Week 8 (July 27th-July 31st)

Lecturer: Richard Zhang *Scribes: Richard Zhang*

As we have seen in the last lecture, finite difference is a starting point but is quite inconvenient when it comes to non-rectangular boundaries and/or discontinuous boundary conditions. We would need a much more flexible method.

Finite element method is a vast class of numerical method in solving engineering and and mathematical physics problems. Compared with the finite difference method, it has its advantage in

- Accurate representation of complex geometric domain
- Easy representation of global solutions
- Capture of local structure effect

We shall first study the finite element method in $1D$

8.1 Finite Element Method in $1D$

As before, we start with the $1D$ Poisson's equation

$$-\frac{d^2u(x)}{dx^2} = f(x) \tag{8.1}$$

$$u(0) = a \tag{8.2}$$

$$u(1) = \beta \tag{8.3}$$

We first need to redefine what it means for a function u to satisfy the equation

8.1.1 The Weak Form

Classically, the meaning of the equation above is that we would like to find a function u whose second derivative is equal to $f(x)$ at any point x within the domain and who is equal to a at $x = 0$ and b at $x = 1$. However, often time this is just not possible. We have seen before that when $f(x) = \delta(x)$, the solution is not differentiable at $x = 0$. However, that is just one point. Shall we reject the entire solution and say that the equation does not have a solution just because of a single point? Probably not. So we need to redefine what it means to satisfy the differential equation above.

For now we assume that $a = \beta = 0$, whence we can define the weak form

Definition 8.1 *u is called the weak solution to the problem above if for any infinitely smoothly functions v such that $v(0) = v(1) = 0$,*

$$\int_0^1 u'v' = \int_0^1 fv \tag{8.4}$$

v is also called a C^∞ function. The motivation of the weak solution comes from the following algebra. If we multiply both sides of the equation by any C^∞ function, v, and integrate over the domain, we have that

$$\int_0^1 -v\frac{d^2u(x)}{dx^2}dx = \int_0^1 f(x)v(x)dx \tag{8.5}$$

$$\tag{8.6}$$

Performing the integration by parts on u, we have that

$$-v\frac{du}{dx}|_0^1 + \int_0^1 v'(x)\frac{du}{dx}dx = \int_0^1 f(x)v(x)dx \tag{8.7}$$

Since we picked $v(0) = v(1) = 0$, the boundary term vanishes, whence

$$\int_0^1 v'(x)u'(x)dx = \int_0^1 f(x)v(x)dx \tag{8.8}$$

8.1.2 The Basis Function

The crux of the finite element method relies on the assumption that we can write u a a linear combination of basis functions, ie.

$$u(x) = \sum_{i=1}^{N} a_i\phi_i \tag{8.9}$$

We then plug it into the weak formulation and find that

$$\int_0^1 v'\sum_{i=1}^{N} a_i\phi_i' dx = \int_0^1 f(x)v(x)dx \tag{8.10}$$

$$\sum_{i=1}^{N} a_i\int_0^1 v'\phi_i' dx = \int_0^1 f(x)v(x)dx \tag{8.11}$$

Therefore, if I now set $v = \phi_j$, for all $j = 1, ..., N$, we have

$$\sum_{i=1}^{N} a_i\int_0^1 \phi_i'\phi_j' dx = \int_0^1 f(x)\phi_j(x)dx \tag{8.12}$$

This can be then cast into a matrix equation, $Ax = b$, where

$$A_{ij} = \int_0^1 \phi_i'\phi_j' dx \tag{8.13}$$

$$b_j = \int_0^1 f(x)\phi_j(x) \tag{8.14}$$

8.1.3 Linear Basis

To set up the problem, let N be the number of inner nodes of the interval $[0, 1]$, so that $x_0 = 0, x_{N+1} = 1$, while $x_i = ih$, for $i = 1, ..., N$ and $h = 1/(N+1)$. We now define the piece linear function function as the basis vectors. For $j = 1, ..., N$, we define

$$\phi_j(x) = \begin{cases} \frac{x-x_{j-1}}{h}, x \in [x_{j-1}, x_j] \\ -\frac{x-x_{j+1}}{h}, x \in [x_j, x_{j+1}] \\ 0, \text{ otherwise} \end{cases} \tag{8.15}$$

These are also called the "hat function" because of their shapes. Then some algebra shows that

$$\int_0^1 {\phi'_j}^2 dx = \frac{2}{h} \tag{8.16}$$

$$\int_0^1 \phi'_i \phi'_j dx = -\frac{1}{h} \tag{8.17}$$

Hence, the matrix A will look like

$$A_{ij} = \frac{1}{h} \begin{cases} 2, & i = j \\ -1, & |i-j| = 1 \\ 0, & \text{Otherwise} \end{cases} \tag{8.18}$$

This is exactly the same as the second difference matrix.

