PHY604 Lecture 16

October 21, 2025

Today’s lecture: Elliptical PDEs

- Relaxation methods
- Spectral methods

Elliptical equations: e.g., Laplace equation

- The PDEs we will discuss here represent boundary-value problems
  - Solution is a static field

- Consider Laplace's equation: $$\frac{\partial^2 \Phi(x,y)}{\partial x^2} + \frac{\partial^2 \Phi(x,y)}{\partial y^2} = 0$$

- Φ is the electrostatic potential

- As usual it is useful to solve a simple problem analytically so that we can benchmark numerical methods

Separation of variables for Laplace's equation

- Write Φ as the product: $\Phi(x, y) = X(x)Y(y)$
- Insert into Laplace's equation and divide by Φ:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} + \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = 0$$

- This equation should hold for all *x* and *y*, so each term must be a constant:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} = -k^2, \qquad \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = k^2$$

  - *k* is a complex constant
  - Writing constant as k^2 to simplify notation later
  - Signs can be switched
- Now we have two ODEs

Solution of Laplace’s eq. ODEs

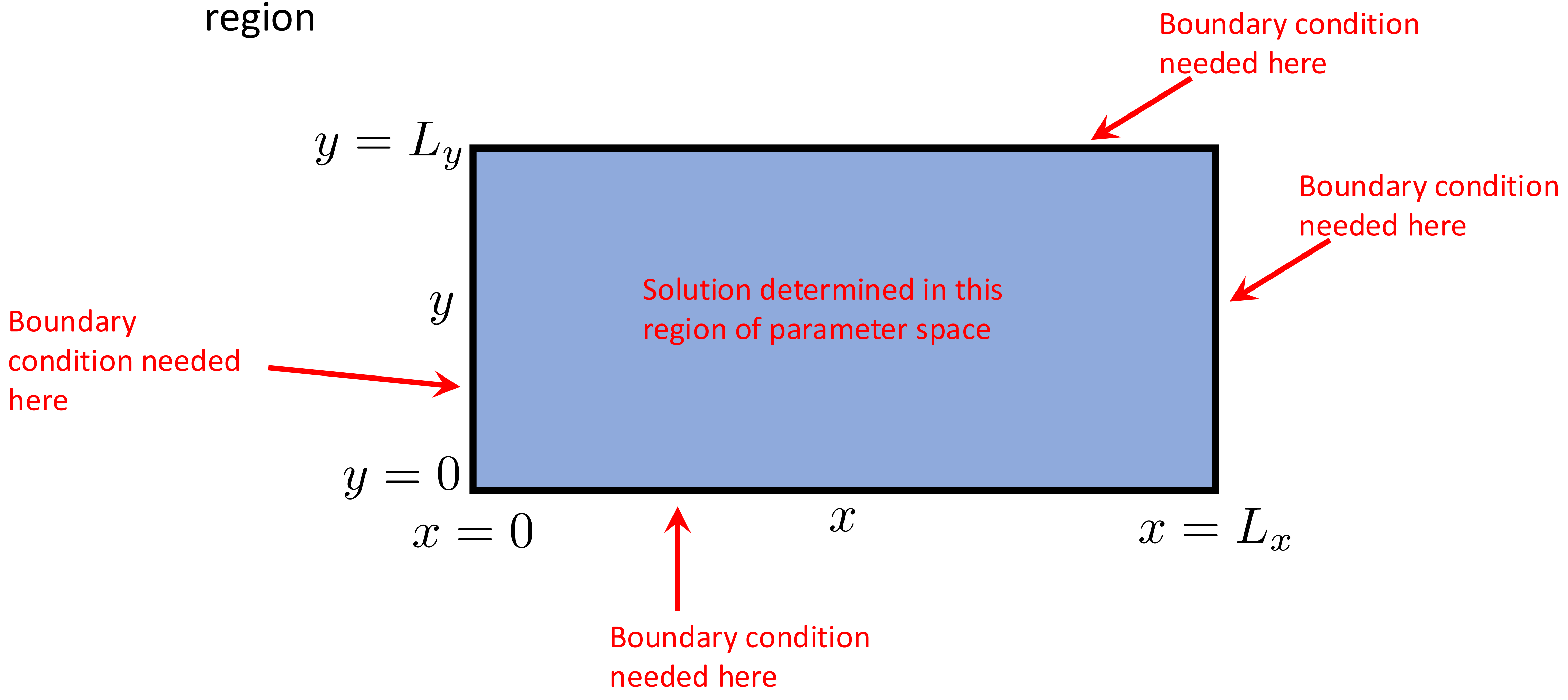
- Solution of these equations are well known:

$$X(x) = C_s \sin(kx) + C_c \cos(kx), \qquad Y(y) = C'_s \sinh(ky) + C'_c \cosh(ky)$$

  - Recall that k is complex, so solutions are “symmetric”
- To get the coefficients, we need to specify the boundary conditions

Boundary value problems

- All boundary values are specified at the outset
  - E.g., Laplace's equation in electrostatics, potential fixed on for sides of spatial region



