Scientific Computing
Lecture 5

Differential equations (part 2)
Partial Differential Equations (PDE)

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October 14, 2021

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Structure of the lecture

- Galerkin approach
- Elliptic equations
- Finite Volumes Method
- Parabolic equations
- Hyperbolic equations
- **EXAMPLE:** 3D Cauchy problem for elliptic equation

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Part 1: Galerkin approach

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Differential operator

The operator equation for differential equations is often written as:

$$D\mathbf{u} = 0,$$

where D represents both mathematical and the right-hand side (observed data); the function $\mathbf{u}$ is an unknown function to be found.

- **Ordinary differential equation (ODE):** Let $x \in \mathbb{R}^1$. ODE of the k-th order can be represented with the operator:

$$D\mathbf{u} = F\Big(x, u(x), u'(x), u''(x), ..., u^{(k)}(x)\Big).$$

- **Partial differential equation (PDE):** Let $\mathbf{x} \in \mathbb{R}^n \equiv (x_1, x_2, ..., x_n)$. PDE of the k-th order can be represented with the following operator:

$$D\mathbf{u} = F\Big(\mathbf{x}, \mathbf{u}(\mathbf{x}), \frac{\partial \mathbf{u}}{\partial x_1}, ..., \frac{\partial \mathbf{u}}{\partial x_n}, \dots \frac{\partial^2 \mathbf{u}}{\partial x_1^2}, ..., \frac{\partial^2 \mathbf{u}}{\partial x_n^2}, \dots \frac{\partial^{(k)} \mathbf{u}}{\partial x_1^{(k)}}, \frac{\partial^{(k)} \mathbf{u}}{\partial x_n^{(k)}}\Big).$$

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- The Galerkin method may be considered an initial point - an **IDEA** - for linear DE/IE solution
- The Method is a base for wavelets analysis, FEM, FDM etc
- The Method shows one of the most general approaches in computational problems
- The Method allows to chose the concrete solution spaces with respect to the problem (may be considered a regularization too)
- Easy to understand
- Easy to research

Consider the Boundary Value problem for the linear differential operator D:

$$Du = 0, \quad \text{in } \Omega \subset \mathbb{R}^n, \quad S(u) = 0, \text{in } \partial\Omega$$

- Assume $u \in U, \quad D : U \to V$, where U, V are some Hilbert spaces.
- Let $\{\varphi_i(\mathbf{x})\}, i = 1, \ldots$ be some basis in U.
- Chose finite number N and approximate

$$u(\mathbf{x}) \approx u_a(\mathbf{x}) = u_0(\mathbf{x}) + \sum_{i=1}^{N} a_i \varphi_i(\mathbf{x}).$$

Consider the Boundary Value problem for the linear differential operator D:

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- Let $\{\varphi_i(\mathbf{x})\}, i = 1, \ldots$ be some basis in U.
- Chose finite number N and approximate the solution u
- Since N is finite, and u_a is only the approximation, we get:

$$D\left(\sum_{i=1}^{N} a_i \varphi(\mathbf{x})\right) + Du_0 = R(a_1, \ldots, a_n, \mathbf{x}).$$

Consider the Boundary Value problem for the linear differential operator D:

$$Du = 0, \quad \text{in } \Omega \subset \mathbb{R}^n, \quad S(u) = 0, \text{in } \partial\Omega$$

- Assume $u \in U, \quad D : U \to V$, where U, V are some Hilbert spaces.
- Let $\{\varphi_i(\mathbf{x})\}, i = 1, \dots$ be some basis in U.
- Chose finite number N and approximate the solution u
- Since N is finite, and u_a is only the approximation, we get the residual $R(a_1, \dots, a_n, \mathbf{x})$
- The function R is never zero... But we can minimize it with respect to the coefficients $\{a_i\}$!

The idea

- Represent (or approximate) the solution u with some weighted sum of functions
- Substitute the approximation or representation into the original equations
- Minimize the residual with respect to weights
- After the weights are calculated, reconstruct the approximate (or, sometimes, exact) solution, substituting the weights into your representation (or approximation) of it
- Be careful: the residual rarely being equal to zero, but it should be small!

Galerkin and FEM

Let the problem be linear: $D, S(u)$ are linear.

$$Du = 0, \quad \text{in } \Omega \subset \mathbb{R}^n, \quad S(u) = 0, \text{in } \partial\Omega$$

- The weak formulation:

$$(Du, v) = 0, \quad v \in U.$$

- Approximate the solution:

$$u = \sum_{i=0}^{N} u_i \varphi_i(\mathbf{x}), \quad \varphi_i(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} = \mathbf{x}_i \\ 0, & \mathbf{x} = \mathbf{x}_j, j \neq i \\ \text{continuous} & \text{elsewhere} \end{cases}$$

- Substitute the approximation into the weak form:

$$\sum_{i=1}^{N} u_i (D\varphi_i, \varphi_j) = 0, \quad \sum_{l:\mathbf{x}_l \in \partial\Omega} u_l S\big(\varphi_l(\mathbf{x})\big) = 0.$$

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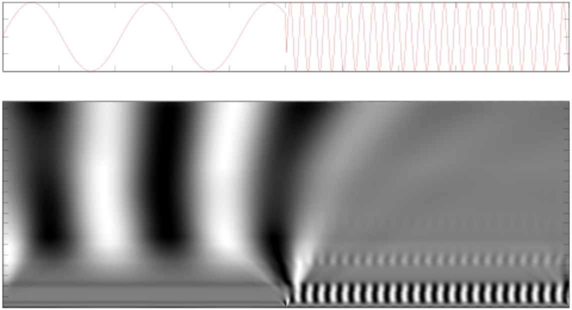
With the wavelets we can analyse not only frequencies (like in Fourier analysis), but both frequencies and its locations in time (scaling and shifting)

$$U(a, b) = \frac{1}{|a|^{\frac{1}{2}}} \int_{\mathbb{R}} u(x)\psi^*\left(\frac{t-b}{a}\right)dt$$



