Computational physics

Partial Differential Equations

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Partial Differential Equations

- Involving more than one independent variable
- Physisc problems → second-order PDEs
- elliptic, parabolic, or hyperbolic

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PDEs in physics

- General form

$$A\frac{\partial^2 U}{\partial x^2} + 2B\frac{\partial^2 U}{\partial x \partial y} + C\frac{\partial^2 U}{\partial y^2} + D\frac{\partial U}{\partial x} + E\frac{\partial U}{\partial y} = F$$

- Elliptic: $AC - B^2 > 0$
- Laplace's equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv \nabla^2 u(,x,y) \equiv \Delta u(x,y) = 0$$

- Poisson's equation:

$$\nabla^2 u(x,y) = -4\pi\rho(x,y)$$

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PDEs in physics

- Parabolic: $AC - B^2 = 0$
- Heat equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \nabla^2 u(x,y,t) = \alpha\frac{\partial u}{\partial t}$$

- Hyperbolic: $AC - B^2 < 0$
- Wave equation:

$$\nabla^2 u(x,y,t) = -c^2\frac{\partial^2 u}{\partial t^2}$$

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Numerical solutions to elliptic equations

- Elliptic equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

- Taylor expansions of the potential $u(x, y)$ to the right and left of (x, y)

$$u(x - \Delta x, y) = u(x, y) - \frac{\partial u}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}(\Delta x)^2 - \cdots [1]$$

$$u(x + \Delta x, y) = u(x, y) + \frac{\partial u}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}(\Delta x)^2 + \cdots [2]$$

$$\overset{1+2}{\Longrightarrow} \frac{\partial^2 u}{\partial x^2} \approx \frac{u(x + \Delta x, y) + u(x - \Delta x, y) - 2u(x, y)}{(\Delta x)^2}$$

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Numerical solutions to elliptic equations

- Taylor expansions of the potential $u(x, y)$ to the right and left of (x, y)

$$u(x, y - \Delta y) = u(x, y) - \frac{\partial u}{\partial y}\Delta y + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}(\Delta y)^2 - \cdots$$

$$u(x, y + \Delta y) = u(x, y) + \frac{\partial u}{\partial y}\Delta y + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}(\Delta y)^2 + \cdots$$

- Adding the two series:

$$\Rightarrow \frac{\partial^2 u}{\partial y^2} \approx \frac{u(x, y + \Delta y) + u(x, y - \Delta y) - 2u(x, y)}{(\Delta y)^2}$$

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Numerical solutions to elliptic equations

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u(x+\Delta x, y) + u(x-\Delta x, y) - 2u(x,y)}{(\Delta x)^2}$$

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{u(x, y+\Delta y) + u(x, y-\Delta y) - 2u(x,y)}{(\Delta y)^2}$$

- Adding the two equations:

$$\Rightarrow \frac{u(x+\Delta x, y) + u(x-\Delta x, y) - 2u(x,y)}{(\Delta x)^2} +$$

$$\frac{u(x, y+\Delta y) + u(x, y-\Delta y) - 2u(x,y)}{(\Delta y)^2} = f(x,y)$$

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Numerical solutions to elliptic equations

- For $\Delta x \equiv h, \Delta y = k$:

$$\frac{u(x+h, y) + u(x-h, y) - 2u(x,y)}{h^2} +$$

$$\frac{u(x, y+k) + u(x, y-k) - 2u(x,y)}{k^2} = f(x,y)$$

$$\Rightarrow 2\left[\frac{h^2}{k^2} + 1\right] u(x,y) - [u(x+h,y) + u(x-h,y)]$$

$$-\frac{h^2}{k^2}[u(x,y+k) + u(x,y-k)] = -h^2 f(x,y)$$

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Numerical solutions to elliptic equations

- For $\Delta x = \Delta y = h$:

$$4u(x,y) - [u(x+h,y) + u(x-h,y)]$$
$$-[u(x,y+h) + u(x,y-h)] = -h^2 f(x,y)$$
$$\Rightarrow 4u(x,y) \approx [u(x+h,y) + u(x-h,y)]$$
$$+[u(x,y+h) + u(x,y-h)] - h^2 f(x,y)$$

- Poisson's equation:

$$4u(x,y) \approx u(x+h,y) + u(x-h,y)$$
$$+ u(x,y+h) + u(x,y-h) + h^2 4\pi\rho(x,y)$$

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Numerical solutions to elliptic equations

- Finite-Difference method: $x \to x_i = x_0 + ih$,

$$y \to y_i = y_0 + jk \,;\, i = 0, \dots, n, j = 0, \dots, m$$

$$\Rightarrow 2\left[\frac{h^2}{k^2} + 1\right] u_{ij} - \left[u_{i+1,j} + u_{i-1,j}\right] - \frac{h^2}{k^2}\left[u_{i,j+1} + u_{i,j-1}\right]$$
$$= -h^2 f(x_i, y_j)$$

