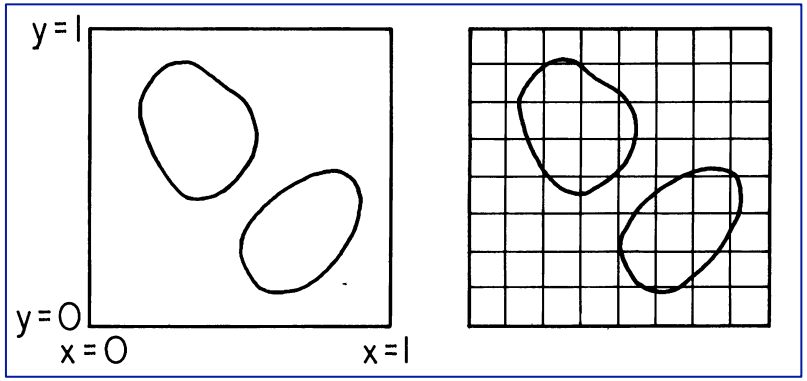
Ch 10
Elliptic Partial Differential Equations

Andrea Mignone
Physics Department, University of Torino
AA 2017-2018

Elliptic PDE:

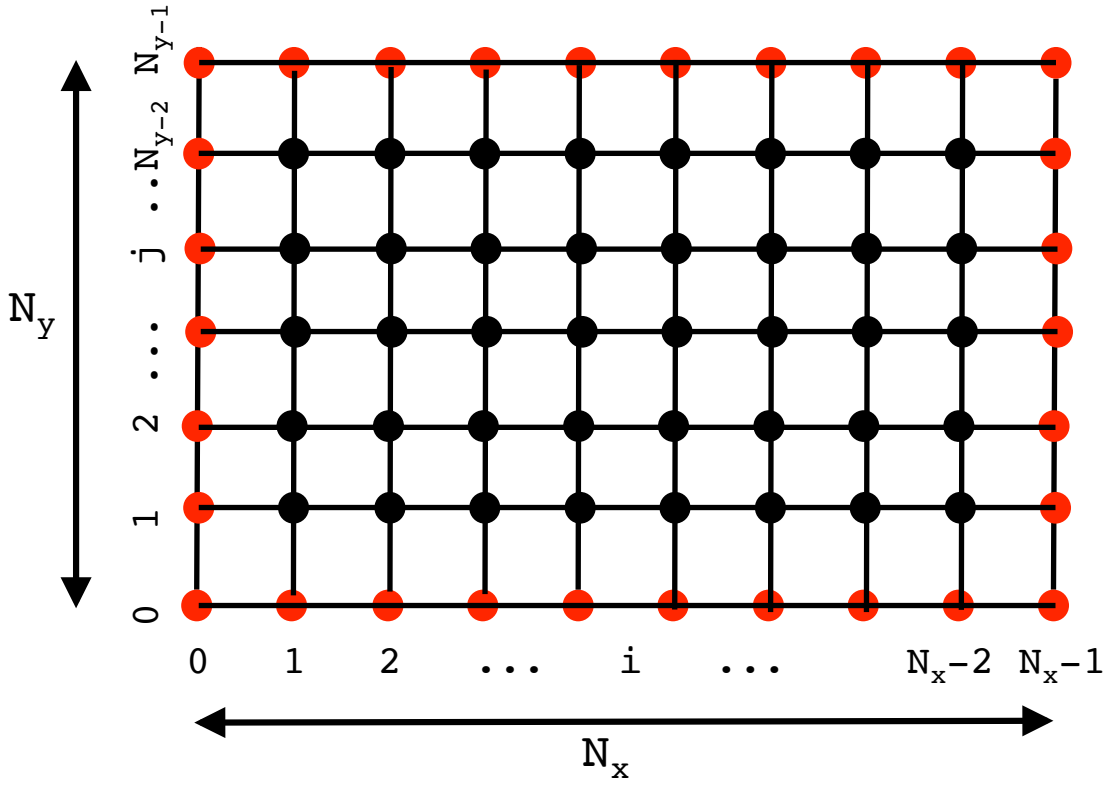
- Several elliptic PDEs can be written (in 2D) as $$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = S(x, y)$$
- Here φ(x,y) is a function of space only and S(x,y) is a source term.
- Although not the most general form, several equations can be written in this way:
  - Poisson equation for electrostatic potential
  - Time independent Schrodinger eq.
  - Heat diffusion with local heat generation/loss
- Elliptic equations are *boundary value problem*.
- The problem is well posed (i.e. the PDE has unique solution) if appropriate boundary conditions (b.c.) are specified (*Dirichlet* or *Neumann*).