Galerkin and wavelets

- Continuous wavelet transform:

$$U(a,b) = \frac{1}{|a|^{\frac{1}{2}}} \int\limits_{\mathbb{R}} u(x)\psi^*\left(\frac{t-b}{a}\right)dt$$

- The continuous wavelet transform (the inverse one, 1D case):

$$u(x) = C_{psi} \int\limits_{\mathbb{R}^2} \frac{1}{a^2} U(a,b)\tilde{\psi}\left(i\frac{t-b}{a}\right)dbda$$

- In discrete case:

$$u(x) = C_\psi \sum_{i,j=-\infty}^{\infty} U_{ij}\psi_{ij}(t), \quad U_{ij} = \int\limits_{\mathbb{R}} u(x)\psi_{ij}^* dt$$

- In n-dimensional case we use separable wavelets: each for one dimension.

Multiresolution analysis

Let $\{V_j\}_{j=-\infty}^{\infty}$ is a sequence of spaces such that:

- $V_j \subset V_{j+1}$
- $\bigcup\limits_{j \in \mathbb{Z}} V_j = L^2(\mathbb{R}), \quad \bigcap\limits_{j \in \mathbb{Z}} V_j = \emptyset$
- $f(t) \in V_j \Rightarrow f(2t) \in V_{j+1}, \quad f(t) \in V_j \Rightarrow f(t-k) \in V_j$
- The mother wavelet ψ defines orthonormal basis in V_j:

$$\psi_{jk} = 2^{j/2}\psi(2^j t - k)$$

- Example: Haar's multiresolution analysis:

$$V_j = \{f \in L^2(\mathbb{R}); \forall k \in \mathbb{Z} : f|_{[2^j k, 2^j(k+1)]} = const\}$$

- After we choose the basis, then do the same: substitute the solution approximated with that basis!

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Part 2: Elliptic equations & FVM

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Partial differential equations of the second order

Partial differential equations of second order

Most of PDE-driven problems can be described with PDEs of second order. The differential operator D can be represented as follows:

$$D\mathbf{u} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(\mathbf{x})\frac{\partial^2 \mathbf{u}}{\partial x_i \partial x_j} + F\left(\mathbf{x}, \mathbf{u}, \frac{\partial \mathbf{u}}{\partial x_1}, ..., \frac{\partial \mathbf{u}}{\partial x_n}\right) \equiv L\mathbf{u} + F(...).$$

The operator L is called the Principle Part and being defined with the matrix:

$$L\mathbf{u} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n1} & \dots & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_1} & \frac{\partial^2 \mathbf{u}}{\partial x_2 \partial x_1} & \dots & \frac{\partial^2 \mathbf{u}}{\partial x_n \partial x_1} \\ \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_2} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_n} & \dots & \dots & \frac{\partial^2 \mathbf{u}}{\partial x_n \partial x_n} \end{pmatrix} = A_L H^T.$$

Here the matrix H is a **Hessian**.

General classification

We are able to find the eigenvalues λ of the matrix A_L:

$$A_L \mathbf{v} = \lambda \mathbf{v}$$

- Suppose we have found several eigenvalues λ_i.
- **Elliptic equation:** $\lambda_i > 0$ or $\lambda_i < 0$ for $\forall i$.
  All-positive of all-negative eigenvalues
- **Parabolic equation:** $\exists k : \lambda_k = 0$ while $\lambda_i > 0$ or $\lambda_i < 0$ for $\forall i \neq k$. There is only one zero eigenvalue while all others have the same sign.
- **Hyperbolic equation:** $\exists k : \lambda_k > 0$ while $\lambda_i < 0 \forall i \neq k$ OR $\exists k : \lambda_k > 0$ while $\lambda_i < 0 \forall i \neq k$
  The signs of eigenvalues are the same excepting one of them, which is non-zero and has contrary sign.

Elliptic equations

The equation

$$Lu + F(...) = 0 \tag{1}$$

is considered elliptic if the coefficient matrix A_L has all-positive or all-negative eigenvalues.

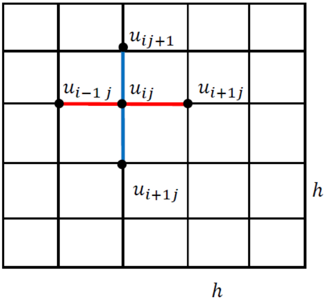
- The solution is as smooth as the coefficients and boundary conditions allow.
- Well suited to describe static or equilibrium states.
- Less suitable for dynamic processes.

Meshed approaches on solution

- Finite Differences Method (FDM)
- Finite Elements Method (FEM)
- Finite Volumes Method (FVM)

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

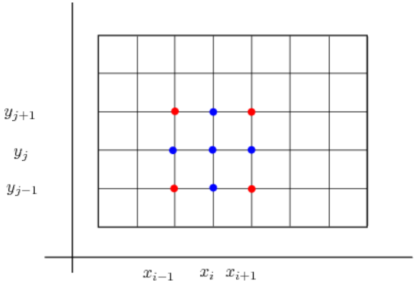
$$u_{yy}(x_i, y_j) \approx \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h_y^2}.$$



The Poisson equation in this approximation takes the form

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

FDM: Mixed derivatives (2D case)

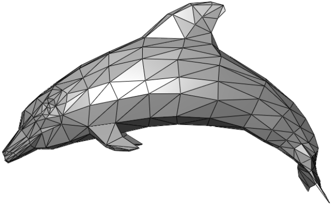


$$\frac{\partial^2 \mathbf{u}}{\partial x \partial y} \approx \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4 h_x h_y}$$

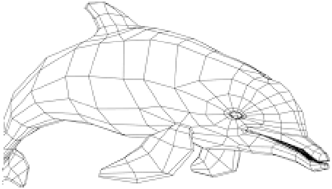
FDM: advantages and disadvantages

- Simplicity of mesh construction; simplicity of working with the mesh.
- In case of uniform meshes and simple boundary of the comp.domain, might work fast.
- In cases of static and slowly evolving systems, gives good accuracy.
- Can be too cumbersome for 3D meshes.
- High interpolation errors due to complex boundaries or complex inner structure.
- Evolving systems need to usage of implicit schemes, which affects on the performance.
- The system can be ill-conditioned.

