

Notes for Lectures 10 & 11

Introduction to grid-based methods for solving Poisson and Laplace Equations

Finite difference methods

The basis for grid-based finite difference methods is a Taylor's series expansion:

$$\Phi(\mathbf{r} + \mathbf{u}) = \Phi(\mathbf{r}) + \mathbf{u} \cdot \nabla \Phi(\mathbf{r}) + \frac{1}{2!}(\mathbf{u} \cdot \nabla)^2 \Phi(\mathbf{r}) + \frac{1}{3!}(\mathbf{u} \cdot \nabla)^3 \Phi(\mathbf{r}) + \frac{1}{4!}(\mathbf{u} \cdot \nabla)^4 \Phi(\mathbf{r}) + \dots \quad (1)$$

We will work out some explicit formulae for a 2-dimensional regular grid with h denoting the step length. For the 2-dimensional Poisson equation we have

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Phi(x, y) = -\frac{\rho(x, y)}{\epsilon_0}. \quad (2)$$

We note that a sum of 4 surrounding edge values gives:

$$\begin{aligned} S_A &\equiv \Phi(x+h, y) + \Phi(x-h, y) + \Phi(x, y+h) + \Phi(x, y-h) \\ &= 4\Phi(x, y) + h^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Phi(x, y) + \frac{h^4}{12} \left(\frac{\partial^4}{\partial x^4} + \frac{\partial^4}{\partial y^4} \right) \Phi(x, y) + (h^6 \dots). \end{aligned} \quad (3)$$

Similarly, a sum of 4 surrounding corner values gives:

$$\begin{aligned} S_B &\equiv \Phi(x+h, y+h) + \Phi(x-h, y+h) + \Phi(x+h, y-h) + \Phi(x-h, y-h) \\ &= 4\Phi(x, y) + 2h^2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Phi(x, y) + \frac{h^4}{6} \left(\frac{\partial^4}{\partial x^4} + \frac{\partial^4}{\partial y^4} + 6 \frac{\partial^2}{\partial x^2} \frac{\partial^2}{\partial y^2} \right) \Phi(x, y) + (h^6 \dots). \end{aligned} \quad (4)$$

We note that we can combine these two results into the relation

$$S_A + \frac{1}{4}S_B = 5\Phi(x, y) + \frac{3h^2}{2}\nabla^2\Phi(x, y) + \frac{h^4}{8}\nabla^2\nabla^2\Phi(x, y) + (h^6 \dots). \quad (5)$$

This result can be written in the form;

$$\Phi(x, y) - \frac{1}{5}S_A - \frac{1}{20}S_B = \frac{3h^2}{10\epsilon_0}\rho(x, y) + \frac{h^4}{40\epsilon_0}\nabla^2\rho(x, y). \quad (6)$$

In general, the right hand side of this equation is known, and most of the left hand side of the equation, except for the boundary values are unknown. It can be used to develop a set of linear equations for the values of $\Phi(x, y)$ on the grid points.

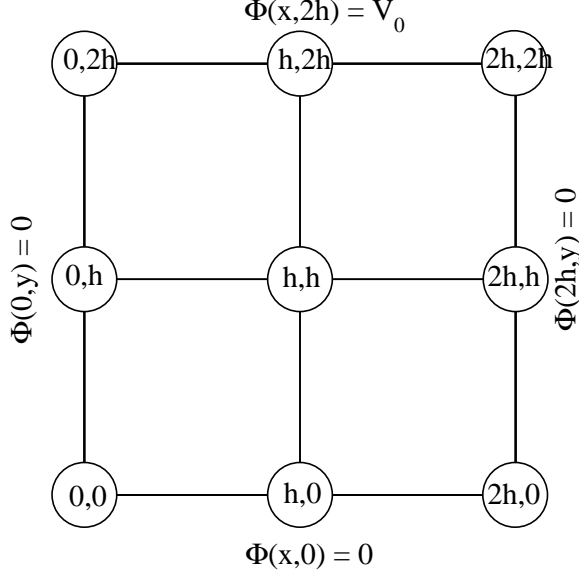


Figure 1: 3×3 grid for solution of the Poisson equation within a 2-dimensional square.