- In a two dimensional space the function φ(x,y) (or its normal derivative) can be specified on the edges of the square and (possibly) on some additional curve within.

Elliptic PDE: Discretization

- We define a 2D lattice of N_x points in the x-direction and N_y points in the y-direction:



- Uniform and equal spacing in both direction is assumed: $h = \Delta x = \Delta y$.
- ***Red*** points should be specified as boundary conditions while ***black*** points are the solution values (unknowns).

Elliptic PDE: Discretization

- To begin with, we discretize the Laplacian operator using 2nd-order approximations to the second derivatives:

$$\frac{\varphi_{i+1,j} - 2\varphi_{i,j} + \varphi_{i-1,j}}{\Delta x^2} + \frac{\varphi_{i,j+1} - 2\varphi_{i,j} + \varphi_{i,j-1}}{\Delta y^2} = S_{i,j}$$

- *Interior points*:
  - $i=1\ldots N_x-2,\ \ j=1\ldots N_y-2$. This is where the solution must be found.

- *Boundary points*:
  - *Bottom:* $i=0\ldots N_x-1$ $j=0$
  - *Top:* $i=0\ldots N_x-1$ $j=N_y-1$
  - *Left:* $i=0$ $j=0\ldots N_y-1$
  - *Right:* $i=N_x-1$ $j=0\ldots N_y-1$

Direct Methods of Solution

- The solution of a discrete elliptic PDE involves $(N_x-2)x(N_y-2)$ equations at just as many grid points.

- For linear PDEs the discretization is naturally framed as a matrix-inversion problem:

$$\mathrm{A}\varphi = \mathbf{b}$$

- Here A is a large sparse matrix of $(N_x-2)^2x(N_y-2)^2$ points.

- A direct methods attempt to solve the system in a fixed number of operations by inverting A (e.g. Gaussian elimination). piuttosto costosi

- We *will not* use direct method for the present purpose.

Iterative Methods of Solution

- An iterative method is one in which a first approximation is used to compute a second approximation which in turn is used to calculate a third one and so on:

$$\varphi_i^{(n+1)} = F(\varphi_{i,j}^{(n)}, \varphi_{i-1,j-1}^{(n)}, \cdots, \varphi_{i+1,j+1}^{(n)})$$

- The iterative procedure is said to be convergent when the differences between the exact solution and the successive approximations tend to zero as the number of iterations increase.

- These methods are also called "relaxation methods" since the iterative process gradually "relax" the solution to the exact solution.

- From the analytical point of view, relaxation method can be understood by decomposing the matrix A as a diagonal component D, strictly lower and upper triangular components L and U:

$$A = D + L + U$$

Iterative Methods of Solution

- Here we will focus on three basic techniques, namely:

1. *Jacobi's* iterative method: we solve for diagonal element by keeping off-diagonal terms on the right hand side at the previous stage:

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \qquad \rightarrow \qquad \boldsymbol{\varphi}^{(k+1)} = D^{-1}\left[\boldsymbol{b} - (L+U)\boldsymbol{\varphi}^{(k)}\right]$$

2. *Gauss-Seidel* iterative method: we solve for the lower triangular part of the system using backsubstitution:

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \quad \rightarrow \quad \boldsymbol{\varphi}^{(k+1)} = (D+L)^{-1}\left[\boldsymbol{b} - U\boldsymbol{\varphi}^{(k)}\right]$$

3. *Successive Over Relaxation* iterative method: a variant of the Gauss-Seidel algorithm based on a constant parameter $\omega > 1$, called the relaxation factor:

converge + velocemente degli altri due

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \quad \rightarrow \quad \boldsymbol{\varphi}^{(k+1)} = (D+\omega L)^{-1}\left[\omega\boldsymbol{b} - (\omega U - (\omega-1)D)\boldsymbol{\varphi}^{(k)}\right]$$