FEM for elliptic problems: the mesh



$r = 3, d = 3$



$r = 4, d = 3$

- nodes: $N \times d$ array with d coordinates of N points in d-dimensional space.
- elements: $K \times r$ array with r indices of vertices in nodes array for K elements.

FEM for elliptic equation: reminder

- The equation: $Au = f, \quad u \in U.$
- Weak formulation:

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

- Approximation with FE:

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

- Substitute $\tilde{u}$ and take $v = \varphi_j, j = 1, ..., N$. The SLAE with respect to u_i:

$$\sum_{i=1}^{N} u_i (A\varphi_i, \varphi_j) = (f, \varphi_j), \quad j = 1, ..., N.$$

- Exclude u_i covered with boundary conditions.

FEM: advantages and disadvantages

- Suitable for computational domains with complex boundaries and/or complex inner structure.
- Not so cumbersome independently on the number of dimensions.
- Complicated procedure of mesh construction.
- The structure of the mesh may be complicated for working with it.
- The system is often being ill-conditioned.

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:

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

- Continuity of the potential and its gradient on interfaces. Let $\partial\Omega_k$ be an intracranial interface. Denote by f^- and f^+ values of some function f nearby the interface, located on two sides of the boundary. Then

$$u^+|_{\partial\Omega_k} = u^-|_{\partial\Omega_k}; \quad \sigma^+\frac{\partial u^+}{\partial n} = \sigma^-\frac{\partial u^-}{\partial n}.$$

3D EEG modelling

The weak formulation of the problem

$$\int_{\Omega} \big(\sigma(\mathbf{x})\nabla V(\mathbf{x})\big) \cdot \nabla h(\mathbf{x}) d\mathbf{x} = \int_{\Omega} (\nabla \cdot \mathbf{J}) h(\mathbf{x}) d\mathbf{x}.$$

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

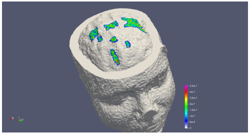
$$\int_{\Omega} \big(\nabla \cdot \mathbf{J}(\mathbf{x})\big) h_m(\mathbf{x}) d\mathbf{x} + \int_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla h_m(\mathbf{x}) d\mathbf{x} = \int_{\partial\Omega} \big(\mathbf{J}(\mathbf{x}) \cdot \mathbf{n}\big) h_m(\mathbf{x}) d\mathbf{x}$$

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

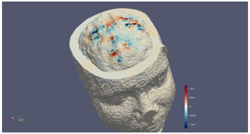
$$Au_h = b, \quad A_{nm} = -\int_{\Omega} \sigma(\mathbf{x}) \nabla h_m(\mathbf{x}) \cdot \nabla h_n(\mathbf{x}) d\mathbf{x},$$

$$b_m = \int_{\Omega} \nabla \cdot \mathbf{J}^i(\mathbf{x}) h_m(\mathbf{x}) d\mathbf{x} \equiv -\int_{\Omega} \mathbf{J}(\mathbf{x}) \cdot \nabla h_m(\mathbf{x})$$

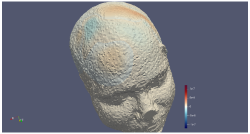
- The system contains $10^6 - 10^7$ equations and the same number of unknown variables;
- The matrix of the system is ill-conditioned;
- It's, however, symmetric and sparse;
- The suitable method to solve: generalized residual method with regularization.



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



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



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

Finite Volumes Method

Non-conservative difference scheme example

Consider the boundary value problem:

$$-\frac{d}{dx}\left(K(x)\frac{du}{dx}\right) = 0, \quad u(0) = 1, u(1) = 0$$

$$K(x) = \begin{cases} 1 & x < 1/2 \\ 5 & x > 1/2 \end{cases}$$

Using

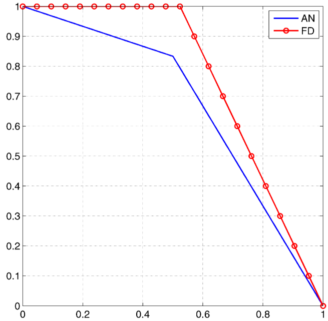
$$-Ku_{xx} - K_x u_x = 0,$$

build the difference scheme:

$$-K_j \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} - \frac{K_{i+1} - K_{i-1}}{2h} \cdot \frac{u_{i+1} - u_{i-1}}{2h} = 0,$$

$$u_0 = 1, \quad u_n = 0$$

Non-conservative difference scheme example



The scheme does not converge!

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Energy balance: conservative schemes

Consider the diffusion equation:

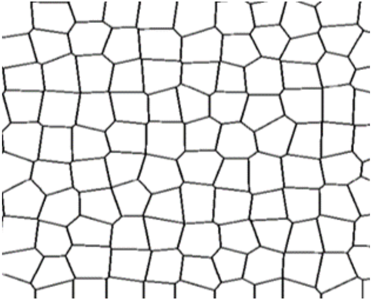
$$-\nabla \cdot (K \nabla U) = f, \quad x \in \Omega,$$
$$u = \varphi, \quad x \in \partial\Omega$$

- $K(x)$ - the thermal conductivity
- $\mathbf{W}$ - the thermal flux

$$\mathbf{W} = -K \nabla u,$$
$$\nabla \cdot \mathbf{W} = f$$

The energy balance equation

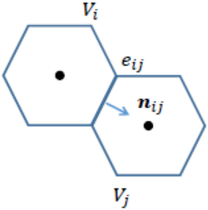
$$\int\limits_{\partial V_i} \mathbf{W} \cdot \mathbf{n}_i dl = \int\limits_{V_i} f dS$$



