Scientific Computing Lecture 5

Discretization Nikolay Koshev, Nikolay Yavich October 14, 2023



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Structure of the lecture

- Introduction
- Finite Differences Method (FDM)
- Finite Elements Method (FEM)
- Galerkin approach
- **EXAMPLE:** 3D Cauchy problem for elliptic equation



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Part 1: Introduction October 14, 2023

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Why do we need to descretize the problem?

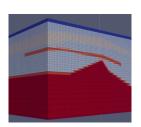
- Generally, the solution of complex problem could be rarely found analytically; and, if if could, you don't need a computer...
- The continuous function f(x) is defined for the infinite number of points
- ► From the point of view of computer, it seems an infinite-dimensional vector
- Having only two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



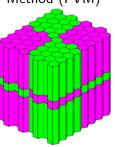
Macroscopic approaches

Three main approaches for macroscopic problems:

Finite Difference Method (FDM)



Finite Volume Method (FVM)



Finite Element Method (FEM)

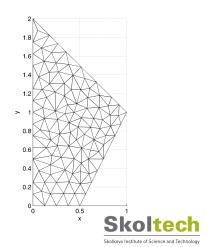




The computational domain: $\Omega \subset \mathbb{R}^n$, n=2 or n=3. The boundary: $\partial \Omega$: the boundary of computational domain;

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

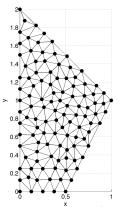
Cover the computational domain with some mesh.



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

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



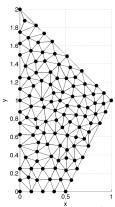


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- Cover the computational domain with some mesh.
- Define the locations of known and unknown variables.
- Construct the system of equations to solve numerically:

$$Au_h=g$$
.

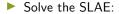




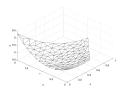
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$$u_h = A^{-1}g$$

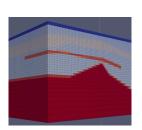




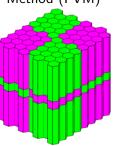
Macroscopic approaches

Three main approaches for macroscopic problems:

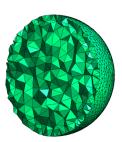
Finite Difference Method (FDM)



Finite Volume Method (FVM)



Finite Element Method (FEM)





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Part 4: Discretization. Finite differences.
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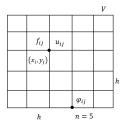
FDM: The mesh

- lacksquare 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.
- $x_n = (x_{n_1}^1, x_{n_2}^2, ..., x_{n_r}^r); n_i = 0, ..., N_i 1,$ where N_i is a number of nodes at *i*-th dimension.
- For example, for r = 3, the nodes will be denoted as: $x_{ijk}, i = 0, ..., N_x 1, j = 0, ..., N_y 1, k = 0, ..., N_k 1$.
- ▶ 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} .

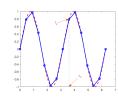


FDM: The uniform mesh

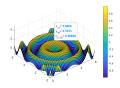
Uniform mesh: $x_n = (n_1 h_1, n_2 h_2, ..., n_r h_r).$



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 $x_i = i/N, y_j = j/N, N = 50$.



FDM: Approximations with a uniform mesh

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:

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

► The same is for other variables;



FDM: Higher derivatives approximation illustration

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

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

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

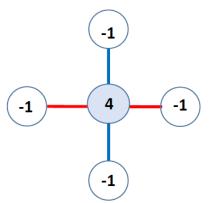
- ▶ The boundary conditions mean we can exclude variables u_{ij} for indices i, j belonging to the boundary, changing them with correspondent values φ_{ij} .
- The scheme has a square matrix: easy to see that indices vary such that $i=1,...,N_i-2, j=1,...,N_j-2$, which means $(N_i-2)*(N_j-2)$ equations.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



The Cross

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

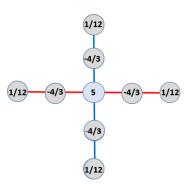
$$-u_{i-1,j} - u_{i+1,j} + 4u_{ij} - u_{i,j-1} - u_{i,j+1} = h^2 f_{ij}$$