For example, consider a solution to the Laplace equation in the square region $0 \leq x \leq a$, $0 \leq y \leq a$ which $\Phi(x, 0) = \Phi(0, y) = \Phi(a, y) = 0$ and $\Phi(x, a) = V_0$. We will first analyze this system with a mesh of 9 points generated with a grid spacing of $h = \frac{a}{2}$. In this case, $\Phi(h, h) \equiv \Phi(\frac{a}{2}, \frac{a}{2})$ is unknown, while $\Phi(0, 2h) = \Phi(h, 2h) = \Phi(2h, 2h) = V_0$ and $\Phi(0, 0) = \Phi(h, 0) = \Phi(2h, 0) = \Phi(0, h) = \Phi(h, 2h) = 0$. For this example, Eq. 6 states

$$\Phi_5 = \frac{1}{5}(\Phi(h, 0) + \Phi(0, h) + \Phi(2h, h) + \Phi(h, 2h)) + \frac{1}{20}(\Phi(0, 0) + \Phi(2h, 0) + \Phi(0, 2h) + \Phi(2h, 2h)) = \frac{3}{10}V_0. \quad (7)$$

This results is within 20% of the exact answer of $\Phi(\frac{a}{2}, \frac{a}{2}) = 0.25V_0$. If analyze this same system with the next more accurate grid, $h = \frac{a}{4}$, using the symmetry of the system $\Phi(x, y) = \Phi(a-x, y)$, we have now 6 unknown values $\{\Phi(h, h), \Phi(2h, h), \Phi(h, 2h), \Phi(2h, 2h), \Phi(h, 3h), \Phi(2h, 3h)\}$ and boundary values $\Phi(0, 4h) = \Phi(h, 4h) = \Phi(2h, 4h) = V_0$ and $\Phi(0, 3h) = \Phi(0, 2h) = \Phi(0, h) = \Phi(0, 0) = \Phi(h, 0) = \Phi(2h, 0) = 0$.

This results in the following relations between the grid points:

$$\Phi(h, 3h) - \frac{1}{5}(\Phi(h, 4h) + \Phi(0, 3h) + \Phi(2h, 3h) + \Phi(h, 2h)) - \frac{1}{20}(\Phi(0, 4h) + \Phi(2h, 4h) + \Phi(2h, 2h) + \Phi(0, 2h)) = 0, \quad (8)$$

$$\Phi(2h, 3h) - \frac{1}{5}(\Phi(2h, 4h) + \Phi(3h, 3h) + \Phi(h, 3h) + \Phi(2h, 2h)) - \frac{1}{20}(\Phi(h, 4h) + \Phi(3h, 4h) + \Phi(3h, 2h) + \Phi(h, 2h)) = 0, \quad (9)$$

$$\Phi(h, 2h) - \frac{1}{5}(\Phi(h, 3h) + \Phi(0, 2h) + \Phi(2h, 2h) + \Phi(h, h)) - \frac{1}{20}(\Phi(0, 3h) + \Phi(2h, 3h) + \Phi(0, h) + \Phi(2h, h)) = 0, \quad (10)$$

$$\Phi(2h, 2h) - \frac{1}{5}(\Phi(2h, 3h) + \Phi(h, 2h) + \Phi(3h, 2h) + \Phi(2h, h)) - \frac{1}{20}(\Phi(3h, 3h) + \Phi(h, 3h) + \Phi(3h, h) + \Phi(h, h)) = 0, \quad (11)$$

$$\Phi(h, h) - \frac{1}{5}(\Phi(h, 2h) + \Phi(0, h) + \Phi(2h, h) + \Phi(h, 0)) - \frac{1}{20}(\Phi(0, 2h) + \Phi(2h, 2h) + \Phi(0, 0) + \Phi(2h, 0)) = 0, \quad (12)$$

$$\Phi(2h, 0) - \frac{1}{5}(\Phi(2h, 2h) + \Phi(3h, h) + \Phi(h, h) + \Phi(2h, 0)) - \frac{1}{20}(\Phi(h, 2h) + \Phi(3h, 2h) + \Phi(h, 0) + \Phi(3h, 0)) = 0. \quad (13)$$