Solution of Laplace’s eq. ODEs

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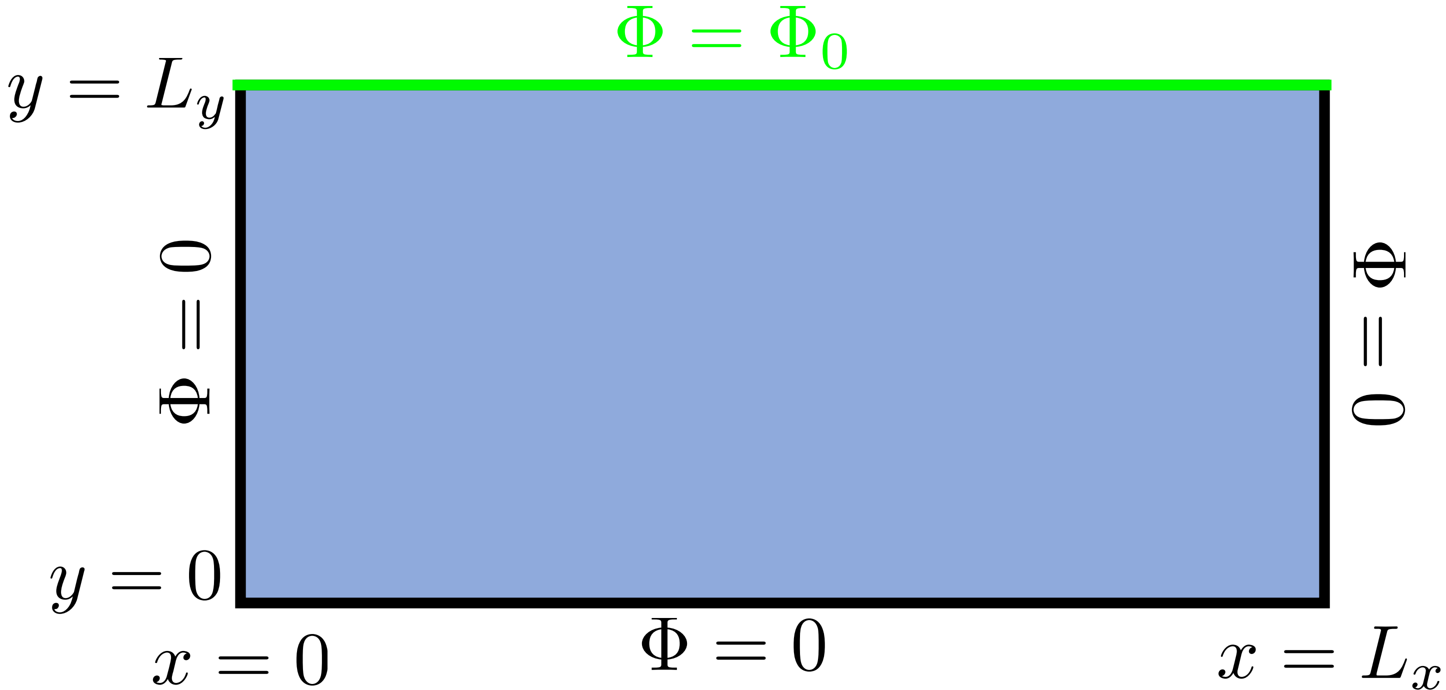
  - Recall that k is complex, so solutions are “symmetric”

- To get the coefficients, we need to specify the boundary conditions

$$\Phi(x=0,y) = \Phi(x=L_x,y) = \Phi(x,y=0) = 0, \quad \Phi(x,y=L_y) = \Phi_0$$



Solution of Laplace’s eq. ODEs

$$X(x) = C_s \sin(kx) + C_c \cos(kx), \qquad Y(y) = C'_s \sinh(ky) + C'_c \cosh(ky)$$

- Use our boundary conditions:

$$\Phi(x=0,y)=0 \quad \Longrightarrow \quad C_c = 0$$

$$\Phi(x,y=0)=0 \quad \Longrightarrow \quad C'_c = 0$$

$$\Phi(x=L_x,y)=0 \quad \Longrightarrow \quad k = \frac{n\pi}{L_x},\ n = 1, 2, \ldots$$

- So, we have solutions of the form:

$$c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

- Any linear combination is also a solution, so:

$$\Phi(x,y) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

Solution of Laplace's equation

- Now we use our last boundary condition:

$$\Phi_0 = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi L_y}{L_x}\right)$$

- To solve the equation, multiply both sides by sin($m\pi x/L_x$) and integrate from 0 to L_x:

$$\int_0^{L_x} dx \Phi_0 \sin\left(\frac{m\pi x}{L_x}\right) = \sum_{n=1}^{\infty} c_n \sinh\left(\frac{n\pi L_y}{L_x}\right) \int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi x}{L_x}\right)$$

- Left-hand side integral:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) = \begin{cases} 2L_x/m\pi, & m \text{ odd} \\ 0, & m \text{ even} \end{cases}$$

Solution of Laplace's equation

- Sum on the right-hand side simplifies because:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi x}{L_x}\right) = \frac{L_x}{2}\delta_{n,m}$$

- So, we have:

$$\Phi_0 \frac{2L_x}{\pi m} = c_m \sinh\left(\frac{m\pi L_y}{L_x}\right)\frac{L_x}{2}, \quad m = 1, 3, 5, \ldots$$

- So:

$$c_m = \frac{4\Phi_0}{\pi m \sinh\left(\frac{m\pi L_y}{L_x}\right)}, \quad m = 1, 3, 5, \ldots$$

Solution of Laplace's equation

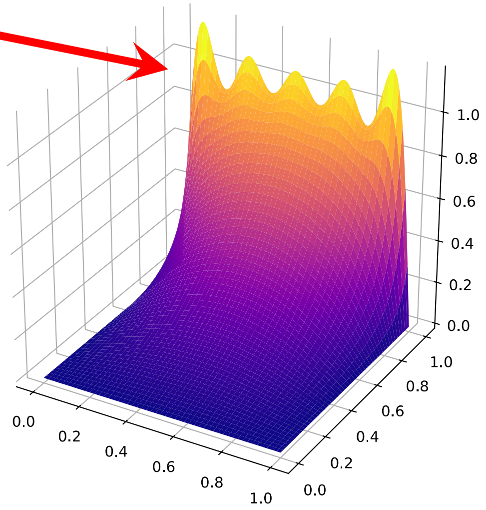
- Our final solution of Laplace's equation with our chosen boundary conditions:

