Partial differential equations

Method of finite differences… Consider the Laplace equation in 2D:

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

Remember how we can calculate 2nd derivatives with step size a:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\psi(x+a,y) + \psi(x-a,y) - 2\psi(x,y)}{a^2}$$

$$\frac{\partial^2 \psi}{\partial y^2} = \frac{\psi(x,y+a) + \psi(x,y-a) - 2\psi(x,y)}{a^2}$$

Combining:

$$\frac{\psi(x+a,y)+\psi(x-a,y)+\psi(x,y+a)+\psi(x,y-a)-4\psi(x,y)}{a^2}=0$$

Or:

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

Note that the above is an equation for the field at every point (x,y), given some spacing value a. We can use the relaxation method (Jacobi method here) for solving it, assuming the field has no crazy shape

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

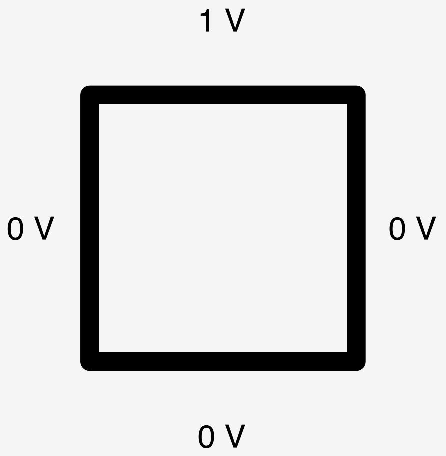
Jacobi method

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

We guess some initial values of the field that respect the boundary conditions we are trying to set. And then we update the field based on the above equation. And repeat until things converge

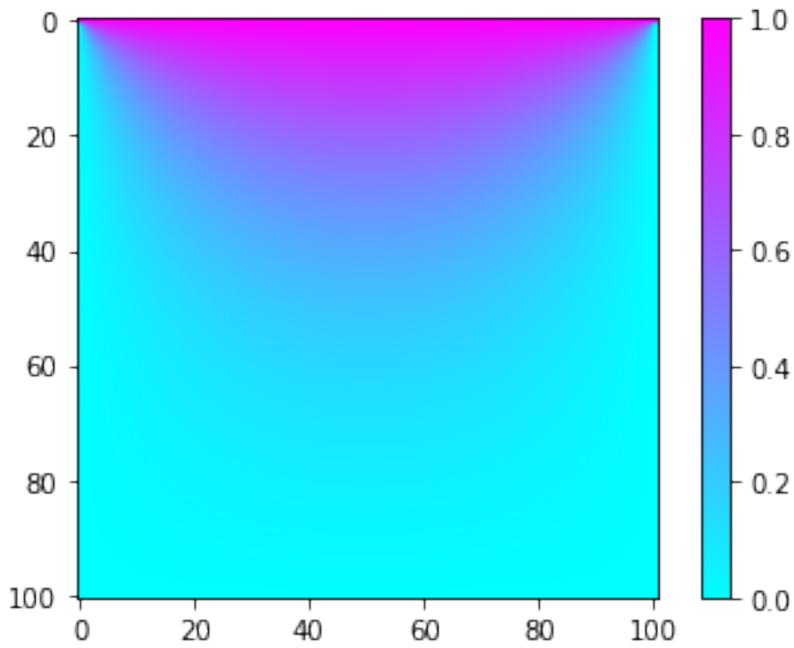
Laplace’s Equation for a simple example

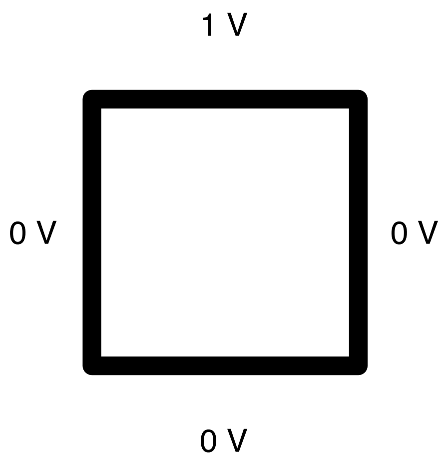

```python
# Laplace's equation for a box at 1 V on the top, 0 V on the sides
from numpy import empty,zeros,max
from pylab import imshow,colorbar,show
import pylab as plt

M = 100
V = 1.0
target = 1e-5

phi = zeros([M+1,M+1],float)
phi[0,:] = V
phiprime = empty([M+1,M+1],float)

delta = 1.0
while delta > target:
  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
  delta = max(abs(phi-phiprime))
  phi,phiprime = phiprime, phi

imshow(phi,cmap=plt.get_cmap('cool'))
colorbar()
show()
```



