higher derivatives approximation illustration

$$u_{xx}(x_i, y_j) \approx \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h_x^2}.$$

$$u_{yy}(x_i, y_j) \approx \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h_y^2}.$$



The Poisson equation in this approximation takes the form

$$-\left(\frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h_x^2} + \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h_y^2}\right) = f_{ij}.$$

Approximation of 2D Neumann problem for Poisson eq.

- **The Poisson equation in this approximation takes the form**

$$-\left(\frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h_x^2} + \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h_y^2}\right) = f_{ij}.$$

- The boundary conditions mean we can exclude variables u_{ij} for indices i, j belonging to the boundary, changing them with correspondent values φ_{ij}.
- The scheme has a square matrix: easy to see that indices vary such that $i = 2, ..., N_i - 1$, $j = 2, ..., N_j - 1$, which means $(N_i - 2) * (N_j - 2)$ equations. Since the boundary values are excluded, so we have the same number of unknown variables.

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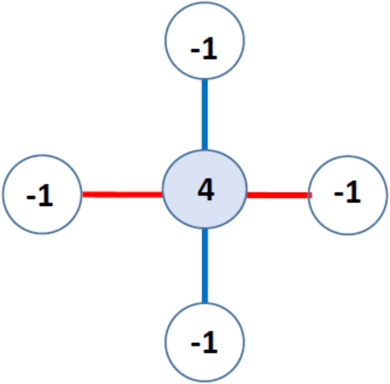
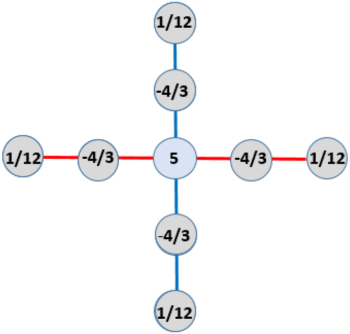
The Cross template consists of five nodes. If the steps $h_x = h_y = h$ (the most often case):

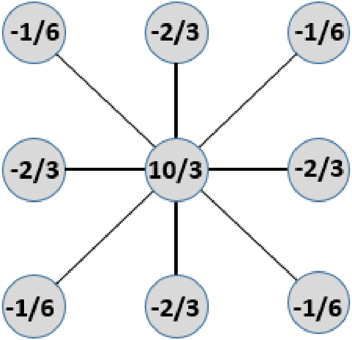
$$-u_{i-1,j} - u_{i+1,j} + 4u_{ij} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$



Fourth order scheme



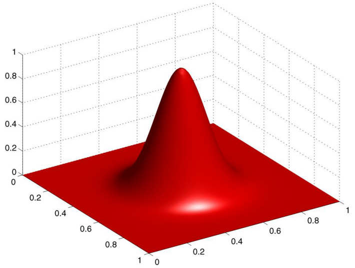
Fourth order compact scheme
(Numerov's scheme)



Non-uniform meshes: example

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

$$u = exp\left(-40\left(x - \frac{1}{2}\right)^2 - 40\left(y - \frac{1}{2}\right)^2 \right)$$



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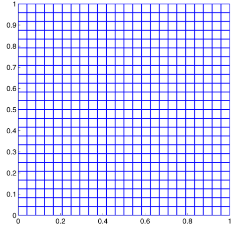
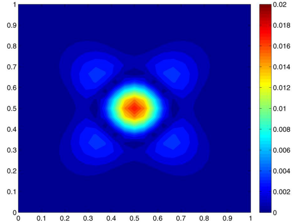
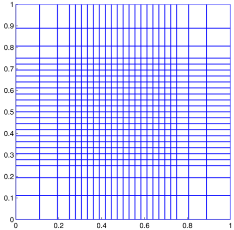
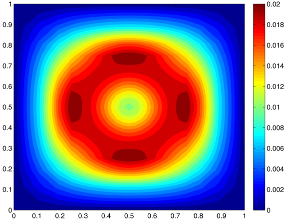
Non-uniform meshes: example