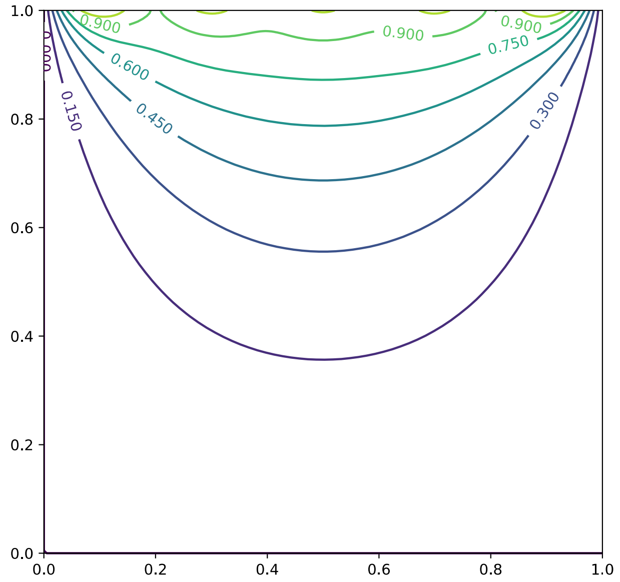
$$\Phi(x,y) = \Phi_0 \sum_{n=1,3,5,\ldots}^{\infty} \frac{4}{\pi n} \sin\left(\frac{n\pi x}{L_x}\right) \frac{\sinh\left(\frac{n\pi y}{L_x}\right)}{\sinh\left(\frac{n\pi L_y}{L_x}\right)}$$

Analytical solution to Laplace equation

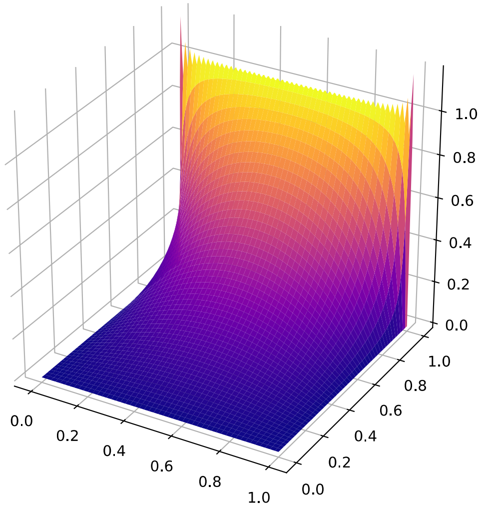
“Gibbs phenomenon,”
oscillations of Fourier series for
discontinuous function

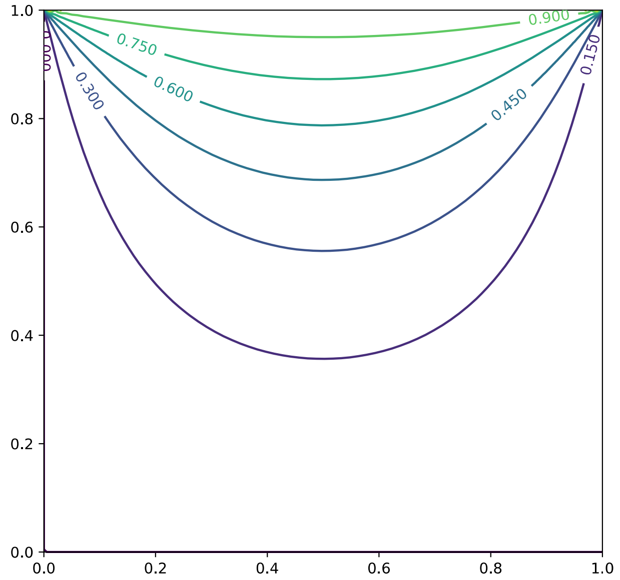
5 terms in the sum:





50 terms in the sum:





Numerical solution of the Laplace equation

- To do this, we'll go back to the *diffusion* equation we have solved previously, this time in two spatial dimensions:

$$\frac{\partial T(x,y,t)}{\partial t} = \kappa \left(\frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2} \right)$$

- Given an initial temperature profile and stationary boundary conditions, the solution will eventually relax to some steady state:

$$\lim_{t \to \infty} T(x,y,t) = T_s(x,y)$$

- In this state $\partial T / \partial t = 0$, so:

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} = 0$$

- We can think of the Laplace equation as the steady-state of the diffusion equation

Relaxation methods

- Methods based on this physical intuition are called relaxation methods
- We can use the FTCS method that we have used previously for the diffusion equation
- Start with the 2D “diffusion” equation:

$$\frac{\partial \Phi}{\partial t} = \mu \left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right)$$

Remember, solving an electrostatic problem, so Φ does not actually have time dependence

Will drop out later

Relaxation methods

- Methods based on this physical intuition are called relaxation methods
- We can use the FTCS method that we have used previously for the diffusion equation
- Start with the 2D “diffusion” equation:

$$\frac{\partial \Phi}{\partial t} = \mu \left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right)$$

- Discretize:

$$\begin{aligned} \Phi_{i,j}^{n+1} = \Phi_{i,j}^{n} &+ \frac{\mu\tau}{h_x^2}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} - 2\Phi_{i,j}^{n}) \\ &+ \frac{\mu\tau}{h_y^2}(\Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n} - 2\Phi_{i,j}^{n}) \end{aligned}$$

- *n* here is not really time, more an improved guess for the solution

Jacobi relaxation method

- Recall that FTCS is stable for $\mu\tau/h^2 \leq 1/2$
- In 2D the stability criteria is :

$$\frac{\mu\tau}{h_x^2} + \frac{\mu\tau}{h_y^2} \leq \frac{1}{2}$$

- If $h_x = h_y = h$, then the criterion is

$$\frac{\mu\tau}{h^2} \leq \frac{1}{4}$$

- Since we want to take *n* to infinity, we choose the largest timestep:

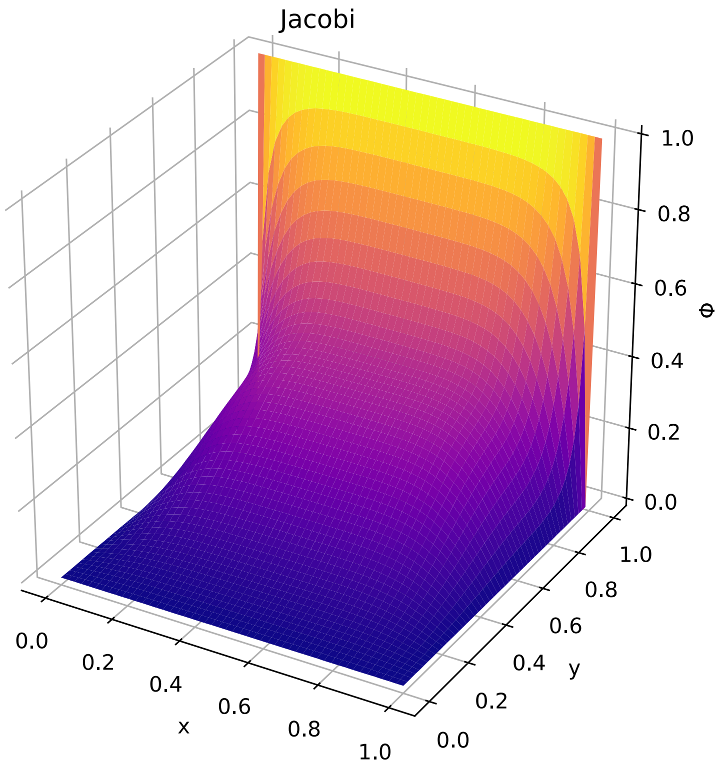
$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n})$$

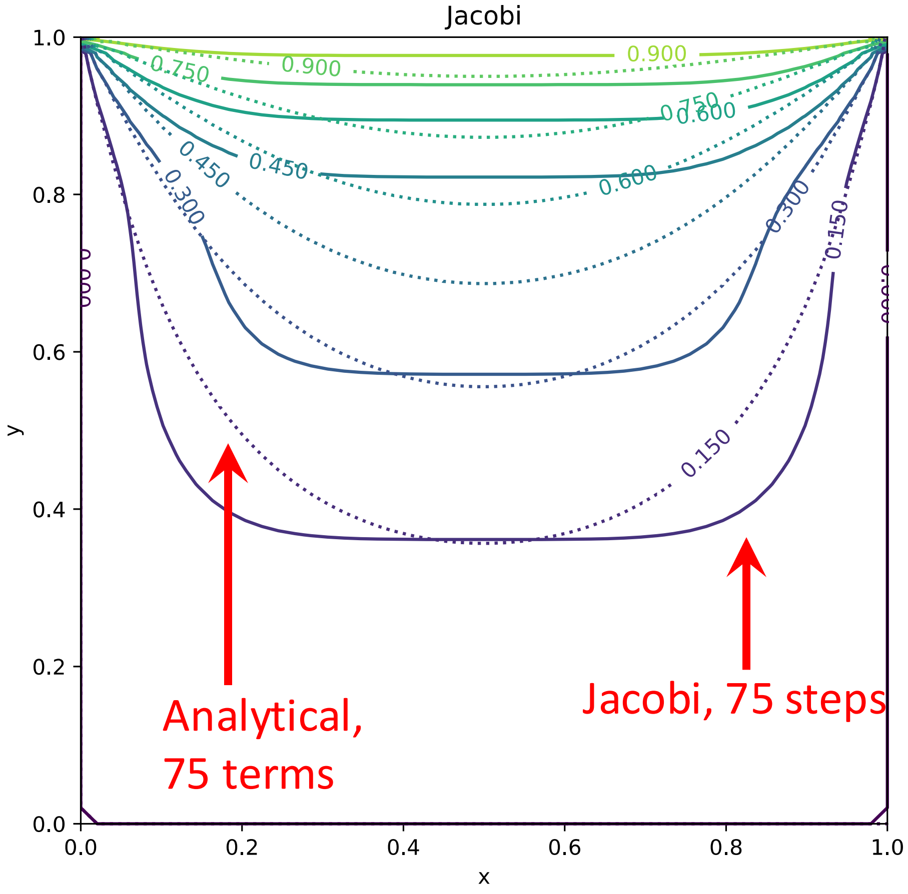
Jacobi method for Laplace equation

$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n})$$

- Note that the μ has dropped out
- Involves replacing the value of the potential at a point with the average value of the four nearest neighbors
  - Discrete version of mean-value theorem for the electrostatic potential
- This equation is for the interior points (exterior are set by boundary conditions)
- Simple to generalize for Poisson equation

Jacobi method for Laplace equation





Gauss-Seidel and simultaneous overrelaxation

- Gauss-Seidel: We can improve the convergence over the Jacobi method by using updated values of the potential as they are calculated:

$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

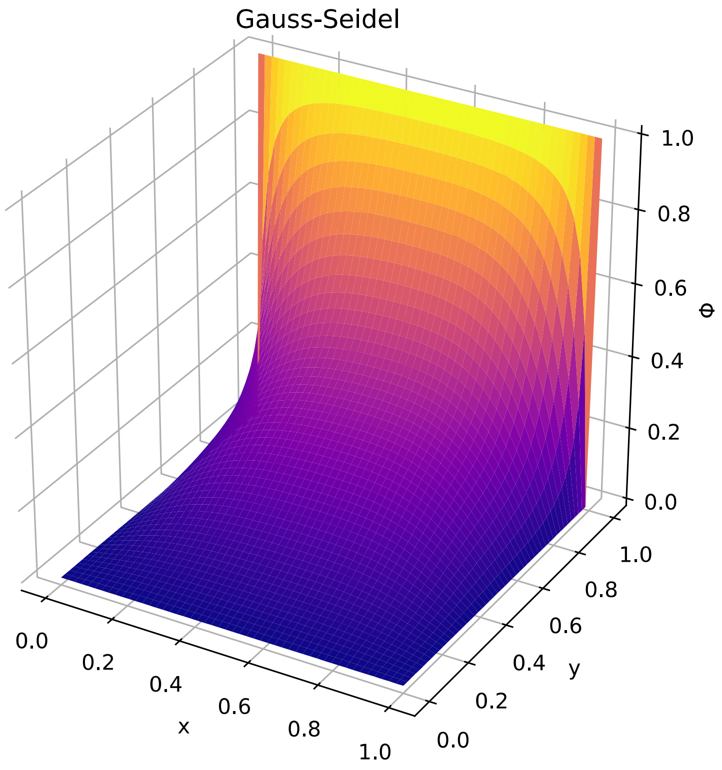
- Simultaneous overrelaxation: Choose a mixing parameter ω:

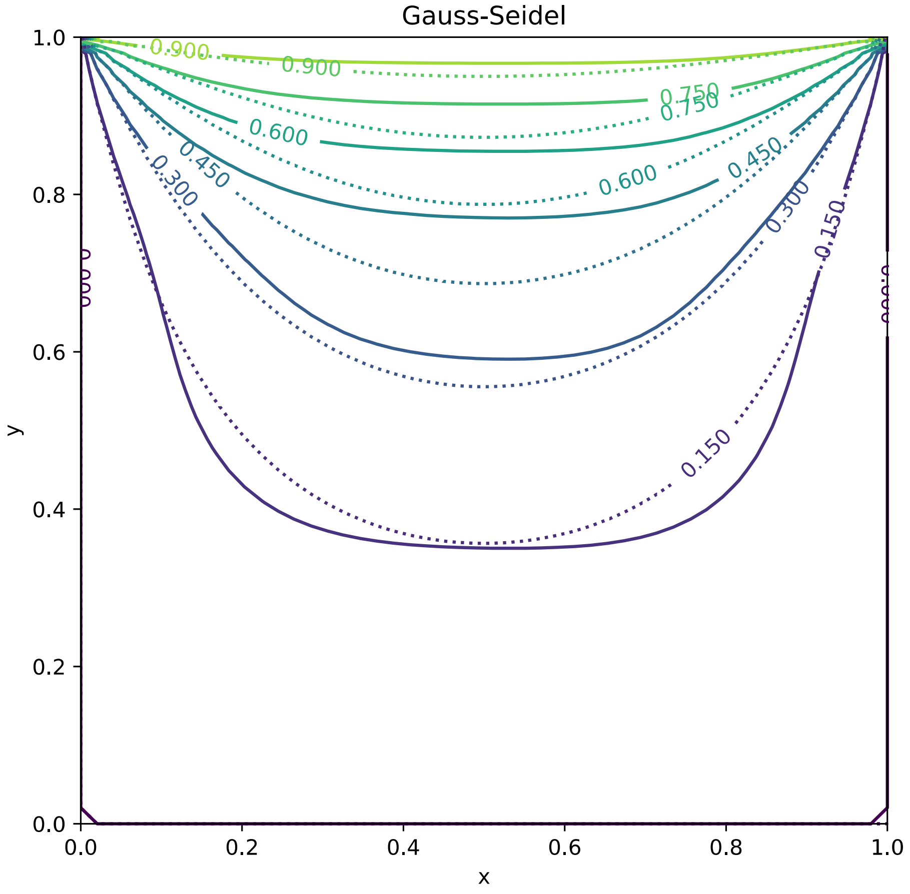
$$\Phi_{i,j}^{n+1} = (1-\omega)\Phi_{i,j}^{n} + \frac{\omega}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

  - $\omega < 1$ slows convergence, $\omega > 2$ is unstable
  - Often chosen by trial and error
  - E.g., for a square geometry with equal discretization, often a good choice:

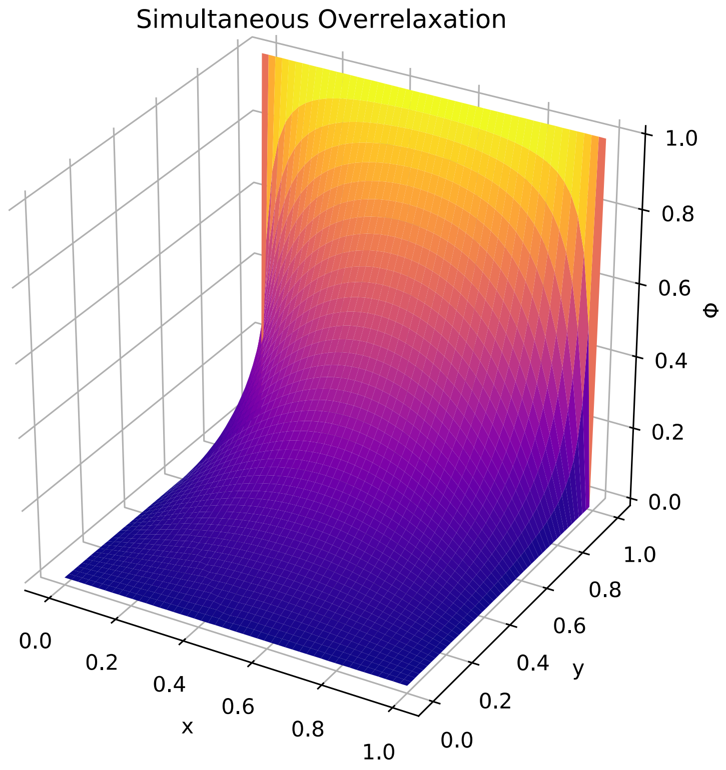
$$\omega_{\text{opt}} = \frac{2}{1 + \sin(\pi/N)}$$

