Electrostatic PDEs via Finite Elements*

Industrial Strength $\neq$ Finite Differences

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Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

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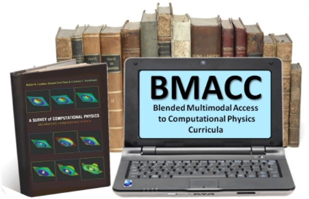
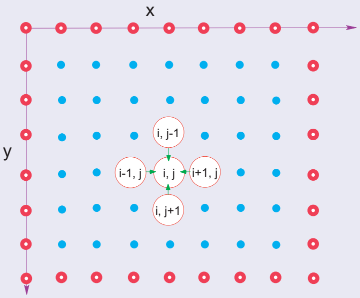
Course: **Computational Physics II**



Finite-Element Method (FEM)

Divide Space into Elements; Approximate Solution on Each

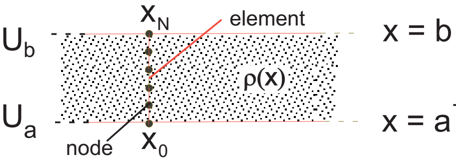


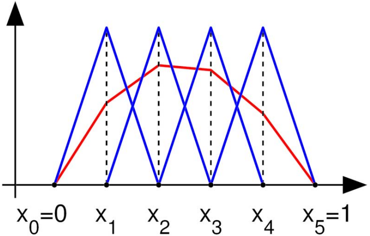
- Finite Difference: how approximate derivatives
- FEM: solution on elements

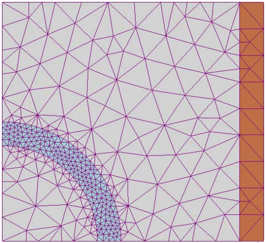
- Match element edges
- Active development, ||
- ↑ convergence, robust, precision
- Flexible, variable domains
- FEM: ↓ computer time
- FEM: ↑ analysis
- Not just “on” grid

Sample 1-D Basis & 2-D Elements (Wikipedia)

1-D elements, 1-D Elemental Solutions



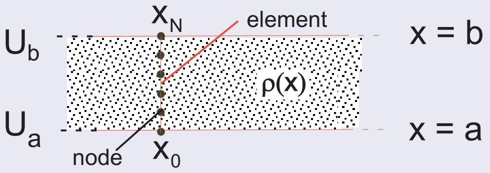




2-D

Electric Field $V(x)$ from Charge Density = ?

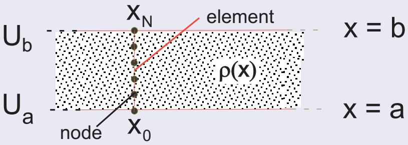
2 Conducting Plates



- Solve Poisson Equation $\frac{d^2U(x)}{dx^2} = -4\pi\rho(x) = -1$
- BC: $U(x = a = 0) = 0, \quad U(x = b = 1) = 1$
- Analytic solution: $U(x) = \frac{x}{2}(3 - x) \quad \surd$

Finite Element Method

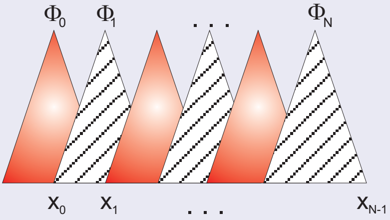
Analytic + Numeric

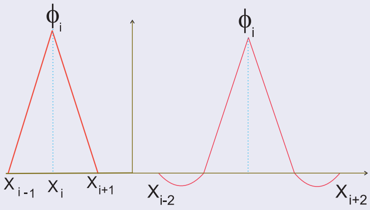


- Split domain into subdomains = *elements*
- Lines = subdomains, Dots = nodes x_i
- Hypothesize trial solution in subdomain
- Global fit trial solution to exact (matching subdomains)
- Via PDE weak form $\equiv$ min $\int$ (approximate - exact)
- Implement BC, Solve linear equations