1. Jacobi's Iterative Method

- Suppose we have found a solution of the discretized equation, then at each grid point:

$$\varphi_{i,j} = \frac{1}{4}\left(\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j+1} + \varphi_{i,j-1} - h^2 S_{i,j}\right)$$

- This is only formal since the r.h.s. is not known. To find the solution, the equations must be solved simultaneously → solving Poisson's equation is essentially a problem in linear algebra.

- Jacobi's iterative method starts with a guess $\varphi^{(0)}$ for the solution at the interior lattice points. Plugging this guess into the r.h.s. yields $\varphi^{(1)}$ at all lattice points. Iterating:

$$\varphi_{i,j}^{(k+1)} = \frac{1}{4}\left(\varphi_{i+1,j}^{(k)} + \varphi_{i-1,j}^{(k)} + \varphi_{i,j+1}^{(k)} + \varphi_{i,j-1}^{(k)} - h^2 S_{i,j}\right)$$

- Formally, using matrix notations, this is the same as

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \qquad \rightarrow \qquad \boldsymbol{\varphi}^{(k+1)} = D^{-1}\left[\boldsymbol{b} - (L+U)\boldsymbol{\varphi}^{(k)}\right]$$

where D^{-1} is trivially inverted.

1. Jacobi's Iterative Method

$$\varphi_{i,j}^{(k+1)} = \frac{1}{4}\left(\varphi_{i+1,j}^{(k)} + \varphi_{i-1,j}^{(k)} + \varphi_{i,j+1}^{(k)} + \varphi_{i,j-1}^{(k)} - h^2 S_{i,j}\right)$$

- In Jacobi's method, the computation of $\varphi^{(k+1)}$ requires neighbor elements at the previous stage.
- We cannot overwrite $\varphi^{(k)}$ with $\varphi^{(k+1)}$ since that value will be needed by the rest of the computation. The minimum amount of storage is *two* vectors of size `n`.
- A necessary and sufficient condition for an iterative method to converge is that the iteration matrix R - in Jacobi's method $R = D^{-1}(L+U)$ – has a spectral radius less than unity.

massimo autovalore

- The eigenvalues of the iteration matrix R are found to be

$$\lambda_{mn} = \frac{1}{2}\left[\cos\frac{m\pi}{M} + \cos\frac{n\pi}{N}\right],\ m = 1,\cdots,M-1,\ \ n = 1,\cdots,N-1$$

- Usually convergence is slow for the lowest and highest frequencies.

2. Gauss-Seidel Iterative Method

- This is a modification of the Jacobi method, which can be shown to converge somewhat faster: the idea is to use the components of $\varphi^{(k+1)}$ as soon as they are computed.

- In fact, if we sweep in order of increasing *i* and *j*. Then the left and lower neighbors of each lattice point are already updated.

- Why not use these (presumably) more accurate values in Jacobi's formula? This results in one form of the Gauss-Seidel algorithm:

$$\varphi_{i,j}^{(k+1)} = \frac{1}{4}\left(\varphi_{i+1,j}^{(k)} + \varphi_{i-1,j}^{(k+1)} + \varphi_{i,j+1}^{(k)} + \varphi_{i,j-1}^{(k+1)} - h^2 S_{i,j}\right)$$

- Formally, this is equivalent to

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \quad \rightarrow \quad \boldsymbol{\varphi}^{(k+1)} = (D+L)^{-1}\left[\boldsymbol{b} - U\boldsymbol{\varphi}^{(k)}\right]$$

- The preconditioner matrix D + L becomes triangular instead of diagonal, but this is still easy to use.

2. Gauss-Seidel Iterative Method

- The computation of $\varphi^{(k+1)}$ uses only the elements of $\varphi^{(k+1)}$ that have already been computed, and the elements of $\varphi^{(k)}$ that have not yet to be advanced to iteration k+1.

- This means that, unlike the Jacobi method, only *one storage array* is required as elements can be overwritten as they are computed (advantageous for very large problems).

