Supporting textbook chapters for week 8: Chapters 9.1, 9.2, 9.3.1

Lecture 8, topics:

- Classifying PDEs
- Elliptic equation solvers: Jacobi, Gauss-Seidel, overrelaxation
- Parabolic equation solver: FTCS (Forward Time, Centered Space)
- Stability.

Classifying PDEs

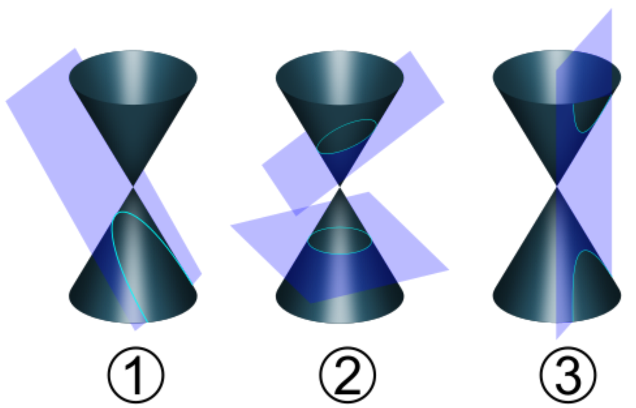
Recall conical equations in geometry:

$$\alpha x^2 + \beta x y + \gamma y^2 + \delta x + \varepsilon y = f,$$

classified using

$$\Delta = \beta^2 - 4\alpha\gamma.$$

1. $\Delta = 0$: equation for a parabola,
2. $\Delta < 0$: equation for an ellipse,
3. $\Delta > 0$: equation for a hyperbola.



Similar for PDEs:

$$\alpha\frac{\partial^2\phi}{\partial x^2} + \beta\frac{\partial^2\phi}{\partial x\partial y} + \gamma\frac{\partial^2\phi}{\partial y^2} + \delta\frac{\partial\phi}{\partial x} + \varepsilon\frac{\partial\phi}{\partial y} = f.$$

Imagine Fourier modes to convince yourself of the connection:

$$\begin{pmatrix}\phi\\ f\end{pmatrix} = \begin{pmatrix}\Phi\\ F\end{pmatrix}e^{i(kx+\ell y)} \Rightarrow -\alpha k^2 - \beta k\ell - \gamma\ell^2 + i\delta k + i\varepsilon\ell = \frac{F}{\Phi}.$$

$$\Rightarrow (x, y) \leftrightarrow (ik, i\ell)$$

$$\alpha\frac{\partial^2\phi}{\partial x^2} + \beta\frac{\partial^2\phi}{\partial x\partial y} + \gamma\frac{\partial^2\phi}{\partial y^2} + \delta\frac{\partial\phi}{\partial x} + \varepsilon\frac{\partial\phi}{\partial y} = f.$$

With $\Delta = \beta^2 - 4\alpha\gamma$,

1. $\Delta = 0$: parabolic PDE,
2. $\Delta < 0$: elliptic PDE,
3. $\Delta > 0$: hyperbolic PDE.

1. Canonical parabolic PDE: the diffusion equation, $\kappa\frac{\partial^2 T}{\partial x^2} - \frac{\partial T}{\partial t} = 0$,
$$x \to x, \quad y \to t, \quad \alpha \to \kappa, \quad \varepsilon \to -1, \quad \beta, \gamma, \delta, f \to 0 \quad \Rightarrow \quad \beta^2 - 4\alpha\gamma = 0.$$
2. Canonical elliptic PDE: the Poisson equation, $\nabla^2\phi = \rho$,
$$x \to x, \quad y \to y, \quad \alpha, \gamma \to 1, \quad f \to \rho, \quad \beta, \delta, \varepsilon \to 0 \quad \Rightarrow \quad \beta^2 - 4\alpha\gamma = -4 < 0.$$
3. Canonical hyperbolic PDE: the wave equation, $c^2\frac{\partial^2\phi}{\partial x^2} - \frac{\partial^2\phi}{\partial t^2} = 0$.
$$x \to x, \quad y \to t, \quad \alpha \to c^2, \quad \gamma \to -1, \quad \beta, \delta, \varepsilon, f \to 0 \quad \Rightarrow \quad \beta^2 - 4\alpha\gamma = 4c^2 > 0.$$

Note: we use these expressions even when the spatial operator is $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$, i.e., for 4D PDEs.