- with $u_{ij} \equiv u(x_i, y_j)$; $i = 1, \dots, n-1$, $j = 1, \dots, m-1$
- And boundary conditions

$$u_{0j} = g(x_0, y_j), u_{nj} = g(x_n, y_j) \,, j = 0, \dots, m$$
$$u_{i0} = g(x_i, y_0), u_{im} = g(x_i, y_m) \,, i = 0, \dots, n$$

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Numerical solutions to elliptic equations

$h = k$

- Poisson's equation

$$u_{ij} = \frac{1}{4}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right] + h^2 \pi \rho(x_i, y_j)$$

- With boundary conditions

$$u_{0j} = g(x_0, y_j), u_{nj} = g(x_n, y_j)\ , j = 0, \dots, m$$
$$u_{i0} = g(x_i, y_0), u_{im} = g(x_i, y_m)\ , i = 0, \dots, n$$

- This Poisson's equation is equivalent to a system of linear equations! We will use the Gauss-Seidel method to solve it

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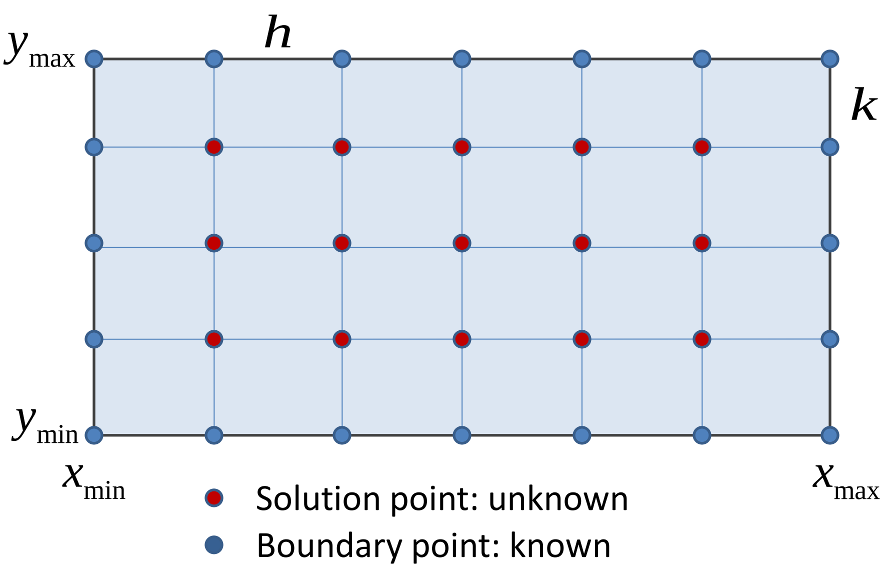
Numerical solutions to elliptic equations



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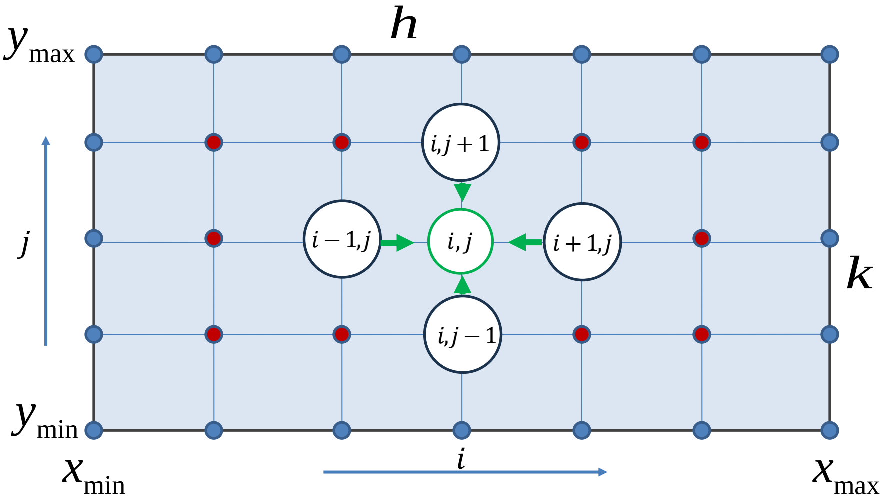
Numerical solutions to elliptic equations