- However, unlike the Jacobi method, the computations for each element cannot be done in parallel and the values at each iteration are dependent on the order of the original equations.

- Again, convergence is ensured if the spectral radius of the iteration matrix $\mathtt{R} = (\mathtt{D}+\mathtt{L})^{-1}\mathtt{U}$ is less than one.

- The eigenvalues are $$\lambda_{mn,\max} = \frac{1}{4}\left[\cos\frac{\pi}{M} + \cos\frac{\pi}{N}\right]^2$$

- This means that the Gauss Seidel method is twice as fast as the Jacobi's method.

3. Successive Over Relaxation (SOR)

- Both Jacobi and Gauss-Seidel do not use the value of $\varphi_{i,j}$ at the same lattice point during the update step.

- The convergence of the iteration can be improved considerably by using a linear combination of the new and old solutions as follows:

$$\varphi_{i,j}^{(k+1)} = (1-\omega)\varphi_{i,j}^{(k)} + \frac{\omega}{4}\left(\varphi_{i+1,j}^{(k)} + \varphi_{i-1,j}^{(k+1)} + \varphi_{i,j+1}^{(k)} + \varphi_{i,j-1}^{(k+1)} - h^2 S_{i,j}\right)$$

- In matrix notation, this is the same as

$$A\boldsymbol{\varphi} = (D+L+U)\boldsymbol{\varphi} = \boldsymbol{b} \quad \rightarrow \quad \boldsymbol{\varphi}^{(k+1)} = (D+\omega L)^{-1}\left[\omega \boldsymbol{b} - (\omega U - (\omega-1)D)\boldsymbol{\varphi}^{(k)}\right]$$

The preconditioner matrix is still in triangular form.

3. Successive Over Relaxation (SOR)

- The over-relaxation parameter ω can be tuned to optimize the convergence. It can be shown that
  - SOR converges only for $0<\omega<2$;
  - It is faster than Gauss-Seidel only if $1<\omega<2$;
  - It converges fastest for a square lattice if $\omega \approx 2/(1+\pi/N)$, where N is the number of points in the x or y directions.

- It can be shown that the eigenvalues of the SOR matrix are

$$\mu^{1/2} = \frac{1}{2}\left[\lambda\omega + \sqrt{\lambda^2\omega^2 - 4(\omega - 1)}\right]$$

where λ is an eigenvalue of the Jacobi matrix.

- The minimum occurs at $\omega_{\text{opt}} = \dfrac{2}{1+\sqrt{1-\lambda_{\max}^2}}$

Convergence Checking

- We need to decide when the solution has converged sufficiently.
- Since we presumably do not know the exact solution, one criterion is to ask that the approximate solution does not change significantly from one iteration to the next.
- One possibility is to compute the iteration error

$$\epsilon = \sum_{ij} \left| \varphi_{ij}^{(k+1)} - \varphi_{ij}^{(k)} \right|$$

where summation should be extended to *interior points only*.

- Alternatively, convergence can also be checked by computing the residual defined as

$$\epsilon_r = \sum_{ij} \left| \delta_x^2 \varphi_{ij} + \delta_y^2 \varphi_{ij} - h^2 S_{ij} \right|$$

where $\delta^2\varphi$ are the undivided approximations to the 2nd derivatives:

$$\delta_x^2 \varphi_{ij} = \varphi_{i+1,j} - 2\varphi_{ij} + \varphi_{i-1,j} \,, \qquad \delta_y^2 \varphi_{ij} = \varphi_{i,j+1} - 2\varphi_{ij} + \varphi_{i,j-1}$$

Convergence Rate

- If we denote with r the number of iterations required to reduce the overall error by a factor 10^{-p} for the 2D Laplacian equation is (see NR, Sect. 19.5):

$$r = \begin{cases} pN^2/2 & [\text{Jacobi}] \\ pN^2/4 & [\text{Gauss} - \text{Seidel}] \\ pN/3 & [\text{SOR}] \end{cases}$$

- Thus SOR converges in $\approx N$ iteration (provided an optimal choice for ω is used) while Jacobi and Gauss-Seidel are much slower.

