PHY407 – University of Toronto
Lecture 8: Partial Differential Equations, part 1/2

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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.

1 Intro

1.1 Classifying PDEs

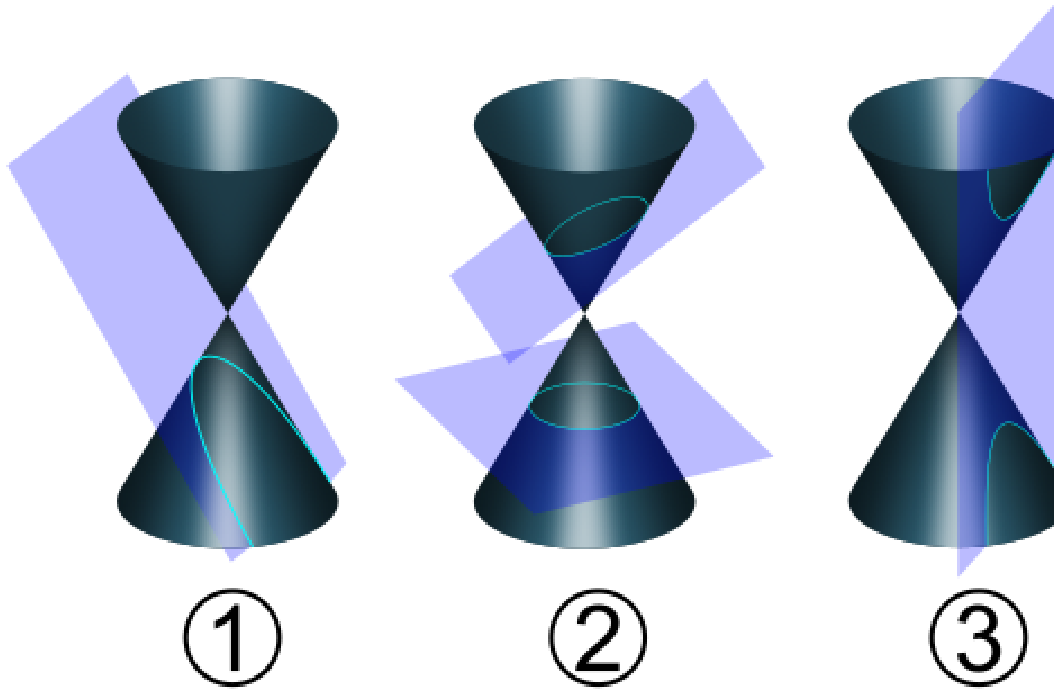
Recall conical equations in geometry:

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

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.



Recall conical equations in geometry:

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

classified using

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

What does it have to do with 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:

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

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

What does it have to do with PDEs?

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

With $\Delta = \beta^2 - 4\alpha\gamma$, 1. $\Delta = 0$: parabolic PDE, 3. $\Delta < 0$: elliptic PDE, 2. $\Delta > 0$: hyperbolic PDE.

1. Canonical parabolic PDE: the diffusion equation, $\kappa\nabla^2\phi - \dfrac{\partial T}{\partial t} = 0$,

$$x \to x, \quad y \to t, \quad \alpha \to \kappa, \quad \varepsilon \to -1, \quad \beta, \gamma, \delta, f \to 0 \quad \Rightarrow \quad \beta^2 - 4\alpha\gamma = 0.$$

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, $c^2\nabla^2\phi - \dfrac{\partial^2\phi}{\partial t^2} = 0$.

$$x \to x, \quad y \to t, \quad \alpha \to c^2, \quad \gamma \to -1, \quad \beta, \delta, \varepsilon, f \to 0 \quad \Rightarrow \quad \beta^2 - 4\alpha\gamma = 4c^2 > 0.$$

Note: we use these expressions even if $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$, i.e., for 4D PDEs. It is a "perversion" of the original classification (see 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 too.