The mesh	$\lvert u - u_h \rvert$



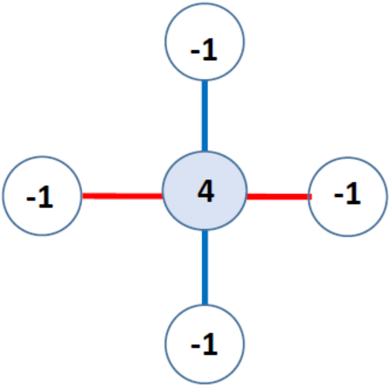






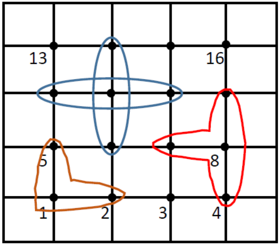
The Cross template consists of five nodes. If the steps $h_x = h_y = h$ (the most often case):

$$-u_{i-1,j} - u_{i+1,j} + 4u_{ij} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$



The structure of SLAE

$$A\, u_h = g$$



$$\left[\begin{array}{cccc|cccc|cccc|cccc}
4 & -1 & & & -1 & & & & & & & & & & & \\
-1 & 4 & -1 & & & -1 & & & & & & & & & & \\
& -1 & 4 & -1 & & & -1 & & & & & & & & & \\
& & -1 & 4 & & & & -1 & & & & & & & & \\
\hline
-1 & & & & 4 & -1 & & & -1 & & & & & & & \\
& -1 & & & -1 & 4 & -1 & & & -1 & & & & & & \\
& & -1 & & & -1 & 4 & -1 & & & -1 & & & & & \\
& & & -1 & & & -1 & 4 & & & & -1 & & & & \\
\hline
& & & & -1 & & & & 4 & -1 & & & -1 & & & \\
& & & & & -1 & & & -1 & 4 & -1 & & & -1 & & \\
& & & & & & -1 & & & -1 & 4 & -1 & & & -1 & \\
& & & & & & & -1 & & & -1 & 4 & & & & -1 \\
\hline
& & & & & & & & -1 & & & & 4 & -1 & & \\
& & & & & & & & & -1 & & & -1 & 4 & -1 & \\
& & & & & & & & & & -1 & & & -1 & 4 & -1 \\
& & & & & & & & & & & -1 & & & -1 & 4
\end{array}\right]$$

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$$
\mathbf{A} = \left[\begin{array}{c|c|c|c}
\mathbf{C} & -\mathbf{E} & & \\ \hline
-\mathbf{E} & \mathbf{C} & -\mathbf{E} & \\ \hline
 & -\mathbf{E} & \mathbf{C} & -\mathbf{E} \\ \hline
 & & -\mathbf{E} & \mathbf{C}
\end{array}\right]
\qquad
\mathbf{C} = \left[\begin{array}{c|c|c|c}
4 & -1 & & \\ \hline
-1 & 4 & -1 & \\ \hline
 & -1 & 4 & -1 \\ \hline
 & & -1 & 4
\end{array}\right]
$$

$$
\left[\begin{array}{cccc|cccc|cccc|cccc}
4 & -1 & & & -1 & & & & & & & & & & & \\
-1 & 4 & -1 & & & -1 & & & & & & & & & & \\
 & -1 & 4 & -1 & & & -1 & & & & & & & & & \\
 & & -1 & 4 & & & & -1 & & & & & & & & \\ \hline
-1 & & & & 4 & -1 & & & -1 & & & & & & & \\
 & -1 & & & -1 & 4 & -1 & & & -1 & & & & & & \\
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 & & & -1 & & & -1 & 4 & & & & -1 & & & & \\ \hline
 & & & & -1 & & & & 4 & -1 & & & -1 & & & \\
 & & & & & -1 & & & -1 & 4 & -1 & & & -1 & & \\
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 & & & & & & & & -1 & & & & 4 & -1 & & \\
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 & & & & & & & & & & -1 & & & -1 & 4 & -1 \\
 & & & & & & & & & & & -1 & & & -1 & 4
\end{array}\right]
$$

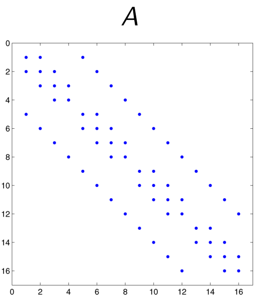
Finite-difference SLAE properties:

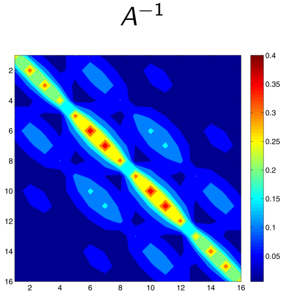
- The system contains a big number of unknown variables and equations
- The matrix is square, sparse, invertible, symmetric, positive definite
- Big condition number (often ill-conditioned):

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

- $H = A^{-1}$ - approximates fundamental (Green's) function.
- H_{ij} - solution in the node i with the point source, located in the node j.
- The matrix A^{-1} is dense while the matrix A is sparse.