Let’s discuss this

Laplace's Equation for a simple example





What if we have charge?

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}$$

As before, we write this as

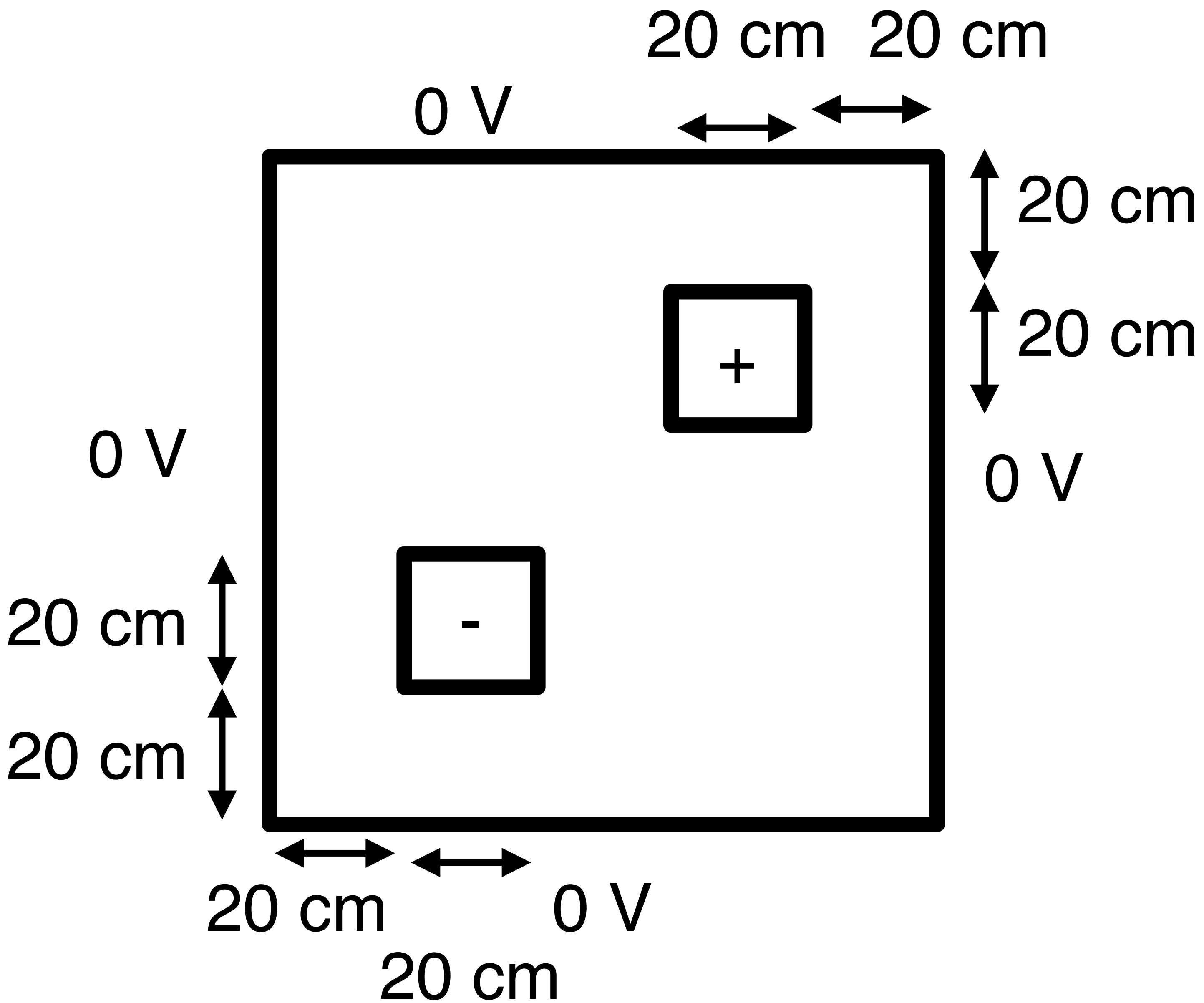
$$\frac{\psi(x+a,y)+\psi(x-a,y)+\psi(x,y+a)+\psi(x,y-a)-4\psi(x,y)}{a^2} = -\frac{\rho}{\epsilon_0}$$