As an example, suppose $N = 3$. Then we have three basis functions that we call ϕ_1, ϕ_2, ϕ_3, and we can formulate the $3 - by - 3$ matrix A and 3-dimensional vector b so that $Ac = b$ gives the coefficient vector $c \in \mathbb{R}^3$, where

$$A = \frac{1}{h} \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \tag{8.19}$$

$$b = \begin{bmatrix} \int_0^1 f(x)\phi_1(x)dx \\ \int_0^1 f(x)\phi_2(x)dx \\ \int_0^1 f(x)\phi_3(x)dx \end{bmatrix} \tag{8.20}$$

8.1.3.1 Inhomogenous boundary

In case of inhomogeneous boundary conditions, we are faced with

$$-\frac{d^2u(x)}{dx^2} = f(x) \tag{8.21}$$

$$u(0) = a \tag{8.22}$$

$$u(1) = \beta \tag{8.23}$$

where $a, \beta \neq 0$. We define $w(x)$ to be a line that goes through $(0, a)$ and $(1, \beta)$, namely

$$w(x) = (\beta - a)x + a \tag{8.24}$$

Then if we define $\tilde{u} = u(x) - w(x)$, $\tilde{u}$ would satisfy that

$$-\frac{d^2\tilde{u}}{dx^2} = -\frac{d^2u}{dx^2} - \frac{d^2w}{dx^2} \tag{8.25}$$

$$= f(x) \tag{8.26}$$

$$\tilde{u}(0) = u(0) - w(0) \tag{8.27}$$

$$= 0 \tag{8.28}$$

$$\tilde{u}(1) = u(1) - w(1) \tag{8.29}$$

$$= 0 \tag{8.30}$$

which brings us back to the homogeneous case. Therefore, to solve for u, we just have to apply the machinery from the homogeneous problem before subtracting w to get the final answer.

From here, we can go in several directions, including

- Higher order $1D$ Poisson: rather than having linear basis element, we run it for quadratic, cubic, or higher-degree polynomials Poisson
- Linear basis for $2D$ Poisson's equation with triangular meshes: we can generalize this process $2D$ with triangular meshes
- Linear basis for $2D$ Poisson's equation with rectangular meshes: we can generalize this process for $2D$ Poisson's equation with rectangular meshes
- Higher order basis for $2D$ Poisson's equation
- Linear or higher order basis for $3D$ Poisson's equation

The book does the first bullet point, and we will explore the second bullet point here. You will have a chance to explore the remaining bullets in other courses such as numerical partial differential equations, computational fluid dynamics, computational mechanics, etc.

8.2 Finite Element Method in $2D$

Solving the Poisson's equation in $2D$ is very nontrivial compared with $1D$. The first thing we will need to do is dividing up the domain into meshes, which would support the basis functions.

Suppose for now that we are solving the Poisson's equation with zero boundary conditions, ie.

$$-\Delta u = g \tag{8.31}$$

$$u|_{\partial\Omega} = 0 \tag{8.32}$$

8.2.1 Weak Solution in Higher Dimensions

Definition 8.2 *u is called the weak solution of the system above if for any $v \in \mathbb{C}^\infty$ such that $v|_{\partial\Omega} = 0$*

$$\int_\Omega \nabla u \cdot \nabla v dx dy = \int_\Omega g v dx dy \tag{8.33}$$

The motivation comes from the following calculation. Starting with $\Delta u = g$, we have that, for every smooth function v,

$$-v\Delta u = gv \tag{8.34}$$

$$-\int_\Omega v\Delta u dx dy = \int_\Omega g v dx dy \tag{8.35}$$

The higher dimensional integration by parts comes from the following identity: if v is a scalar and F is a vector, $\nabla \cdot (vF) = \nabla v \cdot F + v\nabla \cdot F$. Now if we let $F = \nabla \cdot u$, we get that

$$\nabla \cdot (v\nabla u) = \nabla u \cdot v + u\Delta u \tag{8.36}$$

In that way,

$$\int_\Omega \nabla \cdot (v\nabla u)dxdy = \int_\Omega \nabla u \cdot vdxdy + \int_\Omega u\Delta udxdy \tag{8.37}$$