It is a departure from the original classification (see http://www.math.toronto.edu/courses/apm346h1/20129/LA.html (http://www.math.toronto.edu/courses/apm346h1/20129/LA.html)), but usually harmless in Physics.

- Solving partial differential equations is one of the pinnacles of computational physics, bringing together many methods.

- Parabolic, hyperbolic, elliptic PDE: each type comes with design decisions on how to discretize and implement numerical methods,
- Stability is crucial.
- Accuracy is crucial too.

General approach

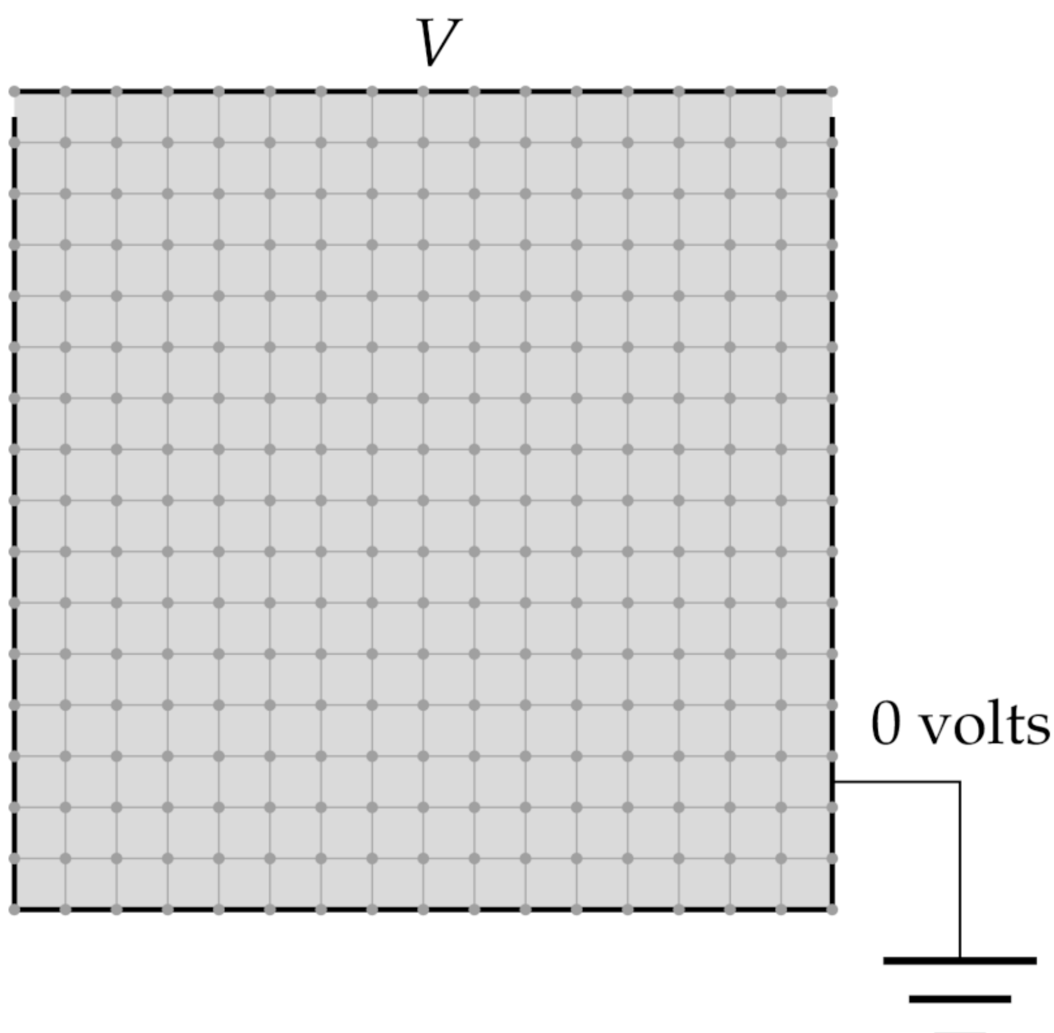
- Discretize system spatially and temporally: can use finite difference, spectral coefficients, etc.
- $\Rightarrow$ set of coupled ODEs that you need to solve in an efficient way.
- Spatial derivatives bring information in from neighbouring points $\Rightarrow$ coupling,
- $\Rightarrow$ errors depend on space and time and can get wave-like characteristics.
- For 2nd derivatives, recall central difference calculation (§5.10.5, p.197):