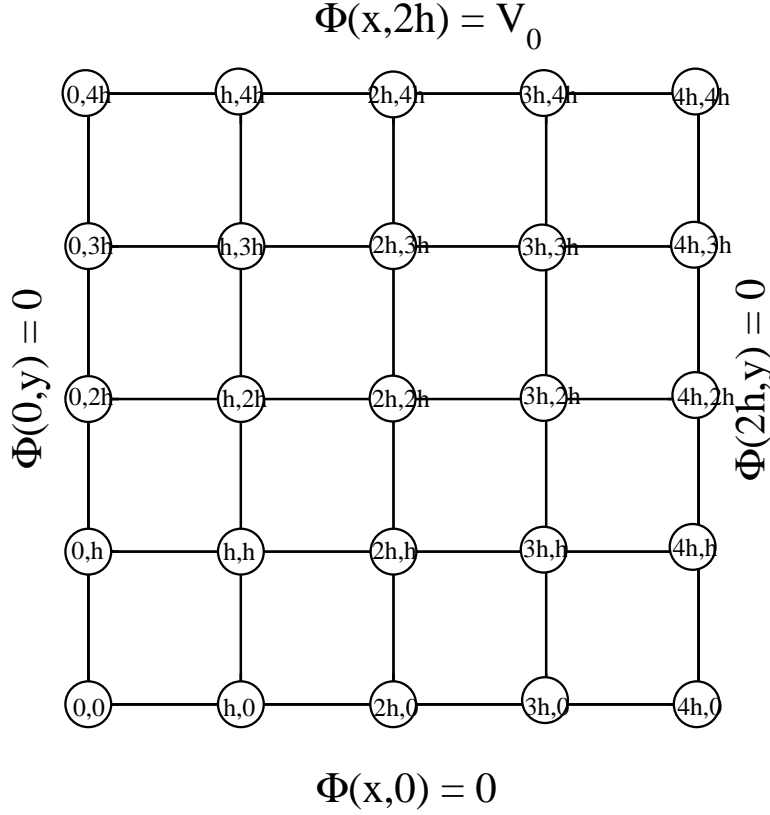


Figure 2: 5×5 grid for solution of the Poisson equation within a 2-dimensional square.

These equations can be cast into the form of a matrix problem which can be easily solved using Maple:

$$\begin{pmatrix} 1 & -1/5 & -1/5 & -1/20 & 0 & 0 \\ -2/5 & 1 & -1/10 & -1/5 & 0 & 0 \\ -1/5 & -1/20 & 1 & -1/5 & -1/5 & -1/20 \\ -1/10 & -1/5 & -2/5 & 1 & -1/10 & -1/5 \\ 0 & 0 & -1/5 & -1/20 & 1 & -1/5 \\ 0 & 0 & -1/10 & -1/5 & -2/5 & 1 \end{pmatrix} \begin{pmatrix} \Phi(h, 3h) \\ \Phi(2h, 3h) \\ \Phi(h, 2h) \\ \Phi(2h, 2h) \\ \Phi(h, h) \\ \Phi(2h, h) \end{pmatrix} = \begin{pmatrix} 3/10 \\ 3/10 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} V_0. \quad (14)$$

The solution to these equations and the exact results are found to be:

$$\begin{pmatrix} \Phi(h, 3h) \\ \Phi(2h, 3h) \\ \Phi(h, 2h) \\ \Phi(2h, 2h) \\ \Phi(h, h) \\ \Phi(2h, h) \end{pmatrix} = \begin{pmatrix} 0.4628135839 \\ 0.5566467694 \\ 0.1920222635 \\ 0.2615955473 \\ 0.07150923611 \\ 0.1001250302 \end{pmatrix} V_0; \text{ (exact)} = \begin{pmatrix} .4320283318 \\ .5405292183 \\ .1820283318 \\ 0.25 \\ .06797166807 \\ .09541411792 \end{pmatrix} V_0. \quad (15)$$

We see that the accuracy has improved considerably with the new mesh.

Introduction to Finite element method

The finite element approach is based on an expansion of the unknown electrostatic potential in terms of known grid-based functions of fixed shape. In two dimensions, using the indices $\{i, j\}$ to reference the grid, we can denote the shape functions as $\{\phi_{ij}(x, y)\}$. The finite element expansion of the potential in two dimensions can take the form:

$$4\pi\epsilon_0\Phi(x, y) = \sum_{ij} \psi_{ij}\phi_{ij}(x, y), \quad (16)$$

where ψ_{ij} represents the amplitude associated with the shape function $\phi_{ij}(x, y)$. The amplitude values can be determined for a given solution of the Poisson equation:

$$-\nabla^2 (4\pi\epsilon_0\Phi(x, y)) = 4\pi\rho(x, y), \quad (17)$$

by solving a linear algebra problem of the form

$$\sum_{ij} M_{kl,ij}\psi_{ij} = G_{kl}, \quad (18)$$

where

$$M_{kl,ij} \equiv \int dx \int dy \nabla\phi_{kl}(x, y) \cdot \nabla\phi_{ij}(x, y) \quad \text{and} \quad G_{kl} \equiv \int dx \int dy \phi_{kl}(x, y) 4\pi\rho(x, y). \quad (19)$$