- This makes SOR of more practical interest while leaving both Jacobi and Gauss-Seidel only of theoretical interest.

Boundary conditions

- *Dirichilet* b.c. specify the value of the solution itself, e.g. at a left boundary:

$$\varphi(x_0, y) = \alpha(y)$$

- *Neumann* b.c. specify the value of the derivative, e.g. $\left.\frac{\partial \varphi}{\partial x}\right|_{x_0} = \sigma(y)$

  - In order to introduce the Neumann b.c. one could use a 1st order discretization,

$$\begin{cases} (\varphi_{0,j} - 2\varphi_{1,j} + \varphi_{2,j}) + (\varphi_{1,j-1} - 2\varphi_{1,j} + \varphi_{1,j+1}) = h^2 S_{1,j} \\ \dfrac{\varphi_{1,j} - \varphi_{0,j}}{h} = \sigma = \left.\dfrac{\partial \varphi}{\partial x}\right|_{x_0} \end{cases}$$

  Eliminating $\varphi_{0,j}$ and solving for $\varphi_{1,j}$ → $\varphi_{1,j} = \frac{1}{3}\left[-h\sigma + \varphi_{2,j} + \varphi_{1,j+1} + \varphi_{1,j-1} - h^2 S_{1,j}\right]$

  - An even better approach can be obtained by introducing a fictitious point $\varphi_{-1,j}$ outside the domain and using a 2nd order approximation

$$\begin{cases} (\varphi_{-1,j} - 2\varphi_{0,j} + \varphi_{1,j}) + (\varphi_{0,j-1} - 2\varphi_{0,j} + \varphi_{0,j+1}) = h^2 S_{0,j} \\ \dfrac{\varphi_{1,j} - \varphi_{-1,j}}{2h} = \left.\dfrac{\partial \varphi}{\partial x}\right|_{x_0} \end{cases}$$

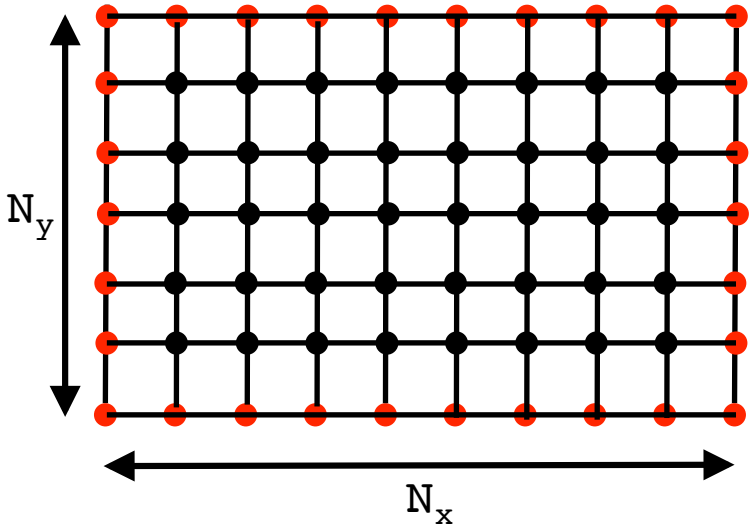
Eliminating $\varphi_{-1,j}$ from the two eqns: $\varphi_{1,j} = \frac{1}{4}\left[2\varphi_{2,j} - 2h\sigma + \varphi_{1,j-1} + \varphi_{1,j+1} - h^2 S_{1,j}\right]$

(same as re-defining $\varphi_{0,j} \leftarrow \varphi_{2,j} - 2h\sigma$)

Algorithm Implementation

- Here's a sketch on how your code should be correctly written:

```
- allocate memory for 2D arrays φ⁰[NX][NY] and φ¹[NX][NY] to store solution
  values at the current and next iteration;

- define grid arrays x[i] and y[j];

- initialize solution array (e.g. φ⁰[i][j] = 0) in the interior points;

- Assign boundary conditions on all sides;

- Iterate solution on interior points until convergence;

- Write solution to disk;
```