1.2 Calculating the second derivative

- Recall central difference calculation of 2nd derivative (§5.10.5):

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

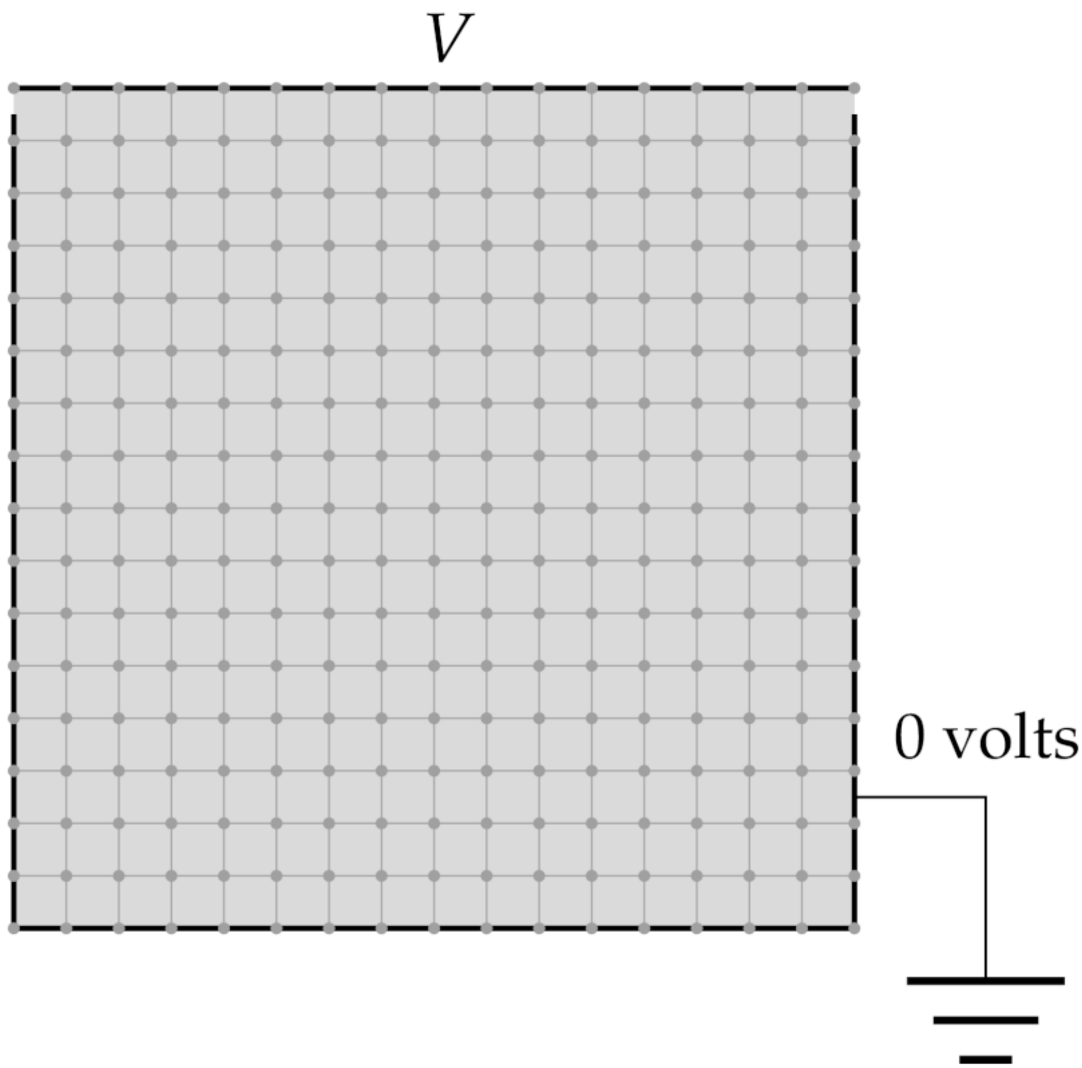
1.3 General approach

- 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.