It's better to avoid usage of inverse matrices in real computations.





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Scientific Computing
Lecture 3

Part 5: FEM discretization

Nikolay Koshev

October 4, 2021

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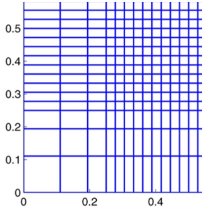
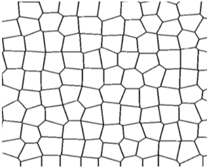
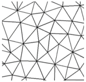
FDM: rectangular cells: fast and simple mesh construction; issues: discontinuous coefficients, complex geometries

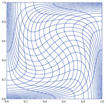


Finite Volumes Method: more flexible with respect to geometry

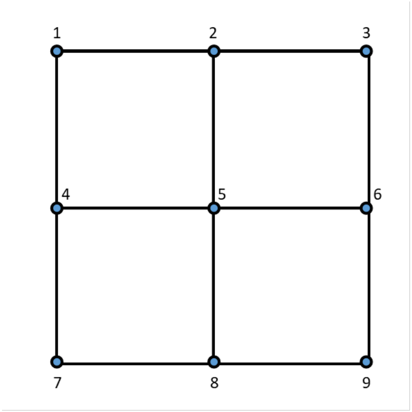


Finite Elements Method: Unstructured grids, complex geometries, stability



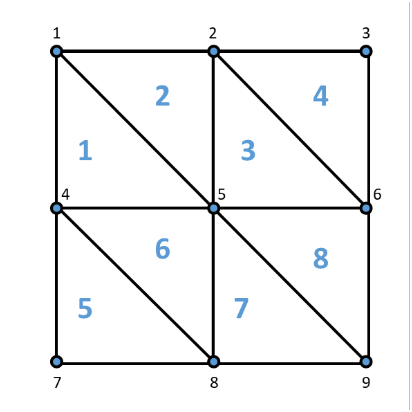


The FEM mesh notations



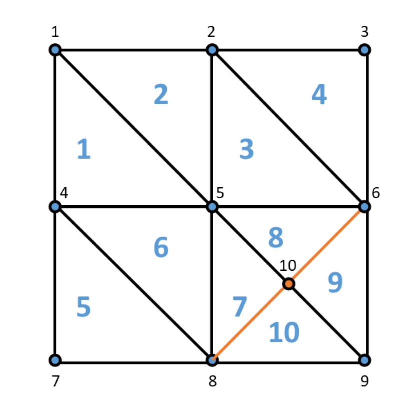
- The number of nodes: N;
- The nodes:
  $\mathbf{x}_i \in \mathbb{R}^d, \quad \text{for } i = 0, \ldots, N-1.$

The FEM mesh notations



- The number of nodes: N (here $N = 9$);
- The nodes: $\mathbf{x}_i \in \mathbb{R}^d, \quad \text{for } i = 0, ..., N-1.$
- The Mesh Cell (Triangle, tetrahedron, etc.): $K_i, 0 = 1, ..., N_e - 1$
- The number of mesh cells: N_e (here $N_e = 8$);

The FEM mesh notations



- The number of nodes here: $N = 10$;
- The number of elements here: $N_e = 10$;
- Sometimes, we are unable to enumerate nodes with appropriate order. Such grids called **unstructured grids.**

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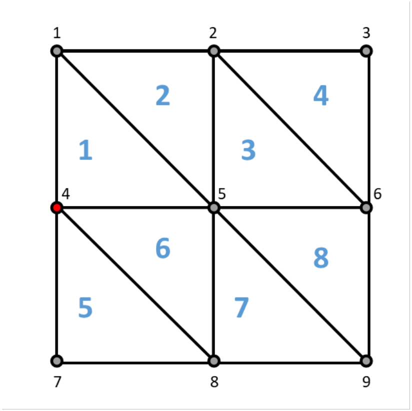
The FEM mesh approximation