- Solution point: unknown
- Boundary point: known

Jacobi iterative method

- The Jacobi iterative method is obtained by solving the i-th equation in $A\boldsymbol{x} = \boldsymbol{b}$ for x_i to obtain (provided $a_{ii} \neq 0$)

$$x_i = \frac{1}{a_{ii}}\left[\sum_{j=1, j\neq i}^{n} -a_{ij}x_j + b_i\right], i = 1, 2, \dots, n$$

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{cases} \Rightarrow x_i = \frac{1}{a_{ii}}\left[\sum_{j=1, j\neq i}^{n} -a_{ij}x_j + b_i\right]$$

Jacobi iterative method

- For each $k \geq 1$, generate the components $x_i^{(k)}$ ["new"] of $\boldsymbol{x}^{(k)}$ from the components of $\boldsymbol{x}^{(k-1)}$ ["old" / known/ đã biết/ đã có] by

$$x_i^{(k)} = \frac{1}{a_{ii}}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} -a_{ij}x_j^{(k-1)} + b_i\right], i = 1, 2, \ldots, n$$

$$x_i^{(\text{new})} = \frac{1}{a_{ii}}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} -a_{ij}x_j^{(\text{old})} + b_i\right], i = 1, 2, \ldots, n$$

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Gauss-Seidel method

- Jacobi's method

$$x_i^{(k)} = \frac{1}{a_{ii}}\left[-\sum_{j=1}^{n} a_{ij}x_j^{(k-1)} + b_i\right], i = 1,2 \ldots, n$$

- Gauss-Seidel method

$$x_i^{(k)} = \frac{1}{a_{ii}}\left[-\sum_{j=1}^{i-1} a_{ij}x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k-1)} + b_i\right]$$

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Gauss-Seidel Iterative Algorithm

- Step 1: Set $k = 1$ // k: k-th iteration [lần lặp thứ k]
- Step 2: While $(k \leq N)$ do Step 3 -6
  - Step 3: For $i = 1, n$
    Set $x_i = \frac{1}{a_{ii}}\left[-\sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}XO_j + b_i\right]$
  - Step 4: If $\|x - XO\| < \epsilon$ then OUTPUT $x_1, \ldots, x_n$
    STOP
  - Step 5: Set $k = k + 1$
  - Step 6: For $i = 1, n$ set $XO_i = x_i$
- Step 7: OUTPUT "Maximum number of iterations exceeded!"
  STOP (The procedure was unfortunately unsuccessful ☹)

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Numerical solutions to elliptic equations

- Sử dụng PP Gauss-Seidel cho PT Poisson:

$$u_{ij} = \frac{1}{4}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right] + h^2\pi\rho(x_i, y_j)$$

- for $i = 1, \ldots, n-1$; $j = 1, \ldots, m-1$
- Điều kiện biên

$$u_{0j} = g(x_0, y_j), u_{nj} = g(x_n, y_j), j = 0, \ldots, m$$
$$u_{i0} = g(x_i, y_0), u_{im} = g(x_i, y_m), i = 0, \ldots, n$$

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Numerical solutions to elliptic equations

- Sử dụng PP Gauss-Seidel cho PT Poisson:

$$u_{ij}^{(new)} = \frac{1}{4}\left[u_{i+1,j}^{(old)} + u_{i-1,j}^{(new)} + u_{i,j+1}^{(old)} + u_{i,j-1}^{(new)}\right] + h^2\pi\rho(x_i, y_j)$$

- Or

$$u_{ij}^{(k)} = \frac{1}{4}\left[u_{i+1,j}^{(k-1)} + u_{i-1,j}^{(k)} + u_{i,j+1}^{(k-1)} + u_{i,j-1}^{(k)}\right] + h^2\pi\rho(x_i, y_j)$$

- Điều kiện biên

$$u_{0j} = g(x_0, y_j), u_{nj} = g(x_n, y_j)\ , j = 0, \dots, m$$
$$u_{i0} = g(x_i, y_0), u_{im} = g(x_i, y_m)\ , i = 0, \dots, n$$

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Numerical solutions to elliptic equations

- Sử dụng PP Gauss-Seidel cho PT Laplace:

$$u_{ij}^{(new)} = \frac{1}{4}\left[u_{i+1,j}^{(old)} + u_{i-1,j}^{(new)} + u_{i,j+1}^{(old)} + u_{i,j-1}^{(new)}\right]$$

- Or

$$u_{ij}^{(k)} = \frac{1}{4}\left[u_{i+1,j}^{(k-1)} + u_{i-1,j}^{(k)} + u_{i,j+1}^{(k-1)} + u_{i,j-1}^{(k)}\right]$$

- Điều kiện biên

$$u_{0j} = g(x_0, y_j), u_{nj} = g(x_n, y_j)\ , j = 0, \dots, m$$
$$u_{i0} = g(x_i, y_0), u_{im} = g(x_i, y_m)\ , i = 0, \dots, n$$