Approximate Subdomain Solutions $\phi_i(x)$

Solution on Element = Basis





- Overlapping elemental solutions $\phi_i(x)$
- Essentially basis functions
- Elements cover space
- $\phi_i(x)$ within 1 element

- Left: Piecewise-linear
- Right: -quadratic
- Match ϕ_is together
- 1-D elements: lines
- 2-D: rectangles, triangles

Weak Form of PDE (Global Best Fit)

$U(x)$ = Solution: $-\frac{d^2U(x)}{dx^2} = 4\pi\rho(x)$

- Best possible global agreement with exact
- Assume *basis* $\Phi(a) = \Phi(b) = 0$, adjust for BC later
- Convert to integral/weak form, ODE $\times\Phi$, integrate by parts

$$-\frac{d^2U(x)}{dx^2}\Phi(x) = 4\pi\rho(x)\Phi(x) \quad (1)$$

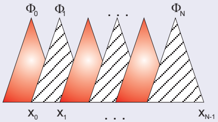
$$-\frac{dU(x)}{dx}\Phi(x)\,\Big|_a^b + \int_a^b dx\,\frac{dU(x)}{dx}\Phi'(x) = \int_a^b dx\,4\pi\rho(x)\,\Phi(x) \quad (2)$$

$$\Rightarrow \quad \int_a^b dx\,\frac{dU(x)}{dx}\Phi'(x) = \int_a^b dx\,4\pi\rho(x)\,\Phi(x) \quad (3)$$

Spectral Decomposition of Solution $U(x)$ (Galerkin)

Hat Basis: Linear Interpolation of $U(nodes)$

$$U(x) \simeq \sum_{j=0}^{N-1} \alpha_j \, \phi_j(x) \qquad (1)$$

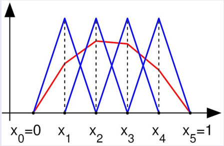


- ϕ_i: elemental solution =??
- α_j = ?
- Simple: Piecewise-cont
- $\phi_i(A, B) = 0$, otherwise

$$\phi_i(x) = \begin{cases} \frac{x - x_{i-1}}{h_{i-1}}, & \text{for } \; x_{i-1} \le x \le x_i, \\ \frac{x_{i+1} - x}{h_i}, & \text{for } \; x_i \le x \le x_{i+1}, \end{cases} \qquad (h_i = x_{i+1} - x_i) \qquad (2)$$

- $\phi_i(x_i) = 1 \;\; \Rightarrow \alpha_i = U(x_i)$ (nodes)

$$U(x) \simeq \sum_{j=0}^{N-1} U(x_j)\phi_j(x) \qquad (3)$$



Determine α_j via Linear Equations

$U(x) \;\simeq\; \sum \alpha_j\, \phi_j(x) = \sum \alpha_j\, U(x_{node})$

- Sub $U(x)$, $\Phi(x) = \phi_i$ into integral Poisson Eq:

$$\int_a^b dx \sum_{j=0}^{N-1} \alpha_j \frac{d\phi_j(x)}{dx} \frac{d\phi_i}{dx} = \int_a^b dx\, 4\pi\rho(x)\phi_i(x), \qquad i = 0, N-1 \quad (1)$$

- $\Rightarrow$ N linear equations for α_j's

$$\alpha_0 \int_a^b \phi_i' \phi_0'\, dx + \alpha_1 \int_a^b \phi_i' \phi_1'\, dx + \cdots + \alpha_{N-1} \int_a^b \phi_i' \phi_{N-1}'\, dx$$

$$= \int_a^b 4\pi\rho\phi_i\, dx, \quad i = 0, N-1 \qquad (2)$$

- ϕ_i = known hat functions $\Rightarrow \int \phi_i' \phi_{N-1}'\, dx = h_i$ = known