In obtaining this result, we have assumed that the boundary values vanish. This will be ensured by our choice of the functional form of the shape functions $\phi_{ij}(x, y)$. In order for this result to be useful, we need to be able evaluate the integrals for $M_{kl,ij}$ and for G_{kl} . In the latter case, we need to know the form of the charge density. The form of $M_{kl,ij}$ only depends upon the form of the shape functions. If we take these functions to be:

$$\phi_{ij}(x, y) \equiv \mathcal{X}_i(x)\mathcal{Y}_j(y), \quad (20)$$

where

$$\mathcal{X}_i(x) \equiv \begin{cases} \left(1 - \frac{|x-x_i|}{h}\right) & \text{for } x_i - h \leq x \leq x_i + h \\ 0 & \text{otherwise} \end{cases}, \quad (21)$$

and $\mathcal{Y}_j(y)$ has a similar expression in the variable y . Then

$$M_{kl,ij} \equiv \int dx \int dy \left[\frac{d\mathcal{X}_k(x)}{dx} \frac{d\mathcal{X}_i(x)}{dx} \mathcal{Y}_l(y)\mathcal{Y}_j(y) + \mathcal{X}_k(x)\mathcal{X}_i(x) \frac{d\mathcal{Y}_l(y)}{dy} \frac{d\mathcal{Y}_j(y)}{dy} \right]. \quad (22)$$

There are four types of non-trivial contributions to these values:

$$\int_{x_i-h}^{x_i+h} (\mathcal{X}_i(x))^2 dx = h \int_{-1}^1 (1 - |u|)^2 du = \frac{2h}{3}, \quad (23)$$

$$\int_{x_i-h}^{x_i+h} (\mathcal{X}_i(x)\mathcal{X}_{i+1}(x)) dx = h \int_0^1 (1-u)u du = \frac{h}{6}, \quad (24)$$

$$\int_{x_i-h}^{x_i+h} \left(\frac{d\mathcal{X}_i(x)}{dx}\right)^2 dx = \frac{1}{h} \int_{-1}^1 du = \frac{2}{h}, \quad (25)$$

and

$$\int_{x_i-h}^{x_i+h} \left(\frac{d\mathcal{X}_i(x)}{dx} \frac{d\mathcal{X}_{i+1}(x)}{dx}\right) dx = -\frac{1}{h} \int_0^1 du = \frac{-1}{h}. \quad (26)$$

These basic ingredients lead to the following distinct values for the matrix:

$$M_{kl,ij} = \begin{cases} \frac{8}{3} & \text{for } k = i \text{ and } l = j \\ -\frac{1}{3} & \text{for } k - i = \pm 1 \text{ and/or } l - j = \pm 1 \\ 0 & \text{otherwise} \end{cases} . \quad (27)$$

For problems in which the boundary values are 0, Eq. 18 then can be used to find all of the interior amplitudes ψ_{ij} . In our case, we have the boundary conditions $\Phi(x, 0) = \Phi(0, y) = \Phi(a, y) = 0$ and $\Phi(x, a) = V_0$. Using the same indexing as in Fig. 2, this means that $\Psi(0, 4h) = \Psi(h, 4h) = \Psi(2h, 4h) = V_0$. The finite element approach for this problem thus can be put into the matrix form for analysis by Maple:

$$\begin{pmatrix} 8/3 & -1/3 & -1/3 & -1/3 & 0 & 0 \\ -2/3 & 8/3 & -2/3 & -1/3 & 0 & 0 \\ -1/3 & -1/3 & 8/3 & -1/3 & -1/3 & -1/3 \\ -2/3 & -1/3 & -2/3 & 8/3 & -2/3 & -1/3 \\ 0 & 0 & -1/3 & -1/3 & 8/3 & -1/3 \\ 0 & 0 & -2/3 & -1/3 & -2/3 & 8/3 \end{pmatrix} \begin{pmatrix} \Phi(h, 3h) \\ \Phi(2h, 3h) \\ \Phi(h, 2h) \\ \Phi(2h, 2h) \\ \Phi(h, h) \\ \Phi(2h, h) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} V_0. \quad (28)$$

The solution to these equations and the exact results are found to be:

$$\begin{pmatrix} \Phi(h, 3h) \\ \Phi(2h, 3h) \\ \Phi(h, 2h) \\ \Phi(2h, 2h) \\ \Phi(h, h) \\ \Phi(2h, h) \end{pmatrix} = \begin{pmatrix} 0.5070276498 \\ .5847926267 \\ 0.1928571429 \\ 0.2785714286 \\ 0.07154377880 \\ 0.1009216590 \end{pmatrix} V_0; \text{ (exact)} = \begin{pmatrix} .4320283318 \\ .5405292183 \\ .1820283318 \\ 0.25 \\ .06797166807 \\ .09541411792 \end{pmatrix} V_0. \quad (29)$$

We see that the results are similar to those obtained using the finite difference approach.