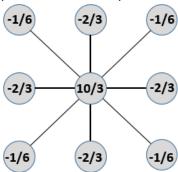


Higher order FDM schemes

Fourth order scheme



Fourth order compact scheme (Numerov's scheme)



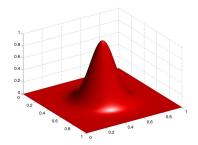


Non-uniform meshes: example

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

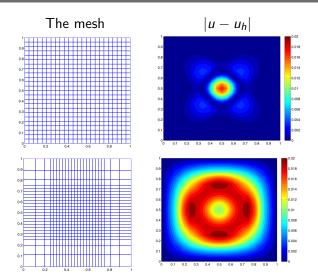
$$u = \varphi, \quad \text{in}\Gamma.$$

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





Non-uniform meshes: example

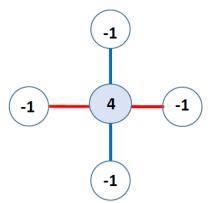




The Cross

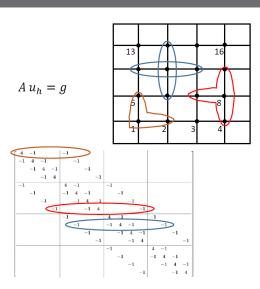
The Cross template consists of five nodes. If the steps $h_x = h_y = h$ (the most often case):

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





The structure of SLAE





The structure of SLAE

$$\mathbf{A} = \begin{bmatrix} \mathbf{C} & -\mathbf{E} & & & & \\ -\mathbf{E} & \mathbf{C} & -\mathbf{E} & & & \\ & -\mathbf{E} & \mathbf{C} & -\mathbf{E} & & \\ & & -\mathbf{E} & \mathbf{C} & \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} \mathbf{4} & -\mathbf{1} & & & \\ -\mathbf{1} & \mathbf{4} & -\mathbf{1} & & \\ & -\mathbf{1} & \mathbf{4} & -\mathbf{1} & \\ & & -\mathbf{1} & \mathbf{4} & -\mathbf{1} \end{bmatrix}$$

4 −1	-1									
-1 4 -1	-1									
-1 4 -1		-1								
-1 4		-1								
-1	4 -1		-1							
-1	-1 4	-1		$^{-1}$						
-1	-1	-1			$^{-1}$					
-1		-1 4				-1				
	-1		4	-1			-1			
	-1		-1	4	$^{-1}$			-1		
		-1		-1	4	-1			-1	
		-1			$^{-1}$	4				-1
			-1				4	-1		_
				-1			-1	4	-1	
					$^{-1}$			-1	4	-1
						-1			-1	4



SLAE: Matrix spectral properties

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):

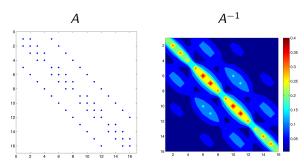
$$\kappa(A) = O\left(\frac{1}{h^2}\right)$$



SLAE: Inverse matrix

- $ightharpoonup H = A^{-1}$ approximates fundamental (Green's) function.
- ▶ H_{ij} solution in the node i with the point source, located in the node i.
- ▶ 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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Part 5: FEM discretization Nikolay Koshev October 14, 2023



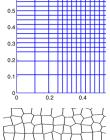
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The motivation

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



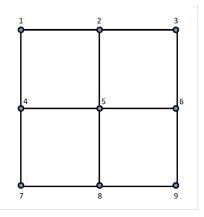








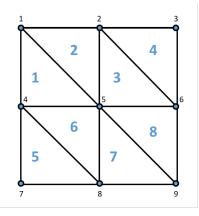
The FEM mesh notations



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



The FEM mesh notations



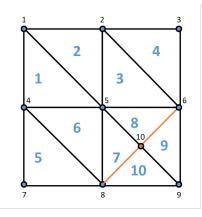
- The number of nodes: N (here N = 9);
- The nodes: $\mathbf{x}_i \in \mathbb{R}^d$, for i = 0, ..., N 1.
- ► The Mesh Cell (Triangle, tetrahedron, etc.):

$$K_i, 0 = 1, ..., N_e - 1$$

The number of mesh cells: N_e (here $N_e = 8$);



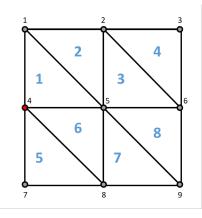
The FEM mesh notations



- 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.