As Matrix Equations for α_j

Stn Form: Stiffness Matrix **A**, Unknown Load Vector **y**

$$\mathbf{A}\,\mathbf{y} = \mathbf{b} \tag{1}$$

$$\mathbf{y} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \ddots \\ \alpha_{N-1} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} \int_{x_0}^{x_1} dx\, 4\pi\rho(x)\phi_0(x) \\ \int_{x_1}^{x_2} dx\, 4\pi\rho(x)\phi_1(x) \\ \ddots \\ \int_{x_{N-1}}^{x_N} dx 4\pi\rho(x)\phi_{N-1}(x) \end{pmatrix} \tag{2}$$

$$\mathbf{A} = \begin{pmatrix} \frac{1}{h_0} + \frac{1}{h_1} & -\frac{1}{h_1} & -\frac{1}{h_0} & 0 & \cdots \\ -\frac{1}{h_1} & \frac{1}{h_1} + \frac{1}{h_2} & -\frac{1}{h_2} & 0 & \cdots \\ \ddots & \ddots & -\frac{1}{h_{N-1}} & -\frac{1}{h_{N-2}} & \frac{1}{h_{N-2}} + \frac{1}{h_{N-1}} \end{pmatrix}$$

- **A**: known, no Δ with ρ, **b**: known analytic or quadrature

Impose Dirichlet (Function) Boundary Conditions

$\phi_{ends} = 0 \;\Rightarrow U_{ends} = 0$

- $\phi_N(x)$ satisfies homogeneous eq (Laplace) $\nabla^2 \phi_N = 0$
- Add particular solution to satisfy BC @ A (B later)

$$U(x) = \sum_{j=0}^{N-1} \alpha_j \phi_j(x) + U_a \phi_N(x)$$

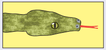
- Sub $U(x) - U_a\phi_N(x)$ into weak form (homo BC):

$$\mathbf{A} = \begin{pmatrix} A_{0,0} & \cdots & A_{0,N-1} & 0 \\ & \ddots & & \\ A_{N-1,0} & \cdots & A_{N-1,N-1} & 0 \\ 0 & 0 & \cdots & 1 \end{pmatrix}, \quad \mathbf{b}' = \begin{pmatrix} b_0 - A_{0,0} U_a \\ \ddots \\ b_{N-1} - A_{N-1,0} U_a \\ U_a \end{pmatrix}$$

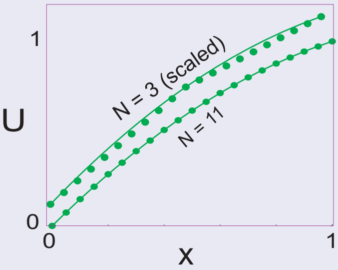
$$b'_i = b_i - A_{i,0} U_a, \quad i = 1, \dots, N-1, \quad b'_N = U_a$$

Implementation

LaplaceFEM.py CODE

- Solve $\mathbf{A}\mathbf{y} = \mathbf{b}'$
- 1-D: $\sim$ 100–1000 eqs
- 3-D: $\sim$ millions
- Number of calcs $\sim N^2$
- $\Rightarrow$ keep N small
- 

• 3 elements (dots) poor



• $N = 11$ excellent

FEM Exercise

1. Examine solution for $a = 0, \quad b = 1, \quad U_a = 0, \quad U_b = 1$
2. Compare piecewise-quadratic basis
3. Solve $3 \le N \le 1000$ elements
4. Check stiffness matrix $\mathbf{A}$ triangular
5. Verify accuracy of integrations in load vector $\mathbf{b}$
6. Verify solution of $\mathbf{A}\mathbf{y} = \mathbf{b}$
7. Plot $U(x)$; $N = 10, 100, 1000$; compare analytic

$$\#\text{ Rel error} = \log_{10} \frac{1}{b-a} \int_a^b dx \left| \frac{U_{\mathrm{FEM}}(x) - U_{\mathrm{exact}}(x)}{U_{\mathrm{exact}}(x)} \right|$$

8. Plot error *versus* x, $N = 10, 100, 1000$