Finite Volumes Method

- e_{ij} - the link between the cell V_i and neighboring cell V_j
- $\mathbf{n}_{ij}$ - the normal to e_{ij} with the direction to V_j
- W_{ij} - mean normal transfer through e_{ij}

$$W_{ij} = \frac{1}{|e_{ij}|} \int_{e_{ij}} \mathbf{W} \cdot n_{ij} dl$$



- $$f_i = \frac{1}{|V_i|} \int_{V_i} f dS, u_i = \frac{1}{|V_i|} \int_{V_i} u dS$$

- Finally, the energy balance equation takes the form:

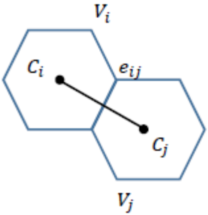
$$\sum_j |e_{ij}| W_{ij} = |V_i| f_i$$

- We need to express W_{ij} in terms of u_{ij}. Since $\mathbf{W} = -K\nabla u$:

$$\frac{W_{ij}}{K} = -\nabla u \mathbf{n}_{ij}$$

- Let us integrate the latter identity between points C_i and C_j:

$$W_{ij} \int\limits_{C_i C_j} \frac{1}{K} dl = - \int\limits_{C_i C_j} \nabla u \cdot n_{ij} dl$$



- The length of interval $C_i C_j$ is h_{ij} and is divided into equal parts by the link e_{ij}. $K|_{V_i} = K_i$. Thus

$$W_{ij} = (u_i - u_j) \frac{2}{h_{ij}} \frac{K_i K_j}{K_i + K_j}$$

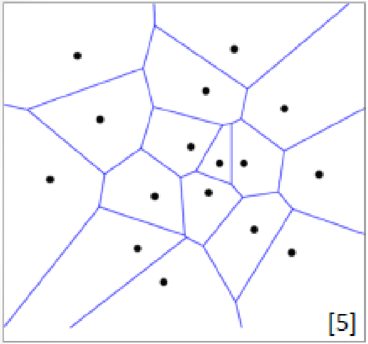
Thus, combining all reasoning above, we have:

$$\sum_j (u_i - u_j)\frac{|e_{ij}|}{h_{ij}}\frac{2K_iK_j}{K_i + K_j} = |v_i|f_i$$

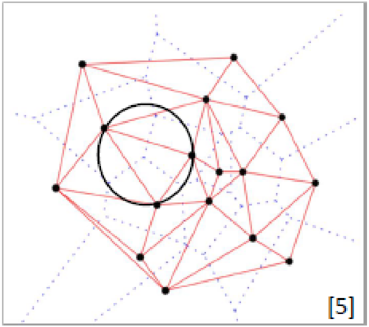
The latter is SLAE with respect to u_i.

- In case of rectangular cells and constant K this SLAE is the same as Finite-difference SLAE
- The geometry is more flexible in comparison with FDM
- The accuracy: $O(h^2)$

Voronoi diagram



Let we have the set of point S. Each cell is consisting of all points closer to that seed than to any other.



The dual: Delaunay triangulation.

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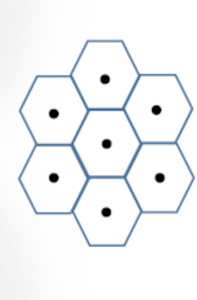
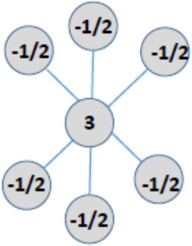
$$-\Delta u = f$$

Mesh constructed from regular hexagons

$$|e_{ij}| = \frac{h_{ij}}{2}, \quad K_{ij} = 1.$$

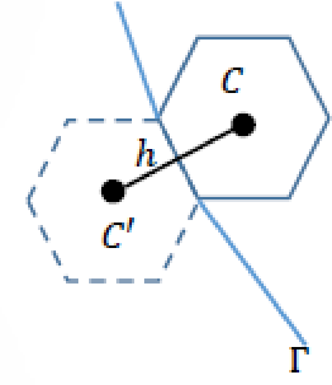




The Dirichlet boundary condition

$$u|_\Gamma = \varphi$$

can be taken into account using the fictitious cell:



$$\varphi = \frac{u_C + u_{C'}}{2} + O(h^2)$$

$$W_{CC'} = -K\frac{u_C - u_{C'}}{h}$$

thus,

$$W_{CC'} = -K\frac{2u_C - 2\varphi}{h}$$

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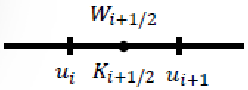
FVM templates

$$-\frac{d}{dx}\left(k\frac{du}{dx}\right) = 0, \quad u(0) = 1, u(1) = 0$$

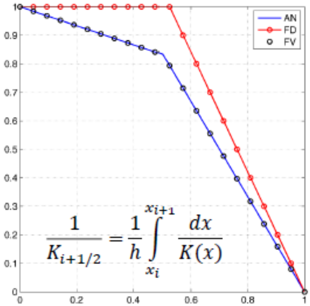
$$K(x) = \begin{cases} 1 & x < 1/2 \\ 5 & x > 1/2 \end{cases}, \quad W = -K(x)u_x, \quad W_x = 0.$$



Finite volume scheme:

$$W_{i+1/2} = -K_{i+1/2}\frac{u_{i+1} - u_i}{h}$$

$$\frac{W_{i+1/2} - W_{i-1/2}}{h} = 0$$



$$\frac{1}{K_{i+1/2}} = \frac{1}{h}\int_{x_i}^{x_{i+1}} \frac{dx}{K(x)}$$

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Part 3: Parabolic equations

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Parabolic equations

The equation

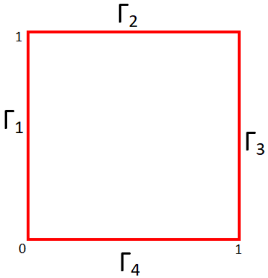
$$L\mathbf{u} + F(...) = 0 \tag{2}$$

is considered parabolic if the coefficient matrix $\{a_{ij}\}$ has one zero eigenvalue, while all others have the same sign (positive or negative)

- May be represented in form $u_t = -L\mathbf{u}$, where $\mathbf{u}$ is an elliptic operator.
- Are well suited to describe the smoothly evolving processes such diffusion or heat transfers.
- The solution is generally smoother than the initial value.