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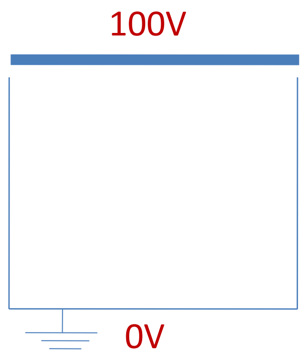
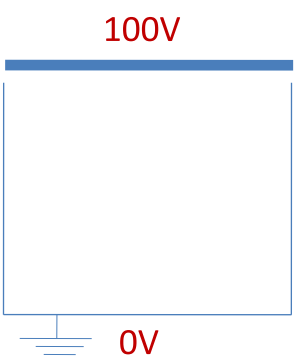
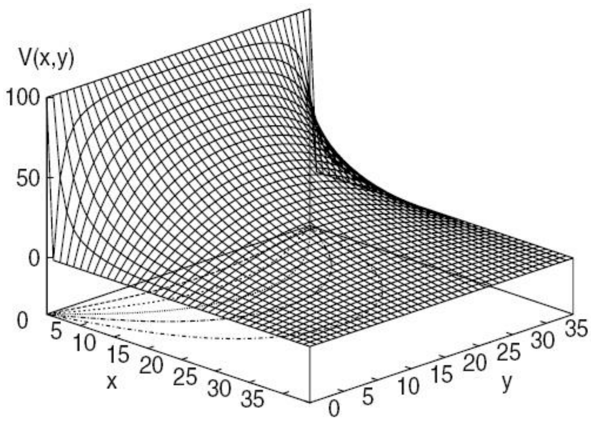
Electrostatic Potentials

- "Find the electric potential for all points *inside the charge-free* square shown in the above Fig. The bottom and sides of the region are made up of wires that are "grounded" (kept at 0 V). The top wire is connected to a battery that keeps it at a constant 100V."



Electrostatic Potentials





R. Landau et al. [2015] chương 19

G-S Iterative Algorithm for Electrostatic Potentials/ Laplace Equations

Step 1: Input N [Maximum number of iterations], n, m [nếu $n \neq m$];

Bound conditions $u_{i,0} [i = 0, n-1], u_{0,j}\ [j = 0, m-1]$;

and $u_{ij}^{(0)}\ [i = 1, n-2, j = 1, m-2]$.

S2: For $k = 0, N-1$ // vòng lặp/iteration [thay cho "While"][do Step 3]

S3: For $i = 1, n-2$ // hướng x: x-direction

For $j = 1, n\ -2$ //hướng y . Nếu $m \neq n$ thì cần cho $j = 1, m$

Set $u_{i,j} = (u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1})$

S4: // OUTPUT

For $i = 0, n-1$ // x:

For $j = 0, n-1$ // y. nếu $m \neq n$ thì cần cho $j = 1, m$

Output $x_0 + i * h, y_0 + j * h$, $u_{i,j}$

...

STOP

Nếu muốn chương trình dừng lại khi đạt được độ chính xác TOL [ε] thì cần thay đổi những gì trong code?

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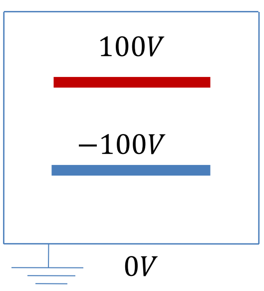
Thực hành

1. Lập trình giải bài toán thế tĩnh điện vừa xét ở slides trước và vẽ thế tĩnh điện. Ma trận A của hệ PT ứng với Laplace eq. có dạng thế nào?
2. Hiệu chỉnh code để dừng khi đạt được độ chính xác ε, và cho biết lần lặp thứ k tương ứng với độ chính xác này. [Nội dung PP G-S đã xét đến.]
3. Giải số và vẽ thế cho bài toán ở hình bên: 2 thanh/sợi (dài bằng nhau) với điện thế 100V và -100V, đặt bên trong sợi hình vuông nối đất. Tính và vẽ điện thế bên trong sợi hình vuông. [Tự 'set' chiều dài thanh, khoảng cách giữa 2 thanh.] [Tham khảo hình 19.4 sách của R. Landau et al. (2015)]



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Thực hành

4. Giải PT Poisson cho thế tĩnh điện tạo ra bởi 1 điện tích điểm [vd, electron] được đặt tại giữa "box" [2D]. Cần xác định điều kiện biên như thế nào? Chọn độ chính xác, vd, $\varepsilon = 10^{-6}$; thử tăng giảm ε và quan sát số lần lặp tương ứng.
   Vẽ thế tĩnh điện của điện tích điểm.