- Introduce **the basis:** the set of continuous functions $\varphi_i(\mathbf{x}), i = 0, ..., N-1$, associated with the nodes, such that:

$$\varphi_i(\mathbf{x}) = \begin{cases} 1, & \text{at } i\text{-th node} \\ 0, & \text{at other nodes} \end{cases}$$

- Each basis function is connected to the node: $\varphi_j(\mathbf{x}), j = 0, ..., N-1$.
- The basis functions being sometimes called **Elements**

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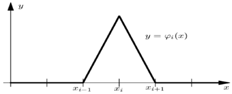
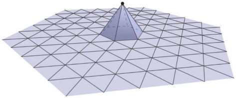
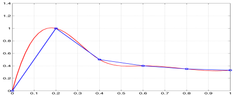






- **The function $u(\mathbf{x})$ can be approximated as follows:**

$$u(\mathbf{x}) \approx \sum_{i=0}^{N-1} u_i \varphi_i(\mathbf{x})$$

- **The derivatives:** $\nabla u(\mathbf{x}) = \sum_{i=0}^{N-1} u_i \nabla \varphi_i(\mathbf{x})$
- **The integrals:**

$$\int_\Omega u(\mathbf{x}) d\mathbf{x} \approx \sum_{i=0}^{N-1} u_i \int_\Omega \varphi_i(\mathbf{x}) d\mathbf{x}, \qquad \int_\Omega \nabla u(\mathbf{x}) d\mathbf{x} \approx \sum_{i=0}^{N-1} u_i \int_\Omega \nabla \varphi_i(\mathbf{x}) d\mathbf{x}$$

The weak formulation

Let U be a Banach space, and F be a Hilbert space. The equation to be solved:

$$Au = f, \quad u \in U, f \in F, A : U \to F.$$

The latter equation is an equivalent to finding $u \in U$ such that:

$$(Au, v)_F = (f, v)_F \quad \forall v \in U.$$

The function v is called a test function. For Poisson equation it means, since $\Delta u \in L_2(\Omega)$, that:

$$(\Delta u, v)_{L_2(\Omega)} = -(f, v)_{L_2(\Omega)}.$$

The pipeline of the FEM

0. **Original equation:** $Au = f, \quad u \in U, f \in F$
1. **Weak formulation:** $(Au, v)_F = (f, v)_F, \quad \forall v \in F$
2. **Approximation (assuming linearity of A):**

$$u(\mathbf{x}) \approx \sum_{i=0}^{N-1} u_i \varphi_i(\mathbf{x}) \quad \Longrightarrow \quad \sum_{i=0}^{N-1} u_i \left(A\varphi_i, v\right)_F = (f, v)_F$$

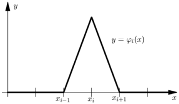
3. **The system:** since $v \in F$ is a certain function, we put $v = \varphi_j, \quad j = 0, 1, ..., N-1$ in order to obtain N equations with respect to unknown u_i:

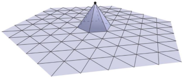
$$\sum_{i=0}^{N-1} u_i \left(A\varphi_i, \varphi_j\right)_F = (f, \varphi_j)_F$$

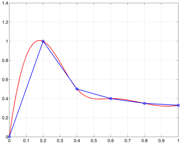
4. Solve the system above.
5. Profit!

Kinds of Finite Elements

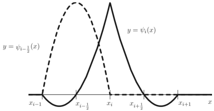
- Linear elements:







- Quadratic elements:



- Bicubic, exponential, etc.
- Since $v \in F$, the elements may imply requirements for U, F spaces!

3D EEG FEM modelling example

3D EEG modelling: statement of the problem

The Neumann problem for Poisson equation in complex heterogeneous area

- The governing equation:

$$\nabla \cdot \big(\sigma(\mathbf{x})\nabla u(\mathbf{x})\big) = \nabla \cdot J(\mathbf{x}), \quad \mathbf{x} \in \Omega \subset \mathbb{R}^3$$

- The Neumann boundary condition:

$$\frac{\partial u}{\partial n}\Big|_{\partial\Omega} = 0.$$

3D EEG modelling: the weak formulation

The weak formulation of the problem

$$-\int_{\Omega} \left(\sigma(\mathbf{x})\nabla u(\mathbf{x})\right) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \left(\nabla \cdot \mathbf{J}(\mathbf{x})\right) v(\mathbf{x}) d\mathbf{x}.$$