2 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

$$\frac{\partial^2\phi}{\partial x^2} \approx \frac{\phi(x+a,y) - 2\phi(x,y) + \phi(x-a,y)}{a^2}, \tag{1}$$

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

Gauss's law:

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

- 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. How would you handle these?
- 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.

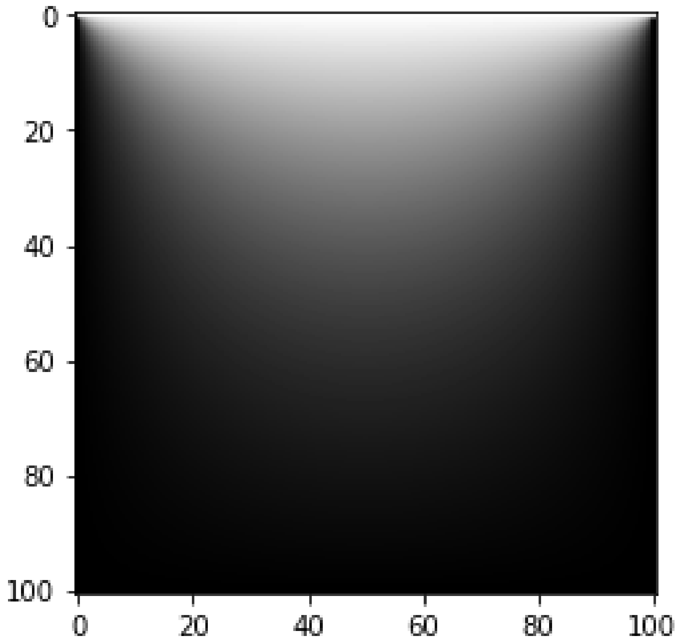
2.1 Jacobi relaxation method

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

* Iterate the rule $\underbrace{\phi'(x,y)}_{\text{"}\phi\text{ prime"}} = \frac{1}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right].$ * 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`

[1]:
```python
# %load laplace.py
# Newman's laplace.py
from numpy import empty, zeros, max
from pylab import imshow, gray, show

# Constants
M = 100         # Grid squares on a side
V = 1.0         # Voltage at top wall
target = 1e-6   # [V] Target accuracy

# Create arrays to hold potential values
phi = zeros([M+1, M+1], float)
phi[0, :] = V
phiprime = empty([M+1, M+1], float)

# Main loop
delta = 1.0
while delta > target:

    # Calculate new values of the potential
    for i in range(M+1):
        for j in range(M+1):
            if i == 0 or i == M or j == 0 or j == M:
                phiprime[i, j] = phi[i, j]
            else:
                phiprime[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 = max(abs(phi-phiprime))
```