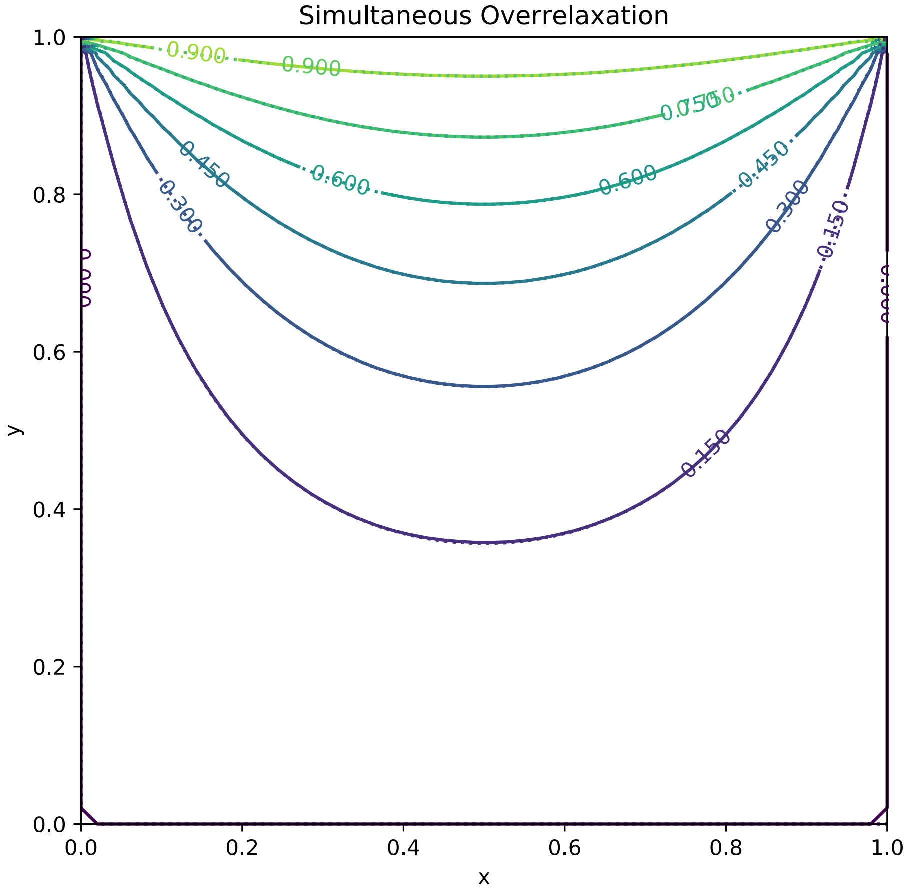
Gauss-Seidel for Laplace equation





Simultaneous overrelaxation for Laplace eq.





Recall: Jacobi iterative method

- Starting with a linear system:

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
\vdots \qquad\quad \vdots \qquad\qquad\quad \vdots \qquad & \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n
\end{aligned}
$$

- Pick initial guesses $\mathbf{x}^k$, solve equation *i* for *i*th unknown to get an improved guess:

$$
\begin{aligned}
x_1^{k+1} &= -\frac{1}{a_{11}}(a_{12}x_1^k + a_{13}x_2^k + \cdots + a_{1n}x_n^k - b_1) \\
x_2^{k+1} &= -\frac{1}{a_{22}}(a_{21}x_1^k + a_{23}x_2^k + \cdots + a_{2n}x_n^k - b_2) \\
\vdots \qquad & \qquad \vdots \qquad\qquad\qquad\qquad \vdots \qquad\qquad \vdots \\
x_n^{k+1} &= -\frac{1}{a_{nn}}(a_{n1}x_1^k + a_{n2}x_2^k + \cdots + a_{n,n-1}x_{n-1}^k - b_n)
\end{aligned}
$$

Recall: Jacobi iterative method

- We can write an element-wise formula for **x**:

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

- Or:

$$\mathbf{x}_i^{k+1} = \mathbf{D}^{-1} \left(\mathbf{b} - (\mathbf{A} - \mathbf{D}) \mathbf{x}^k \right)$$

  - Where **D** is a diagonal matrix constructed from the diagonal elements of **A**

- Convergence is guaranteed if matrix is diagonally dominant (but works in other cases):

$$a_{ii} > \sum_{j=1, j \neq i}^{N} |a_{ij}|$$

The iterative methods discussed here are the same as we used to solve linear systems

- Can interpret Φ as a vector, so are solving **A**Φ=**b**
- Going back to our initial discretization of the Laplace equation (for $h_x = h_y$):

$$\frac{1}{h^2}(\Phi^n_{i+1,j} + \Phi^n_{i-1,j} + \Phi^n_{i,j+1} + \Phi^n_{i,j-1} - 4\Phi^n_{i,j}) = 0$$

- Note that **A** is a banded matrix with 4's on the diagonal, 1's on off-diagonal elements
- This is when the Jacobi method is guaranteed to be accurate (diagonally dominated)!
- Same holds for Gauss-Seidel and SOR

Today's lecture: Elliptical PDEs

- Relaxation methods
- Spectral methods

A different way to represent the potential

- Consider again the Poisson equation:

$$\nabla^2\Phi(\mathbf{r}) = -\frac{1}{\epsilon_0}\rho(\mathbf{r})$$

- For simplicity, square geometry: $0 \le x \le L, \quad 0 \le y \le L$
- Relaxation methods discretize space and solve for $\Phi_{i,j}$
- We constructed out analytical solution as in infinite sum of trigonometric functions
- Let's build an approximate solution as a finite sum:

$$\begin{aligned}\Phi(x,y) &= a_1 f_1(x,y) + a_2 f_2(x,y) + \cdots + a_K f_K(x,y) + T(x,y) \\ &= \sum_{k=1}^{K} a_k f_k(x,y) + T(x,y) \\ &= \Phi_a(x,y) + T(x,y)\end{aligned}$$