Can use the same relaxation method approach:

$$\psi(x,y) = \frac{1}{4}\left[\psi(x+a,y)+\psi(x-a,y)+\psi(x,y+a)+\psi(x,y-a)\right] + \frac{a^2}{4\epsilon_0}\rho(x,y)$$

But we have to be careful, grid spacing no longer cancels out!

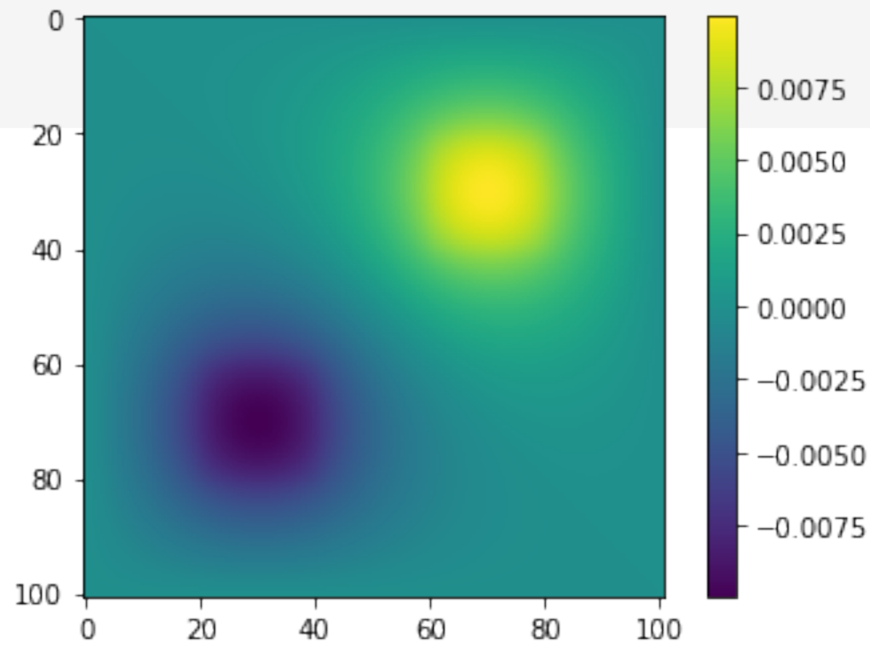
What if we have charge?



What if we have charge? (Exercise 9.1)


```
# Exercise 9.1

from numpy import empty,zeros,max
from pylab import imshow, colorbar,show

# Constants
L = 1.0 # box length
M = 100 # squares on a side
a = L/M # size of square
rho0 = 1.0 # Charge density
epsilon0 = 1.0 # our units
target = 1e-6 # Target accuracy

# Create arrays
phi = zeros([M+1,M+1],float)
phiprime = zeros([M+1,M+1],float)
rho = zeros([M+1,M+1],float)
rho[20:41,60:81] = rho0
rho[60:81,20:41] = -rho0
```

```
# Main loop
delta = 1.0
while delta > target:
  # Calculate new values of potential
  phiprime[0,:] = 0.0
  phiprime[M,:] = 0.0
  phiprime[:,0] = 0.0
  phiprime[:,M] = 0.0
  phiprime[1:M,1:M] = (phi[0:M-1,1:M] + phi[2:M+1,1:M] + phi[1:M,0:M-1] + phi[1:M,2:M+1])/4 \
                        + rho[1:M,1:M]*a*a/(4*epsilon0)
  # Calculate max change
  delta = max(abs(phi-phiprime))
  # Swap the two arrays
  phi,phiprime = phiprime,phi

# Make plot
imshow(phi)
colorbar()
show()
```