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

# Make a plot
imshow(phi)
gray()
show()
```



2.2 Overrelaxation method

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

* When it works, it ususally speeds up the calculation. * Not always stable! How to choose ω is not always reproducible. * see Lab #4 (Newman's exercise 6.11) for a similar problem for finding $f(x) = x$.

2.3 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': 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:

[ ]:
```
# Calculate new values of the potential
for i in range(M+1):
    for j in range(M+1):
        if i == 0 or i == M or j == 0 or j == M:
            phiprime[i, j] = phi[i, j]
        else:
            phiprime[i, j] = (phi[i+1, j] + phi[i-1, j]
                              + phi[i, j+1] + phi[i, j-1])/4
```

becomes:

[ ]:
```
# Calculate new values of the potential
for i in range(1, M):  # CHANGE HERE: boundaries never updated
    for j in range(1, M):  # CHANGE HERE
        phi[i, j] = (phi[i+1, j] + phi[i-1, j]  # NO PHIPRIME
                     + phi[i, j+1] + phi[i, j-1])/4
```

3 Parabolic PDEs: FTCS method

- Stands for "Forward Time, Centred Space".
- 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

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

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

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

Step 2: Discretize in time

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

Let $t_n = nh$, h the time step.

Let $T_m(t_n) \equiv T_m^n$.

$$\Rightarrow \left.\frac{\partial T}{\partial t}\right|_{x=ma,t=nh} \approx \frac{T_m^{n+1}-T_m^n}{h} \equiv \kappa \frac{T_{m+1}^n - 2T_m^n + T_{m-1}^n}{a^2} \text{ (``Forward (Euler) Time'', FT).}$$

$\Rightarrow$ **Explicit FTCS method:**

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

4 Intro to stability analysis

4.1 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:

$$T_m^n = \sum_k \widehat{T}_k^n \exp(ikx_m)$$

- If $T_m^n = \widehat{T}_k^n \exp(ikx_m) = \widehat{T}_k^n \exp(ikam)$ (one Fourier mode in x), and

$$T_m^{n+1} = T_m^n + \frac{\kappa h}{a^2}\left(T_{m+1}^n - 2T_m^n + T_{m-1}^n\right)$$

  becomes

$$\widehat{T}_k^{n+1} e^{ikam} = \left(1 - \frac{2\kappa h}{a^2}\right)\widehat{T}_k^n e^{ikam} + \frac{\kappa h}{a^2}\left(\widehat{T}_k^n e^{ika(m+1)} - \widehat{T}_k^n e^{ika(m-1)}\right)$$

$$\Rightarrow \left|\frac{\widehat{T}_k^{n+1}}{\widehat{T}_k^n}\right| = 1 + \frac{\kappa h}{a^2}\left(e^{ika} + e^{-ika} - 2\right) = \left|1 - \frac{4h\kappa}{a^2}\sin^2\left(\frac{ka}{2}\right)\right|.$$

- This is the growth factor, and it should be less than unity if the solution is not meant to grow, i.e.:

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

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

4.2 FTCS for the wave equation

- 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: $\dfrac{\partial^2 \phi_m}{\partial t^2} \approx \dfrac{c^2}{a^2}\left(\phi_{m+1} - 2\phi_m + \phi_{m-1}\right), \quad m = 1, \ldots, M-1.$
- Now transform to pairs of 1st-order ODEs:

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

  and discretize using forward Euler ($2M$ ODEs).

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

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:

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

Recall

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

Consider a single Fourier mode,

$$\begin{bmatrix} \phi_m^n \\ \psi_m^n \end{bmatrix} = \begin{bmatrix} \widehat{\phi}_k^m \\ \widehat{\psi}_k^m \end{bmatrix} \exp(ikma)$$

and we obtain, after some algebra

$$\begin{bmatrix} \widehat{\phi}_k^{m+1} \\ \widehat{\psi}_k^{m+1} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \widehat{\phi}_k^m \\ \widehat{\psi}_k^m \end{bmatrix} \exp(ikma),$$

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

which **does** depend on k.

$$\begin{bmatrix} \widehat{\phi}_k^{m+1} \\ \widehat{\psi}_k^{m+1} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \widehat{\phi}_k^m \\ \widehat{\psi}_k^m \end{bmatrix} \exp(ikma),$$

$$\text{with} \quad \mathbf{A} = \begin{bmatrix} 1 & h \\ -hr^2 & 1 \end{bmatrix} \quad \text{and} \quad r = \frac{2c}{a}\sin\frac{ka}{2}.$$

- Eigenvalues of $\mathbf{A}$ are $\lambda_\pm = 1 \pm ihr$,
- therefore, $|\lambda_\pm|^2 = 1 + h^2 r^2 \geq 1$.
- Define corresponding eigenvectors $\mathbf{V}_\pm$, suppose initial condition is $\alpha_+\mathbf{V}_+ + \alpha_-\mathbf{V}_-$.
- After p time steps, this becomes $\alpha_+\lambda_+^p\mathbf{V}_+ + \alpha_-\lambda_-^p\mathbf{V}_-$, which will grow without bounds!

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

5 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 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.