By divergence theorem, we have that

$$\int_\Omega \nabla \cdot (v\nabla u)dxdy = \oint_{\partial\Omega} v\nabla u \cdot \hat{n}dS \tag{8.38}$$

However, since we defined $v = 0$ on $\partial\Omega$,

$$\int_\Omega \nabla \cdot (v\nabla u)dxdy = \oint_{\partial\Omega} v\nabla u \cdot \hat{n}dS \tag{8.39}$$

$$= 0 \tag{8.40}$$

whence we have

$$\int_\Omega fvdxdy = -\int_\Omega v\Delta udxdy \tag{8.41}$$

$$\int_\Omega fvdxdy = \int_\Omega \nabla u \cdot \nabla vdxdy \tag{8.42}$$

We can also assume that the solution is a linear combination of different basis functions

$$u(x,y) = \sum_{i=1}^{N} c_i\phi_i(x,y) \tag{8.43}$$

which, upon being plugged in to the weak formulation, becomes

$$\int_\Omega fvdxdy = \sum_{i=1}^{N} \int_\Omega \nabla\phi_i \cdot \nabla vdxdy \tag{8.44}$$

Picking $v = \phi_j$, we have

$$\int_\Omega f\phi_j dxdy = \sum_{i=1}^{N} \left(\int_\Omega \nabla\phi_j \cdot \nabla\phi_i \right) c_i dxdy \tag{8.45}$$

8.2.2 Triangulation

The first step towards solving Poisson using FEM is a proper discretization of the domain. In $1D$, because of its restrictive nature, in $1D$ there aren't a lot of creative ways to discretize the domain. In $2D$, however, the possibilities are endless!

In this lecture, we will focus on triangulating the domain. Triangulating means that we will divide up the domain using triangles. We will consecutively label the following objects

- Nodes
- Edges
- Triangles

See examples

8.2.3 Linear Basis: Pyramid Functions

Once the domain has been triangulated and nodes/edges/triangles established, we can proceed with defining the linear basis functions, ϕ_j, where j runs through all the nodes, $j = 1, ..., N$. The basis functions should enjoy the property of

$$\phi_j(x, y) = \begin{cases} 1, & (x, y) = j^{th} \text{ node} \\ 0, & (x, y) = \text{ neighboring nodes} \end{cases} \tag{8.46}$$

For the linear basis, they should

$$\phi_j(x, y) = ax + by + c \tag{8.47}$$

For instance, if the triangle is defined by $(0, 0), (1, 0)$, and $(0, 1)$, ϕ_j defined at $(0, 0)$ would be

$$\phi_j = 1 - \frac{x}{h} - \frac{y}{h} \tag{8.48}$$

while ϕ_k defined at $(0, 1)$ would be

$$\phi_k = 1 - \frac{x}{h} \tag{8.49}$$

Hence, in this case,

$$\nabla\phi_j = (-1/h, -1/h)^T \tag{8.50}$$
$$\nabla\phi_k = (-1/h, 0)^T \tag{8.51}$$

And hence the corresponding entry, A_{jj},

$$A_{jj} = \int_\Omega \phi_j^2 dxdy \tag{8.52}$$
$$= \int \frac{1}{h^2} dxdy \tag{8.53}$$
$$= \frac{1}{2h^2} \tag{8.54}$$

while A_{jk} would

$$A_{jk} = \int_\Omega \phi_j\phi_k dxdy \tag{8.55}$$
$$= \int_\Omega \frac{1}{h^2} dxdy \tag{8.56}$$
$$= \frac{1}{2h^2} \tag{8.57}$$

etc.