Note: interior points are in black, and looping over them can be done using the indices

```
#define IBEG 1
#define IEND NX-2
```

and similarly for `JBEG, JEND`.
Boundary points are in red and corresponds to

- *φ[0][j], φ[NX-1][j] at left, right bound.;*
- *φ[*][0], φ[*][NY-1] at bottom, top bound.;*

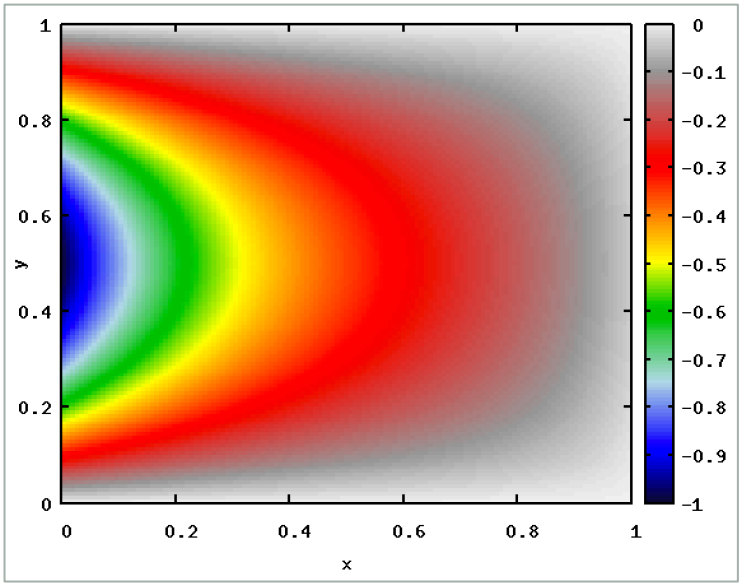
Practice Session #1

- `elliptic.cpp`: solve the Poisson equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} - S(x,y) = 0$$

on the unit square $0 \leq x,y \leq 1$ with S = const. and b.c. given by the exact solution

$$\varphi(x,y) = e^{-\pi x}\sin(-\pi y) + \frac{S}{4}(x^2+y^2)$$



→ Use `NX = NY = 32` and try `S = 0` and then `S = 2` using Jacobi, Gauss-Seidel and SOR. Compare the number of iterations necessary to achieve convergence, using the residual and a tolerance of 10^{-7}. Results are given by the following table

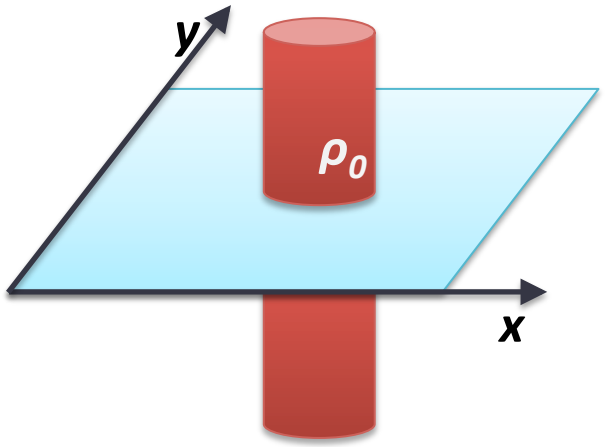
	Jacobi	Gauss-Siedel	SOR
S=0	≈3322	≈1655	≈105
S=2	≈3167	≈1617	≈122

Practice Session #2

- Compute the potential of an infinitely long charged cylinder by solving the Poisson equation

$$\nabla^2\varphi = -\rho\,, \quad \text{with} \quad \rho = \begin{cases} \rho_0 & \text{for} \quad r \le a \\ 0 & \text{otherwise} \end{cases}$$

use $a=0.1$ and $\rho_0=1$.



- As a boundary condition use the exact analytical solution:

$$\varphi(r) = \begin{cases} -\dfrac{\rho_0 r^2}{4} & \text{for} \quad 0 \le r \le a \\ -\dfrac{\rho_0 a^2}{2}\left[\log\left(\dfrac{r}{a}\right) + \dfrac{1}{2}\right] & \text{otherwise} \end{cases}$$

- Solve Poisson eq. on $-1 \le x, y \le 1$ and produce a plot of the solution.