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:

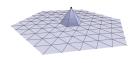
$$\varphi_i(\mathbf{x}) = \begin{cases} 1, & \text{at } i\text{-th node} \\ 0, & \text{at other nodes} \end{cases}$$

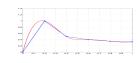
- Each basis function is connected to the node: $\varphi_j(\mathbf{x}), j=0,...,N-1$.
- The basis functions being sometimes called **Elements**



FEM approximation







▶ The function u(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:

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



The weak formulation

Let *F* be a Hilbert space. The equation to be solved:

$$Au = f$$
, $u, f \in F, A : F \rightarrow F$.

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

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

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

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

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

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

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

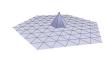
- 4 Solve the system above.
- 5 Profit!

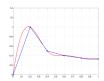


Kinds of Finite Elements

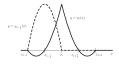
Linear elements:







Quadratic elements:



- ► Bicubic, exponential, etc.
- Since v ∈ 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:

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

► The Neumann boundary condition:

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



3D EEG modelling: the weak formulation

The weak formulation of the problem

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

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

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

Finally, the weak formulation takes the form:

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



3D EEG modelling: the discretization

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

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

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:

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

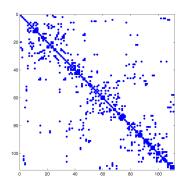
for i, j = 0, 1, ..., N - 1. Thus,

- $ightharpoonup ilde{A}.shape = (N, N), and$
- **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 **b** depends on distribution J(x).



Properties of the matrix

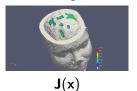
- Square matrix
- ► Sparse and symmetric

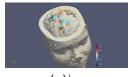




The system properties and methods

- ► 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.









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Galerkin approach, Nikolay Koshev October 14, 2023



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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:

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

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:

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



- ► 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*:

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

- Assume $u \in U$, $D: U \to V$, where U, V are some Hilbert spaces.
- Let $\{\varphi_i(\mathbf{x})\}, i = 1, ...$ 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:

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

- Assume $u \in U$, $D: U \rightarrow V$, where U, V are some Hilbert spaces.
- ▶ Let $\{\varphi_i(\mathbf{x})\}, i = 1, ...$ be some basis in U.
- \triangleright Chose finite number N and approximate the solution u
- \triangleright Since N is finite, and u_a is only the approximation, we get:

$$D\left(\sum_{i=1}^{N}a_{i}\varphi(\mathbf{x})\right)+Du_{0}=R(a_{1},...,a_{n},\mathbf{x}).$$



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

$$Du = 0$$
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- Assume $u \in U$, $D: U \to V$, where U, V are some Hilbert spaces.
- ▶ Let $\{\varphi_i(\mathbf{x})\}, i = 1, ...$ be some basis in U.
- ightharpoonup Chose finite number N and approximate the solution u
- Since N is finite, and u_a is only the approximation, we get the residual $R(a_1, ..., a_n, \mathbf{x})$
- ▶ 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.

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

The weak formulation:

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

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:

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

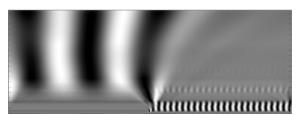


Continuous Wavelet Transform

With the wavelet 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:

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

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

$$u(x) = C \int_{\mathbb{R}^2} \frac{1}{a^2} U(a, b) exp\left(i\frac{t-b}{a}\right) dbda$$

In discrete case:

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

▶ 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:

- $ightharpoonup V_j \subset V_{j+1}$
- ▶ The single-scaling function φ 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!