The quasilinear heat transfer equation:

$$
\begin{aligned}
u_t = \Delta u + aS(u) + F(\mathbf{x}, t), \\
(x, t) \in [0, 1]^3, \\
u(\mathbf{x}, 0) = f(\mathbf{x}), \\
u_{\Gamma_k} = p_k(t), \quad k = 1, 2, 3, 4
\end{aligned}
$$



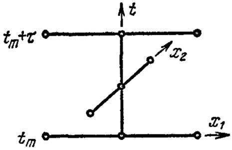
The FDM implicit scheme

- Let τ be the time step.
- Consider three time layers: t, $\tilde{t} = t + \frac{\tau}{2}$, and $\hat{t} = t + \tau$.
- The layer $\tilde{t}$ is named 'half-layer', and any function $\tilde{f} = f(\mathbf{x}, \tilde{t})$.
- The layer $\hat{t}$ - the 'next' layer, and any function $\hat{f} = f(\mathbf{x}, \hat{t})$.
- Assume the values u_{nm} to be known in all nodes at t layer.
- Move from t to $\tilde{t}$ via solution of SLAE:

$$\frac{2}{\tau}(\tilde{u}_{nm} - u_{nm}) = \Lambda_1 \tilde{u}_{nm} + \Lambda_2 u_{nm} + \tilde{f}_{nm}.$$

-

$$\Lambda_1 u = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{2h^2},$$
$$\Lambda_2 u = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{2h^2}$$



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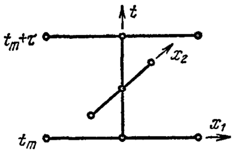
The FDM implicit scheme

- Consider three time layers: t, $\tilde{t} = t + \frac{\tau}{2}$, and $\hat{t} = t + \tau$.
- Assume the values u_{nm} to be known in all nodes at t layer.
- Move from t to $\tilde{t}$.
- Move from $\tilde{t}$ to $\hat{t}$:

$$\frac{2}{\tau}(\hat{u}_{nm} - \tilde{u}_{nm}) = \Lambda_1 \tilde{u}_{nm} + \Lambda_2 \hat{u}_{nm} + \tilde{f}_{nm}.$$



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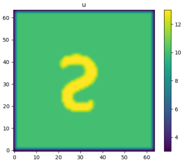
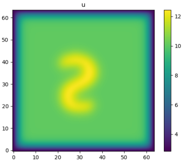
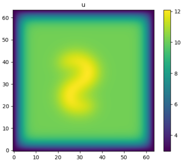
2D Parabolic: result with FDM



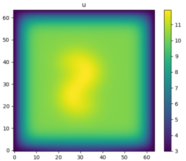
$t = 0$



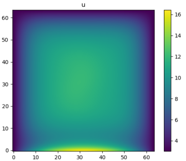
$t = 10s$



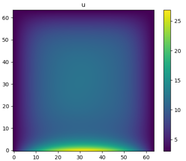
$t = 20s$



$t = 40$



$t = 100s$



$t = 200s$

2D heat transfer: solution using FEM

- The weak formulation:

$$\int_{\Omega} pdu - ftvdx + \int_{\Omega} \nabla u \cdot \nabla vdx - \int_{\Omega} cuvdx$$

- The software to use: Fenics/dolfin (C++/python), OpenFoam.

The ill-posed Cauchy problem for heat transfer equation.

Suppose both initial condition $f(x)$ and the left boundary condition $g(t)$ to be unknown, and the function $q(t) = \partial u / \partial x(1, t)$ to be known:

$$\begin{aligned} u_t = u_{xx} + aS(u) + F(x,t), \quad (x,t) \in [0,1]^2, \\ u(1,t) = p(t), \quad \frac{\partial u}{\partial x}(1,t) = q(t). \end{aligned}$$

Find $u(x,t)$.

The problem is non-linear (quasi-linear), which leads that the cost functional has local minima

Coefficient problem for a heat-transfer equation

Let $\Omega \subset \mathbb{R}^n$ be some domain, $\partial\Omega$ - its boundary, and $\Gamma \subset \partial\Omega$ is some part of this boundary. Consider the problem:

$$u_t = \Delta u + a(\mathbf{x})u, \quad \mathbf{x} \in \Omega$$
$$u_\Gamma(\mathbf{x}, t) = p(\mathbf{x}, t).$$

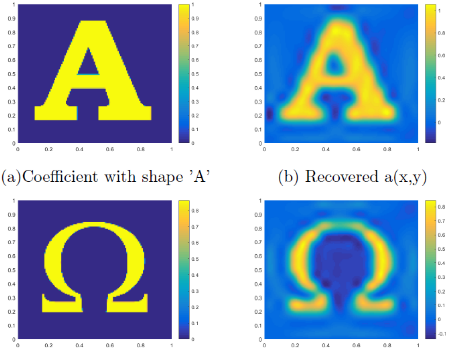
Assuming $u(\mathbf{x}) > 0, \mathbf{x} \in \Omega$ introduce the notation: $u = e^v$, where $v(x, t)$ is some function.

$$v_t u = u\Delta v + u(\nabla v)^2 + a(\mathbf{x})u, \quad v|_\Gamma = ln(p).$$

Dividing the equation by u, we obtain:

$$v_t = \Delta v + (\nabla v)^2 + a(\mathbf{x}).$$

Now, differentiating the latter equation on t, we just exclude the coefficient $a(x)$!