Approximate solution

Approx. solution

Error

$$\Phi(x,y) = \Phi_a(x,y) + T(x,y)$$

- To simplify the approximate solution, we take orthogonal trial functions:

$$\int_0^L dx \int_0^L dy f_k(x,y) f_{k'}(x,y) = A_k \delta_{k,k'}$$

- Insert into the Poisson equation:

$$\nabla^2 \left[\sum_k a_k f_k(x,y) \right] + \frac{1}{\epsilon_0} \rho(x,y) = R(x,y)$$

- Where the residual *R* is:

$$R(x,y) = -\nabla^2 T(x,y)$$

Obtain coefficients with Galerkin method

- Next step is to obtain coefficients a_k
- Galerkin method imposes the condition that the residual is orthogonal to all of the trial functions:

$$\int_0^L dx \int_0^L dy f_k(x,y) R(x,y) = 0$$

- Choice of trial functions motivated by geometry and boundary conditions
- Let's take Neumann boundary conditions:

$$\left.\frac{\partial \Phi}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi}{\partial x}\right|_{x=L} = \left.\frac{\partial \Phi}{\partial y}\right|_{y=0} = \left.\frac{\partial \Phi}{\partial y}\right|_{y=L} = 0$$

- Normal component of electric field zero at the boundaries

Trial functions for our geometry and BCs

- Natural set of trial functions:

$$f_{m,n}(x,y) = \cos\left[\frac{m\pi x}{L}\right]\cos\left[\frac{n\pi y}{L}\right]$$

- Can confirm that these functions are orthogonal:

$$\int_0^L dx \int_0^L dy f_{m,n}(x,y) f_{m',n'}(x,y) = \frac{L^2}{4}(1+\delta_{m,0})(1+\delta_{n,0})\delta_{m,m'}\delta_{n,n'}$$

- Inserting into Poisson equation

$$\nabla^2\left[\sum_k a_k f_k(x,y)\right] + \frac{1}{\epsilon_0}\rho(x,y) = R(x,y)$$

- Gives:

$$-\sum_{m=0}^{M-1}\sum_{n=0}^{M-1} a_{m,n}\frac{\pi^2(m^2+n^2)}{L^2} f_{m,n}(x,y) + \frac{1}{\epsilon_0}\rho(x,y) = R(x,y)$$

Now we need so solve for coefficients

- Apply to both sides of the equation:

$$\int_0^L dx \int_0^L dy f_{m',n'}(x,y)$$

- And use "Galerkin condition":

$$\int_0^L dx \int_0^L dy f_k(x,y) R(x,y) = 0$$

- Which gives:

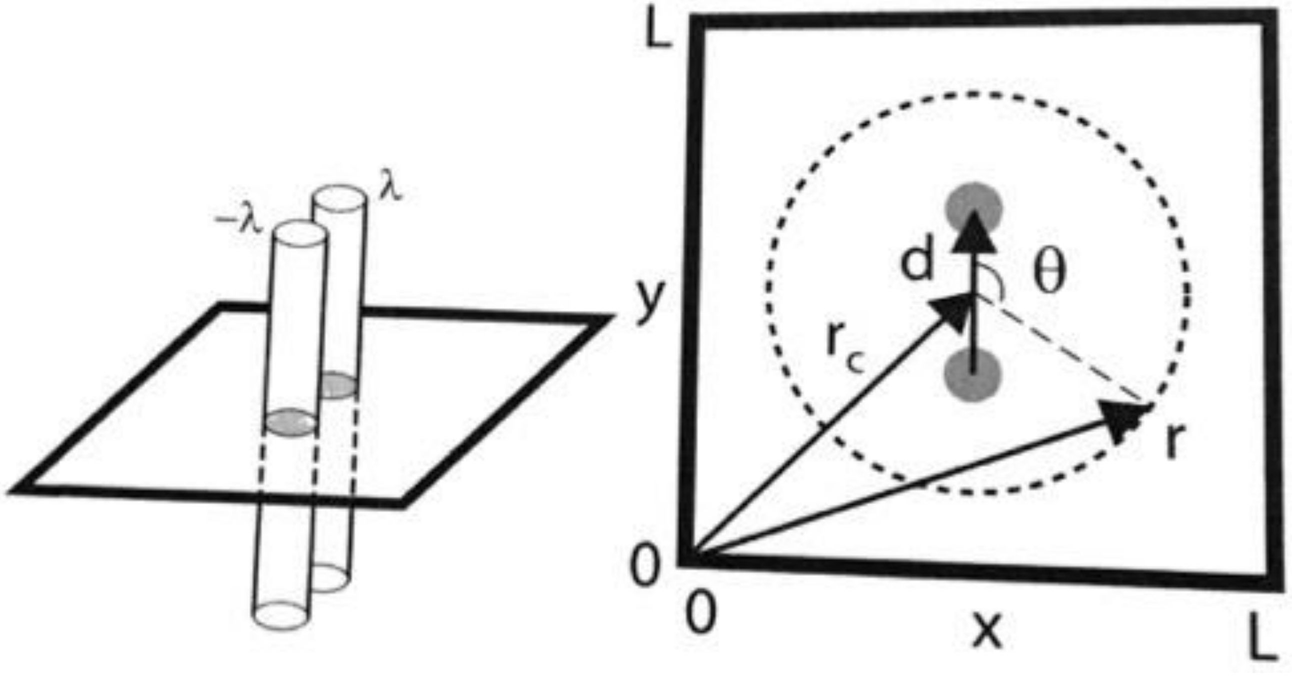
$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2+n^2)(1+\delta_{m,0})(1+\delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x,y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