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}h^2 f^{(4)}(x) + \dots$$

Elliptic equations

- For solutions of Laplace's or Poisson's equation.
- E.g.: electrostatics, with electric potential ϕ s.t. $\vec{E} = \nabla\phi$, in the absence of charges ($\rho \equiv 0$).
- Gauss' law:

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



2D Laplacian:

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2},$$

On regular square grid of cell side length a, finite difference form is

$$\frac{\partial^2\phi}{\partial x^2} \approx \frac{\phi(x+a,y) - 2\phi(x,y) + \phi(x-a,y)}{a^2},$$
$$\frac{\partial^2\phi}{\partial y^2} \approx \frac{\phi(x,y+a) - 2\phi(x,y) + \phi(x,y-a)}{a^2}.$$

Gauss's law:

$$0 \approx \phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a) - 4\phi(x,y)$$

at each location (x, y).

- Put together a series of equations of the form
$$\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a) - 4\phi(x) = 0$$
for each x and y, subject to boundary conditions.
- ϕ or derivative $\partial\phi/\partial\xi$ ($\xi = x,\ y$, or both) given on boundary.
  - If ϕ given, use this value for adjacent points.
  - If $\partial\phi/\partial\xi$ given, find algebraic relationship between points near to boundary using finite difference.
- Could solve using matrix methods $\mathbf{L}\phi = \mathbf{R}\phi$, but a simpler method is possible.

Jacobi relaxation method

$$\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a) - 4\phi(x) = 0$$

- Iterate the rule $\phi_{new}(x,y) = \frac{1}{4}[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)]$.
- Much like the relaxation method for finding solutions of $f(x) = x$,
- For this problem it turns out that Jacobi Relaxation is always stable and so always gives a solution!
- Let's look at `laplace.py`

In [14]:
```
# From Newman's laplace.py
from numpy import empty, zeros, amax
import matplotlib.pyplot as plt

# Constants
M = 10         # Grid squares on a side
V = 1.0         # Voltage at top wall
target = 1e-4   # [V] Target accuracy

# DON'T EXECUTE IN CLASS WITH LARGE M, IT TAKES TOO LONG!
# Create arrays to hold potential values
phi = zeros([M+1, M+1], float)
phi[0, :] = V
phinew = empty([M+1, M+1], float)
```