(a) Coefficient with shape 'A' (b) Recovered a(x,y)

(c) Coefficient with shape 'Ω' (d) Recovered a(x,y)

The result was obtained by Prof. Klibanov (UNCC Charlotte) with co-authors.

Scientific Computing
Lecture 5

Part 2: Hyperbolic equations

Nikolay Koshev, Nikolay Yavich

October 14, 2021

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Hyperbolic equations

The equation

$$Lu + F(...) = 0 \tag{3}$$

is considered hyperbolic if the coefficient matrix $\{a_{ij}\}$ has eigenvalues, the signs of which are the same excepting one of them, which is non-zero and has contrary sign.

- May be represented with elliptic operator: $L\mathbf{u} - a^2 \frac{\partial^2 \mathbf{u}}{\partial t^2} = F(...)$, where L is an elliptic operator.
- Hyperbolic equations solutions retain discontinuities of initial data.
- Well-suited to describe wave processes.

The Maxwell system

- The Gauss Law (in the sourceless domain)

$$\nabla \cdot \mathbf{E} = 0$$

- The Gauss Law for Magnetic induction

$$\nabla \cdot B = 0$$

- The Faraday's Law

$$\nabla \times \mathbf{E} = \frac{\partial \mathbf{B}}{\partial t}$$

- The Ampere's Circuital Law

$$\nabla \times \mathbf{B} = \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

The Wave equation

- Applying curl to the Faraday's law:

$$\nabla \times (\nabla \times \mathbf{E}) = -\mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

- Applying curl to the Ampere's law:

$$\nabla \times (\nabla \times \mathbf{B}) = -\mu_0 \varepsilon_0 \frac{\partial^2 \mathbf{B}}{\partial t^2}$$

- Using the identity $\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \Delta \mathbf{E}$:

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} - \Delta \mathbf{E} = 0$$
$$\frac{1}{c^2}\frac{\partial^2 \mathbf{B}}{\partial t^2} - \Delta \mathbf{B} = 0.$$

The weak form

Consider 1D boundary value problem:

$$\frac{\partial^2 u}{\partial t^2} = k\frac{\partial^2 u}{\partial x^2}, \quad x \in [a, b], t \in [0, T]$$

$$u(x, 0) = 0, \frac{\partial u}{\partial t}(x, 0) = V_0(x), u(a, t) = 0, k\frac{\partial u}{\partial x}(b, t) = t_b(t)$$

- These conditions make the problem well-defined.
- Integrating it:

$$\int_a^b v\frac{\partial^2 u}{\partial t^2}dx = k\int_a^b v\frac{\partial^2 u}{\partial x^2}dx$$

The weak form

Consider 1D boundary value problem:

$$\frac{\partial^2 u}{\partial t^2} = k\frac{\partial^2 u}{\partial x^2}, \quad x \in [a, b], t \in [0, T]$$

$$u(x, 0) = 0, \frac{\partial u}{\partial t}(x, 0) = V_0(x), u(a, t) = 0, k\frac{\partial u}{\partial x}(b, t) = t_b(t)$$

- Integrating the right-hand side by parts, we get:

$$\int_a^b v\frac{\partial^2 u}{\partial t^2}dx = vt_b(t) - \int_a^b \frac{\partial v}{\partial x}\frac{\partial u}{\partial x}(x, t)dx$$

- In nD case:

$$\int_\Omega \frac{\partial^2 u}{\partial t^2}vd\mathbf{x} = \Phi(\partial\Omega) - k\int_\Omega \nabla u \cdot \nabla vd\mathbf{x}$$

- Finite elements:

$$u(x,t) = \sum_{i=1}^{N} u_i(t)\varphi_i(x)$$

- Substituting it to the weak form, we get the system:

$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) - t_b(t) = 0,$$

$$M_{ij} = \int_a^b \varphi_i(x)\varphi_j(x)dx, \quad K_{ij} = \int_a^b \frac{\partial \varphi_i}{\partial x} \cdot \frac{\partial \varphi_j}{\partial x},$$

$$i, j = 1, 2, ..., N.$$

- The system
$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) - t_b(t) = 0,$$
- Rewrite it in the form:
$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{u}(t)\\ \mathbf{M}\dot{\mathbf{u}}(t)\end{pmatrix} = \begin{pmatrix}\dot{\mathbf{u}}(t)\\ -\mathbf{K}\mathbf{u}(t) + t_b(t)\end{pmatrix}$$
- Discretization on t (backward Euler scheme, $\mathbf{v} = \dot{\mathbf{u}}$):
$$\begin{pmatrix}\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n}}{h_t}\\ \mathbf{M}\left(\frac{\mathbf{v}^{n+1}-\mathbf{v}^{n}}{h_t}\right)\end{pmatrix} = \begin{pmatrix}\mathbf{v}^{n+1}\\ -\mathbf{K}\mathbf{u}^{n+1} + t_b(t^{n+1})\end{pmatrix}$$

Consider the BV problem:

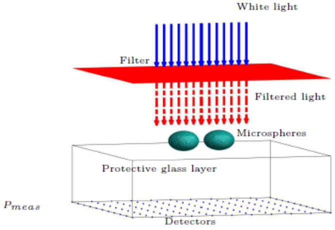
$$
\begin{aligned}
u_{tt} = c^2 u_{xx} + f(x,t), \quad 0 < x < a, 0 < t \leq T \\
u(x,0) = \mu_1(x), u_t(x,0) = \mu_2(x), \quad 0 < x < a \\
u(0,t) = \mu_3(t), u(a,t) = \mu_4(t), 0 \leq t \leq T.
\end{aligned}
$$

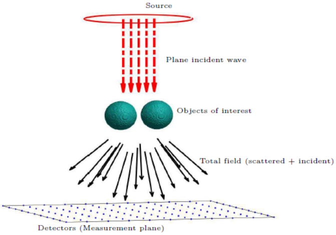
- **The Cross template:**

$$\frac{1}{\tau^2}(\hat{y}_n - 2y_n + \check{y}_n) = \frac{c^2}{h^2}(y_{n+1} - 2y_n + y_{n-1}) + f_n.$$

- On the initial and the next layers the solution is known from initial conditions
- The scheme is explicit and allows to get $\hat{y}_n$ from known $y_n, \check{y}_n$.