Final solution with Galerkin method:

$$\Phi_a(x,y) = \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} a_{m,n} \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

$$a_{m,n} = \frac{4}{\pi^2 \epsilon_0 (m^2+n^2)(1+\delta_{m,0})(1+\delta_{n,0})} \int_0^L dx \int_0^L dy \rho(x,y) \cos\left(\frac{m\pi x}{L}\right) \cos\left(\frac{n\pi y}{L}\right)$$

Ex: charge distribution of 2D dipoles (Garcia Sec. 8.2)



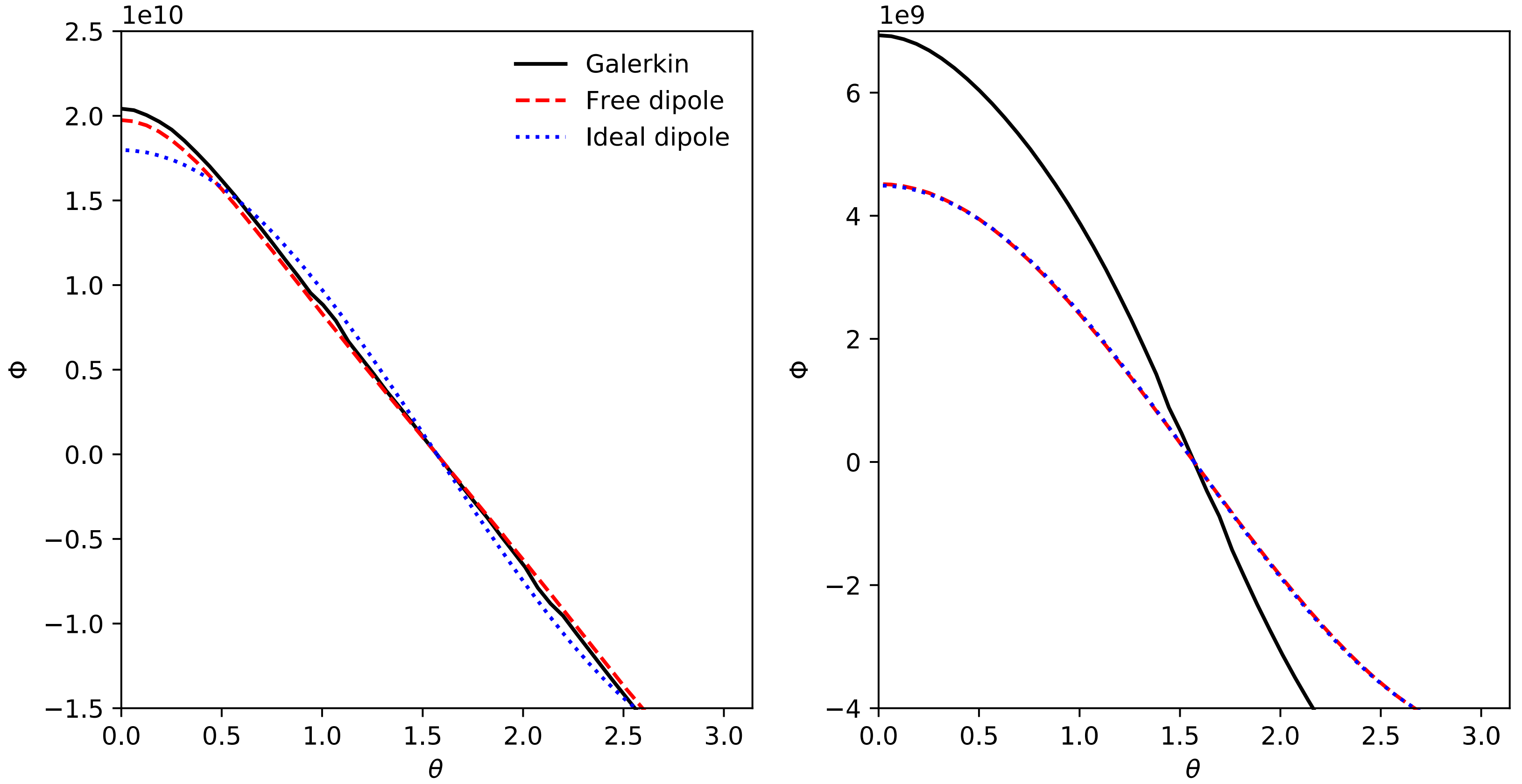
$$\rho(\mathbf{r}) = \lambda[\delta(\mathbf{r} - \mathbf{r}_+) - \delta(\mathbf{r} - \mathbf{r}_-)]$$

- Where:

$$\mathbf{r}_\pm = \mathbf{r}_c \pm \frac{1}{2}\mathbf{d}$$

Galerkin solution to the dipole potential

- Compare to free dipole: $\Phi^{\text{free}}(\mathbf{r}) = -\frac{\lambda}{2\pi\epsilon_0}\left[\ln|\mathbf{r}-\mathbf{r}_+| - \ln|\mathbf{r}-\mathbf{r}_-|\right]$
- Or "ideal" dipole potential (far away): $\Phi^{\text{ideal}}(\mathbf{r}) = \frac{\lambda}{2\pi\epsilon_0}\frac{|\mathbf{d}|}{|\mathbf{r}-\mathbf{r}_c|}\cos\theta$



Comments on the Galerkin method

- Can choose any trial functions that are orthogonal and obey the boundary conditions
  - In contrast to the separation of variables, where we first found general solutions to PDE, the imposed boundary conditions
- Should be interpreted as a spectral transform approach, i.e., representing the solution as a Fourier series
  - In our example, it was a cosine series because of our boundary conditions
- Did not use a spatial grid
  - Convenient if only need the answer at specific points
  - Inefficient if we want to map the potential over the whole range, because of the computation of the prefactors, especially for a more complex potential

After class tasks

- Homework 3 due tomorrow Oct. 22
- Homework 4 will be posted soon

- Readings
  - Garcia Chapters 7 and 8
  - MIke Zingale's notes on computational hydrodynamics