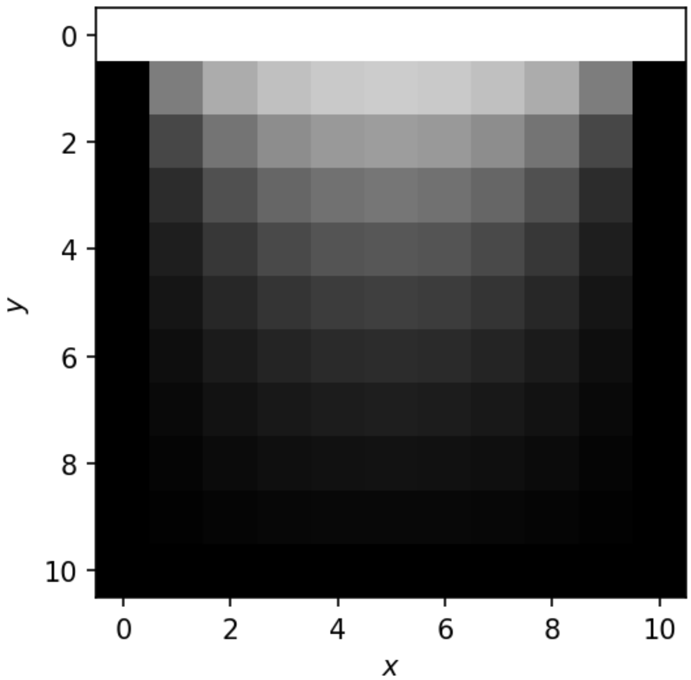
In [15]:
```
# Main loop;
delta = 1.0
while delta > target:

    # Calculate new values of the potential, except on boundaries
    for i in range(1, M):
        for j in range(1, M):
                phinew[i, j] = (phi[i+1, j] + phi[i-1, j] + phi[i, j+1] + phi[i, j-1])/4

    # Calculate maximum difference from old values
    delta = amax(abs(phi-phinew))

    # Swap the two arrays around
    phi, phinew = phinew, phi
```

In [16]:
```
plt.figure(dpi=150)
plt.imshow(phi)
plt.gray()
plt.xlabel('$x$')
plt.ylabel('$y$')
plt.show()
```



Overrelaxation method

$\phi_{new}(x, y) =$

$$(1+\omega)\left[\frac{\phi(x+a, y)+\phi(x-a, y)+\phi(x, y+a)+\phi(x, y-a)}{4}\right]-\omega\phi(x, y)$$

- When it works, it usually speeds up the calculation.
- Not always stable! How to choose ω is not always reproducible.
- see Newman's exercise 6.11 for a similar problem for finding $f(x) = x$.

Gauss-Seidel method

- Replace function on the fly as in
$$\phi(x, y) \leftarrow \frac{\phi(x+a, y)+\phi(x-a, y)+\phi(x, y+a)+\phi(x, y-a)}{4}.$$
- Crucial difference: the LHS is ϕ, not ϕ_{new}: we use newer values as they are being computed (Jacobi used only old values to compute new one).
- This can be shown to run faster.

- Can be combined with overrelaxation.

The old Jacobi code snippet:

In [ ]:
```
# Calculate new values of the potential
for i in range(1, M):
    for j in range(1, M):
          phinew[i, j] = (phi[i+1, j] + phi[i-1, j] + phi[i, j+1] + phi[i, j-1])/4
# Swap the two arrays around
phi, phinew = phinew, phi
```

becomes:

In [ ]:
```
# Calculate new values of the potential
for i in range(1, M):
    for j in range(1, M): #no phi_new in this loop
        phi[i, j] = (phi[i+1, j] + phi[i-1, j] + phi[i, j+1] + phi[i, j-1])/4
```

Parabolic PDEs: Forward Time Centred Space method

- Consider the 1D heat equation:
$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2},$$
- B.Cs.:
$$T(x=0,t) = T_0, \quad T(x=L,t) = T_L.$$
- I.C.:
$$T(x,t=0) = T_0 + (T_L - T_0)\left(\frac{f(x)-f(0)}{f(L)-f(0)}\right)$$

Step 1: Discretize in space

$x_m = \frac{m}{M}L = am, \quad m = 0 \dots M, \quad a = \frac{L}{M},$

$T_m(t) = [T_0(t), \dots, T_M(t)]$

$\left.\frac{\partial^2 T}{\partial x^2}\right|_{x=x_m,t} \approx \frac{T_{m+1} - 2T_m + T_{m-1}}{a^2}$ ("centred space", CS)

Step 2: Discretize in time

$\frac{dT_m}{dt} \approx \kappa \frac{T_{m+1} - 2T_m + T_{m-1}}{a^2}, \quad m = 1 \dots, M-1$

Let $t_n = nh$, h the time step. Let $T_m(t_n) \equiv T_m^n$.