The microscpheres are being irradiated with a plane wave of visible-light frequencies





Source: *A numerical method to solve a phaseless coefficient inverse problem from a single measurement of experimental data.* MV Klibanov, NA Koshev, DL Nguyen, LH Nguyen, A Brettin, VN Astratov *SIAM Journal on Imaging Sciences*, Vol. 11 (4), 2339-2367, 2018

Wave equation to Helmholtz equation

- The equation for the electric field:

$$\frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} - \Delta \mathbf{E} = 0. \tag{4}$$

- Since $\mathbf{E}$ is a plane wave, then $\mathbf{E} = u(x) exp(i\omega t)$
- Substituting it to the equation, we get

$$-\frac{\omega^2}{c^2} u(x) exp(i\omega t) - \Delta u(x) exp(i\omega t) = 0$$

- Dividing by $-exp(...)$ and denoting $\omega^2/c^2 = k^2$:

$$\Delta u(\mathbf{x}) + k^2 u(\mathbf{x}, k) = 0.$$

- The obtained equation is a Helmholtz equation; and it's elliptic!

Integral representation example: the Helmholtz equation

Consider the plane wave propagating in 3D. The governing equation is the Helmholtz equation:

$$\begin{aligned} \Delta u(\mathbf{x}, k) + k^2 n^2(\mathbf{x}) u(\mathbf{x}, k) = 0, &\quad x \in \mathbb{R}^3 \\ \partial_{|\mathbf{x}|} u_{sc}(\mathbf{x}, k) - iku_{sc}(\mathbf{x}, k) = \quad o(|\mathbf{x}|^{-1}) &\quad |\mathbf{x}| \to \infty. \end{aligned}$$

The problem above is called **Scattering problem**.
This is an equivalent for it: the **Lippmann-Schwinger equation:**

$$u(\mathbf{x}, k) = e^{ikx_3} + k^2 \int\limits_{\Omega} \frac{exp(ik|\mathbf{x} - \xi|)}{3\pi|\mathbf{x} - \xi|} \left(n^2(\xi) - 1\right) u(\xi, k) d\xi.$$

$$v(\mathbf{x}, k) g(\mathbf{x}) = e^{ikx_3} + k^2 K * v, \quad K(\mathbf{x}) = \frac{exp(ik|\mathbf{x}|)}{3\pi|\mathbf{x}|}, v = (n^2(\mathbf{x}) - 1) u(\mathbf{x}, k).$$

QUESTION: Classify the IE above.

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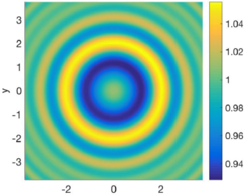
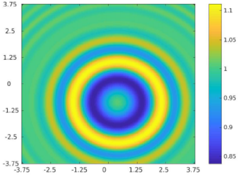
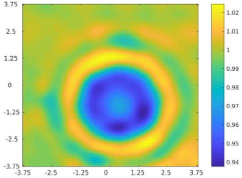
The Plane Wave Diffraction



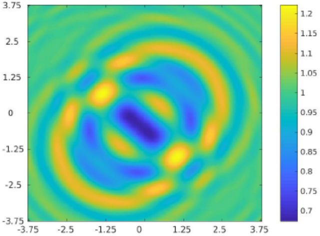
Simulation (MS)



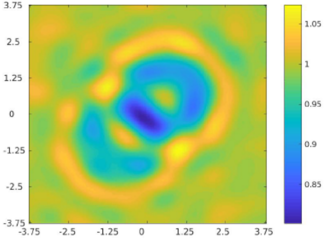
Simulation (LSE, HG)



Experimental



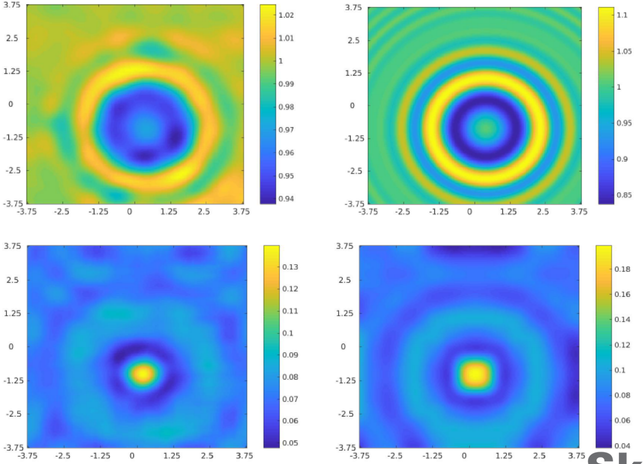
Simulation (LSE, HG)



Experimental

The Backpropagation

By the backpropagation we mean the backwards (inverse) solution of the Lippmann-Schwinger equation in order to 'focus' the data near the protective glass layer (far away from the sensors).