In order to manage the discontinuous function $\mathbf{J}$, we avoid usage of its derivative in the RHS using the known integral identity:

$$\int_{\Omega} \left(\nabla \cdot \mathbf{J}(\mathbf{x})\right) v(\mathbf{x}) d\mathbf{x} + \int_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} \left(\mathbf{J}(\mathbf{x}) \cdot \mathbf{n}\right) v(\mathbf{x}) d\mathbf{x}$$

Finally, the weak formulation takes the form:

$$\int_{\Omega} \left(\sigma(\mathbf{x})\nabla u(\mathbf{x})\right) \cdot \nabla v(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla v(\mathbf{x}) d\mathbf{x}$$

3D EEG modelling: the discretization

- Cover the domain Ω with tetrahedral mesh;
- Approximate the function $u(\mathbf{x})$ and its derivatives:

$$u(\mathbf{x}) \approx u_h(\mathbf{x}) = \sum_{i=0}^{N-1} u_i \varphi_i(\mathbf{x}) \quad \Longrightarrow \quad \nabla u_h(\mathbf{x}) = \sum_{i=0}^{N-1} u_i \nabla \varphi_i(\mathbf{x})$$

- Since the function v may be any function, we can use $v(\mathbf{x}) = \varphi_j(\mathbf{x}), j = 0, 1, ..., N-1$. Substituting the approximation to the weak formulation, we have:

$$\sum_{i=0}^{N-1} u_i \int_{\Omega} \sigma(\mathbf{x}) \nabla \varphi_i(\mathbf{x}) \cdot \nabla \varphi_j(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla \varphi_j(\mathbf{x}) d\mathbf{x},$$

  for $i, j = 0, 1, ..., N-1$.
- Additionally define the obtained system with the values of u on boundaries.

3D EEG modelling: the discretization

After discretization with linear finite elements we get the system to solve:

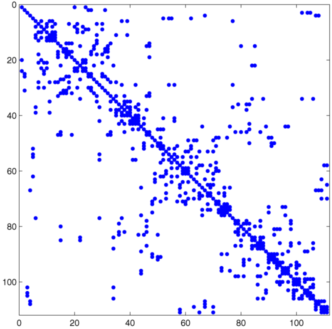
$$\tilde{A}u_h = \mathbf{b}, \quad \tilde{A}_{ij} = \int\limits_{\Omega} \sigma(\mathbf{x})\nabla\varphi_i(\mathbf{x}) \cdot \nabla\varphi_j(\mathbf{x})d\mathbf{x}, \quad b_j = \int\limits_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla\varphi_j(\mathbf{x}),$$

for $i, j = 0, 1, ..., N-1$. Thus,

- $\tilde{A}.shape = (N, N)$, and
- $\mathbf{b}.shape = N$
- The gradients of elements $\nabla\varphi_i(\mathbf{x})$ depend only on mesh and can be pre-calculated.
- The matrix $\tilde{A}$ (called sometimes the *stiffness matrix*) depends only on the mesh and properties of volume (conductivity $\sigma(\mathbf{x})$), and can also be pre-calculated.
- The vector $\mathbf{b}$ depends on distribution $\mathbf{J}(\mathbf{x})$.

Properties of the matrix

- Square matrix
- Sparse and symmetric
- $\kappa(A) = O\left(\frac{1}{h^2}\right)$



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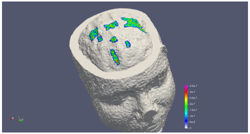
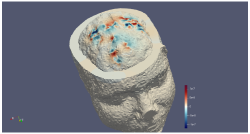
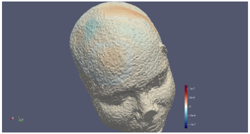
- The system contains $10^6 - 10^7$ equations and the same number of unknown variables;
- The matrix of the system is ill-conditioned;
- It's, however, symmetric and sparse;
- The suitable method to solve: generalized residual method with regularization.



$\mathbf{J}(\mathbf{x})$



$u(\mathbf{x})|_{\partial\Omega_2}$



$u(\mathbf{x})|_{\partial\Omega_1}$

Thank you for your attention!