$\Rightarrow \left.\frac{\partial T}{\partial t}\right|_{x=ma,t=nh} \approx \frac{T_m^{n+1} - T_m^n}{h} \equiv \kappa \frac{T_{m+1}^n - 2T_m^n + T_{m-1}^n}{a^2}$ ("Forward Time", FT).

$\Rightarrow$ **Explicit FTCS method:**
$$\boxed{T_m^{n+1} = T_m^n + \frac{\kappa h}{a^2}\left(T_{m+1}^n - 2T_m^n + T_{m-1}^n\right)}.$$

Von Neumann Stability Analysis

- How can we determine stability in PDEs?
- A simple way is to consider a single spatial Fourier mode.
- T_m^n as an inverse DFT: $\quad T_m^n = \sum_k \widehat{T}_k^n e^{ikx_m}$

- If $T_m^n = \widehat{T}_k^n e^{ikx_m} = \widehat{T}_k^n e^{ikam}$ (one Fourier mode in x), and
$$T_m^{n+1} = T_m^n + \frac{\kappa h}{a^2}\left(T_{m+1}^n - 2T_m^n + T_{m-1}^n\right)$$
Then
$$\widehat{T}_k^{n+1} e^{ikam} = \left(1 - \frac{2\kappa h}{a^2}\right)\widehat{T}_k^n e^{ikam} + \frac{\kappa h}{a^2}\left(\widehat{T}_k^n e^{ika(m+1)} - \widehat{T}_k^n e^{ika(m-1)}\right)$$
$$\Rightarrow \left|\frac{\widehat{T}_k^{n+1}}{\widehat{T}_k^n}\right| = 1 + \frac{\kappa h}{a^2}\left(e^{ika} + e^{-ika} - 2\right) = \left|1 - \frac{4h\kappa}{a^2}\sin^2\left(\frac{ka}{2}\right)\right|.$$
- This is the growth factor, and it should be less than unity if the solution is not meant to grow

Stability criterion:

$$\boxed{h \le \frac{a^2}{2\kappa}}. \qquad \textit{(independent of k!)}$$

FTCS stable for the parabolic equation, provided temporal resolution is adequate ($a \ge \sqrt{2\kappa h}$).

FTCS for hyperbolic equations: instability

- Reminder: wave equation is hyperbolic,
$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2},$$
and is subject to suitable boundary and initial conditions.
- Spatially: $\frac{\partial^2 \phi_m}{\partial t^2} \approx \frac{c^2}{a^2}(\phi_{m+1} - 2\phi_m + \phi_{m-1})\,, \qquad m = 1, \dots, M-1.$
- Temporally: transform to pairs of 1st-order ODEs
$$\frac{\mathrm{d}\phi_m}{\mathrm{d}t} = \psi_m, \quad \text{and} \quad \frac{\mathrm{d}\psi_m}{\mathrm{d}t} = \frac{c^2}{a^2}(\phi_{m+1} - 2\phi_m + \phi_{m-1})$$
and discretize using forward Euler ($2M$ ODEs).

$$\frac{\mathrm{d}\phi_m}{\mathrm{d}t} = \psi_m, \quad \text{and} \quad \frac{\mathrm{d}\psi_m}{\mathrm{d}t} = \frac{c^2}{a^2}(\phi_{m+1} - 2\phi_m + \phi_{m-1})$$