(a) *The propagation of experimental data.* (b) *The propagation of simulated d*

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Scientific Computing
Lecture 5

Part 5: Cauchy problem for Elliptic equation example

Nikolay Koshev, Nikolay Yavich

October 14, 2021

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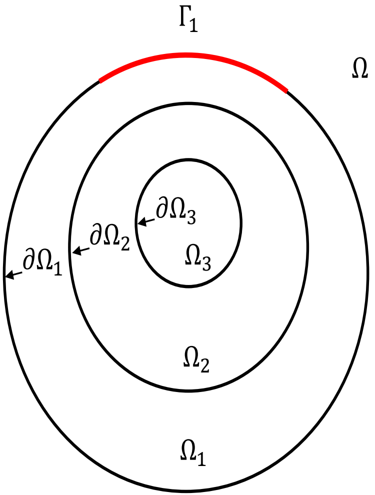
Source localization with data mapping

The EEG Cauchy problem (Data mapping): the domain



- **Notations:**
  - $\Omega \subset \mathbb{R}^3$ - the whole domain.
  - Ω_k, $k = 1, .., N_\Omega - 1$ - the outer 'sourceless' domains ($\sigma(\Omega_k) = \sigma_k = const$).
  - Ω_{N_Ω} - the inner domain containing sources ($\sigma(\Omega_{N_\Omega}) = \sigma_{N_\Omega} = const$)
  - The accessible part of the boundary

$$\Gamma_k = \begin{cases} \Gamma_1, & k = 1 \\ \partial\Omega_k, & k \geq 2. \end{cases}$$

  - The rest of the boundary: Π_k.
- **Assumptions:**
  - Current density volumetric distribution is non-zero only in the inner domain: $\mathbf{J}$: $supp(\mathbf{J}) \in \Omega_{N_\Omega}$
  - Conductivities: $\sigma_k \ll \sigma_{N_\Omega}$, $k = 1, \ldots, N_\Omega - 1$.

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Data mapping: the Cauchy problem

Assume the function $u(\mathbf{x}), \quad \mathbf{x} \in \Pi_1 \subset \partial\Omega_1$ *to be known. Find the function* $U(\mathbf{x}), \quad \mathbf{x} \in \Omega_1$, *such that:*

$$\begin{aligned} \Delta U = 0, &\quad \mathbf{x} \in \Omega_1; \\ U(\mathbf{x}) = u(\mathbf{x}), &\quad \mathbf{x} \in \Gamma_1; \\ \frac{\partial U}{\partial \mathbf{n}}(\mathbf{x}) = g(\mathbf{x}), &\quad \mathbf{x} \in \Gamma_1, \end{aligned}$$

where

$$g(\mathbf{x}) = \begin{cases} 0, & \Gamma_1 \subset \partial\Omega, \\ \frac{\sigma_1}{\sigma_2}\mathbf{n} \cdot \nabla U(\mathbf{x}), & \Gamma_1 \subset \partial\Omega_2. \end{cases}$$

Whenever the function $U(\mathbf{x})$ is found at every point $\mathbf{x} \in \Omega_1$, we obviously have the potential on the rest of a boundary $\Pi_1 = \partial\Omega_1 n \Gamma_1$.

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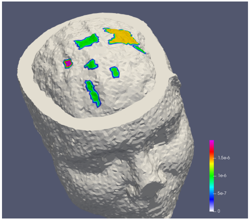
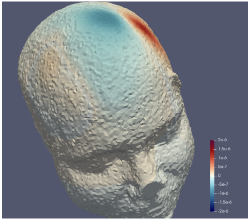
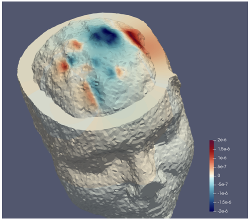
Numerical results: regular currents



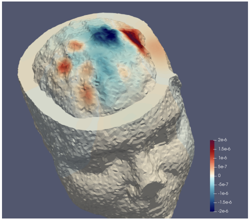
The sources



Potential on the scalp

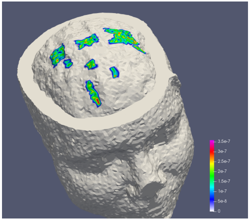


Real potential (brain)

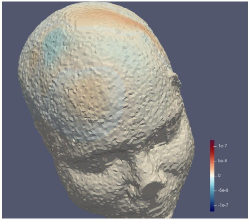


Reconstruction result

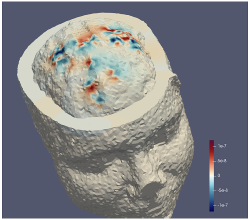
Numerical results: Random currents in each point



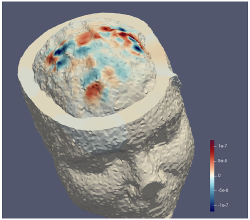
The sources



Potential on the scalp



Real potential (brain)



Reconstruction result

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The algorithm. Let

- Create the FEM mesh allowing to assign appropriate number N_d of subdomains $\Theta_i, i = 1, ..., N_d$
- Solve the Cauchy problem (**??**) for $i = 1$ in order to obtain the function U_1
- For $i = 2, ..., N_d$ do the following:
  - Calculate U_i solving the Cauchy problem (**??**)
  - Calculate the number $e_i = ||U_{i-1} - U_i||_{L^2(\Theta_{i-1})}$
- Find the index i in which $e_i - e_{i-1} > l$, where $l > 0$ is some number, chosen, for example, as a mean value over e_i
- The index $i \equiv s$ due to the consideration above.

The results

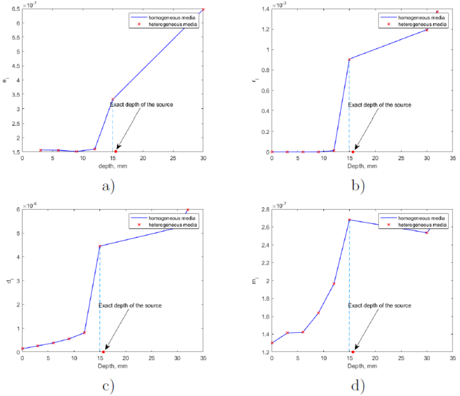

Figure 7: Dependencies on the depth of: a) e_i , b) - relative residual r_i; c) norm of Laplacian of the numerical solution l_i, and d) maximum absolute values of the potential m_i