So the algorithms to solving the Poisson's equation is

- Triangulate the domain and label all the edges, nodes, and face information
- Compute the basis functions defined at each node and their gradients
- Fill in the matrix A and b by computing the integration
- Solve $Ac = b$ to get the coefficients.

8.2.4 Non-homogeneous Boundary

Now suppose we are solving Poisson's equation with non-homogeneous boundary conditions, ie.

$$-\Delta u = g, \text{ in } \Omega \tag{8.58}$$
$$u = f, \text{ on } \partial\Omega \tag{8.59}$$

So we define $\tilde{u} = u - f$. Then we observe that

$$-\Delta \tilde{u} = -\Delta u - \Delta f \tag{8.60}$$
$$= g - \Delta f \tag{8.61}$$
$$\tilde{u}|_{\partial\Omega} = u|_{\partial\Omega} - f \tag{8.62}$$
$$= f - f \tag{8.63}$$
$$= 0 \tag{8.64}$$

Which returns to the homogeneous case. So all we need is to solve the homogeneous differential equation involving $\tilde{u}$ before adding f to it, ie.

$$u = \tilde{u} + f \tag{8.65}$$

8.3 Fourier Transform

We know how to accurately represent periodic functions using sines and cosines, or alternatively, complex exponentials. The coefficients of the Fourier series gives us some insight about substantial information retained at different frequencies. This is best illustrated by the Parseval's theorem.

8.3.1 Parseval Theorem

We shall first state the theorem

Theorem 8.3 *Let $f(x)$ have the following Fourier series representation*

$$f(x) = \sum_{i=0}^{\infty} a_n \cos(nx) + \sum_{i=1}^{\infty} b_n \sin(nx) \tag{8.66}$$

Then

$$\int_{-\pi}^{\pi} |f(x)|^2 dx = \pi(2a_0^2 + a_1^2 + a_3^2 + ...) \tag{8.67}$$

The proof is simply by observing that when expanding $f^2(x)$ and taking the integral, the only surviving terms are those of $\cos^2$ and $\sin^2$. All other terms would vanish due to the orthogonality of sin and cos. This is saying that the energy of the function is stored in the energy of the coefficients. Recall that earlier in simple harmonic oscillator, we can also trigger similar waves with different levels of energies.

Here is an application: computing the following sum

$$\sum_{n=1,3,5,...}^{\infty} \frac{1}{n^2} \tag{8.68}$$

To do that, we take the step function $f(x)$ and compute its L^2 norm

$$\int_{-\pi}^{\pi} |f(x)|^2 dx = 2\pi \tag{8.69}$$
$$= \sum_{1,3,5,\ldots}^{\infty} \frac{16}{k^2\pi^2} \tag{8.70}$$
$$\frac{2\pi^3}{16} = \sum_{k=1,3,5,\ldots}^{\infty} \frac{1}{k^2} \tag{8.71}$$

Hence

$$\sum_{k=1,3,5,\ldots}^{\infty} \frac{1}{k^2} = \frac{\pi^3}{8} \tag{8.72}$$

But how about non-periodic function that decays at infinity? Can we get their power structure in some sense? And how do we represent non-periodic functions in general? We will need a tool called the Fourier transform.

Definition 8.4 *Given a rapidly decaying function, $f(x) : \mathbb{R} \to \mathbb{R}$, $f(x)$ enjoys the following relation with $\hat{f}(k) : \mathbb{R} \to \mathbb{R}$:*

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{8.73}$$
$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dk \tag{8.74}$$

The first relation is called the Fourier transform, while the second is called the inverse Fourier transform.

Before we talk about the applications of the Fourier transform, let's do a few examples of the Fourier transforms

8.3.2 Example 1: Box Function

We start with $f(x)$ defined as

$$f(x) = \begin{cases} 1, & -L \le x \le L \\ 0, & |x| > L \end{cases} \tag{8.75}$$

Let's compute the Fourier transform of f

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{8.76}$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-L}^{L} e^{-ikx} dx \tag{8.77}$$
$$= \frac{1}{\sqrt{2\pi}} \frac{e^{-ikx}}{-ik} |_{x=-L}^{x=L} \tag{8.78}$$
$$= \frac{1}{\sqrt{2\pi}} (2\sin(kL)) \tag{8.79}$$
$$= \sqrt{\frac{2}{\pi}} \sin(kL) \tag{8.80}$$

8.3.3 Example 2: Delta function

Now we let $f(x) = \delta(x)$. Then

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx \tag{8.81}$$
$$= \sqrt{\frac{1}{2\pi}} \tag{8.82}$$

Henceforth, we get to the "weird" statement about the delta function, ie.