Using forward Euler for each:

$$\begin{aligned} \phi_m^{n+1} &= \phi_m^n + h\psi_m^n, \\ \psi_m^{n+1} &= \psi_m^n + h\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right). \end{aligned}$$

or, equivalently:

$$\begin{bmatrix} \phi_m^{n+1} \\ \psi_m^{n+1} \end{bmatrix} = \begin{bmatrix} 1 & h \\ -\frac{2hc^2}{a^2} & 1 \end{bmatrix} \begin{bmatrix} \phi_m^n \\ \psi_m^n \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{c^2 h}{a^2}\left(\phi_{m+1}^n + \phi_{m-1}^n\right) \end{bmatrix}$$

Take $\begin{bmatrix} \phi_m^{n+1} \\ \psi_m^{n+1} \end{bmatrix} = \begin{bmatrix} 1 & h \\ -\frac{2hc^2}{a^2} & 1 \end{bmatrix} \begin{bmatrix} \phi_m^n \\ \psi_m^n \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{c^2 h}{a^2}\left(\phi_{m+1}^n + \phi_{m-1}^n\right) \end{bmatrix}$

and consider single Fourier mode, $\begin{bmatrix} \phi_m^n \\ \psi_m^n \end{bmatrix} = \begin{bmatrix} \widehat{\phi}_k^n \\ \widehat{\psi}_k^n \end{bmatrix} \mathrm{e}^{\mathrm{i}kma}$. Obtain, after some algebra,

$$\begin{bmatrix} \widehat{\phi}_k^{n+1} \\ \widehat{\psi}_k^{n+1} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \widehat{\phi}_k^n \\ \widehat{\psi}_k^n \end{bmatrix},$$
$$\text{with} \quad \mathbf{A} = \begin{bmatrix} 1 & h \\ -hr^2 & 1 \end{bmatrix} \quad \text{and} \quad r^2 = \frac{2c}{a}\sin\frac{ka}{2},$$

which **does** depend on k.

$\begin{bmatrix} \widehat{\phi}_k^{n+1} \\ \widehat{\psi}_k^{n+1} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \widehat{\phi}_k^n \\ \widehat{\psi}_k^n \end{bmatrix}$, with $\mathbf{A} = \begin{bmatrix} 1 & h \\ -hr^2 & 1 \end{bmatrix}$ and $r = \frac{2c}{a}\sin\frac{ka}{2}$.

- Eigenvalues of $\mathbf{A}$ are $\lambda_1 = 1 + \mathrm{i}hr$ and $\lambda_2 = 1 - \mathrm{i}hr$,
  - therefore, $|\lambda_\pm|^2 = 1 + h^2 r^2 \ge 1$.
- Define corresponding eigenvectors $\mathbf{V}_1$ and $\mathbf{V}_2$, project initial condition on eigenvectors, i.e., write $\alpha_1 \mathbf{V}_1 + \alpha_2 \mathbf{V}_2$.
- After p time steps, solution becomes $\alpha_1 \lambda_1^p \mathbf{V}_1 + \alpha_2 \lambda_2^p \mathbf{V}_2$, which grows unbounded!

$\Rightarrow$ **FTCS always unstable for the wave equation!**

Summary

- 2nd-order PDEs can be elliptical, parabolic, hyperbolic.
- Elliptical equations (e.g., Poisson eqn.):
  - Jacobi relaxation (always stable),
  - Speed-up with overrelaxation (not always stable),
  - Gauss-Seidel (overrelaxed or not): replace on the fly; more stable than Jacobi when overrelaxing.

- Parabolic PDEs (e.g., heat eqn):
  - FTCS (Forward Time, Centred Space) scheme: centred finite-diff. in space, forward Euler in time
  - Von Neumann analysis says stable if sufficient resolution in space.
- Hyperbolic PDEs (e.g., wave eqn.):
  - Von Neumann analysis says FTCS never stable.
  - See next week for better schemes.
- Von Neumann stability analysis: plug a Fourier mode, see if it grows or not.