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} dk \tag{8.83}$$

This is weird because the integral is technically not converging. But it is a useful fact for many physics and engineering applications.

8.3.4 Example 3: Gaussian

Let $f(x) = e^{-ax^2}$, where $a > 0$. We will need to compute

$$\hat{f}(k) = \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx \tag{8.84}$$

Computing this integral is beautiful, and the starting point is computing the following integral

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx \tag{8.85}$$

The way to do it is to first compute I^2

$$I^2 = \left(\int_{-\infty}^{\infty} e^{-x^2} \right)^2 \tag{8.86}$$
$$= \int_{-\infty}^{\infty} e^{-x^2} dx \int_{-\infty}^{\infty} e^{-x^2} dx \tag{8.87}$$

Recall that in this case, x is a dummy variable. Therefore, we can just as well replace it by y and get that

$$I^2 = \int_{-\infty}^{\infty} e^{-x^2} dx \int_{-\infty}^{\infty} e^{-y^2} dy \tag{8.88}$$

But then we can put everything into one double integral

$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-x^2} e^{-y^2} dxdy \tag{8.89}$$
$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dxdy \tag{8.90}$$

This is a double integral in Cartesian coordinate. Let's switch to the polar coordinate to make things better.

- In the polar coordinate, $x^2 + y^2 = r^2$
- $dxdy = rdrd\theta$

- The bounds of integration becomes: r goes from 0 to ∞, while θ goes from 0 to 2π

Hence, I^2 becomes

$$I^2 = \int_0^{2\pi} \int_0^{\infty} e^{-(r^2)} r dr d\theta \tag{8.91}$$

A $u-$substitution will have $u = r^2$ and $rdr = du/2$, and so

$$\begin{aligned} I^2 &= \int_0^{2\pi} \int_0^{\infty} e^{-(r^2)} r dr d\theta &(8.92)\\ &= \pi &(8.93) \end{aligned}$$

Hence, $I = \sqrt{\pi}$. Now using a variable substitution, it is not hard to see that

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \tag{8.94}$$

Now let's compute the Fourier transform of e^{-ax^2}.

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx \tag{8.95}$$

To do this, we are going to recall a trick we learned in high school called "completing the square". Essentially, if we know that $(a-b)^2 = a^2 - 2ab + b^2$, we can get $a^2 - ab$ into something similar using

$$\begin{aligned} a^2 \pm ab &= a^2 \pm \frac{2ab}{2} &(8.96)\\ &= a^2 \pm 2(a)\left(\frac{b}{2}\right) + \left(\frac{b}{2}\right)^2 \pm \left(\frac{b}{2}\right)^2 &(8.97)\\ &= \left(a \pm \frac{b}{2}\right)^2 \pm \frac{b^2}{4} &(8.98) \end{aligned}$$

If we look at the exponent of the integrand, we see that

$$-ax^2 - ikx = -a(x^2 + x(ik/a)) \tag{8.99}$$

Hence if we let $a = x$ and $b = ik/a$, we see that

$$-ax^2 - ikx = -a((x + ik/(2a))^2 - (ik/a)^2/4) \tag{8.100}$$

Hence we know that

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ax^2} e^{ikx} dx &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a((x+ik/(2a))^2 - (ik/a)^2/4)} dx &(8.101)\\ &= \frac{e^{-(k^2/(4a))}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a((x+ik/(2a))^2)} dx &(8.102) \end{aligned}$$

Since we are sweeping across the entire real line, the shift on x does not really matter. Hence, we can write that

$$\begin{aligned} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ax^2} e^{ikx} dx &= \frac{e^{-(k^2/(4a))}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ax^2} dx &(8.103)\\ &= \frac{e^{-\frac{k^2}{4a}}}{\sqrt{2a}} &(8.104) \end{aligned}$$