Overrelaxation

Perhaps noticed in previous examples that the code is quite slow. A 100x100 2d grid requires 10^4 updates each cycle, and is also slow to converge

Proposal: In the relaxation method, we are iterating and setting $\phi'(x,y) = \phi(x,y) + \Delta\phi(x,y)$. Let's try and "speed up" the process (at the risk of over-shooting):

$$\phi'(x,y) = \phi(x,y) + (1+\omega)\Delta\phi(x,y)$$

If $\omega == 0$, then we get back our old method, any positive value means over-relaxation

Overrelaxation

$$\phi_\omega(x,y) = \phi(x,y) + (1+\omega)\Delta\phi(x,y)$$

$$\phi_\omega(x,y) = \phi(x,y) + (1+\omega)\left[\phi^{'}(x,y) - \phi(x,y)\right]$$

$$\phi_\omega(x,y) = (1+\omega)\phi^{'}(x,y) - \omega\phi(x,y)$$

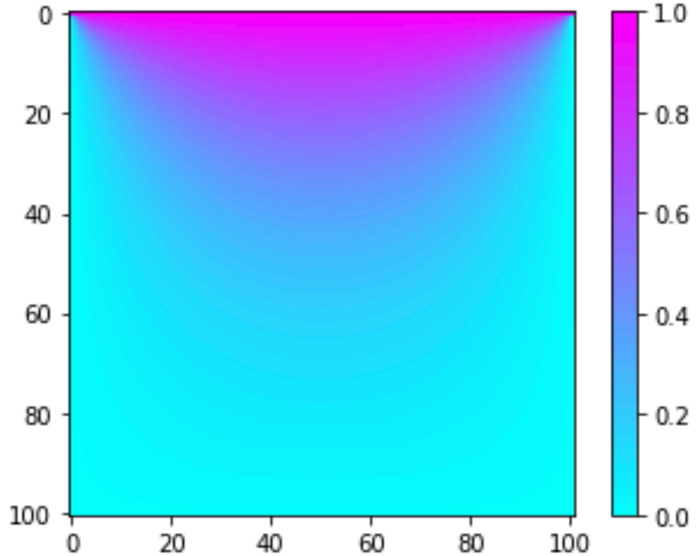
$$\phi_\omega(x,y) = \frac{1+\omega}{4}\left[\phi(x+a,y) + \phi(x-a,y) + \phi(x,y+a) + \phi(x,y-a)\right] - \omega\phi(x,y)$$

Overrelaxation example (9.2)

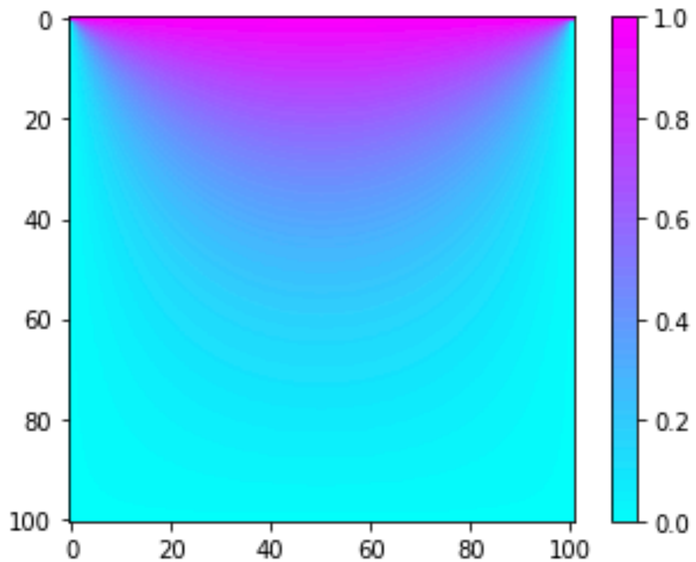
```
[26] # Laplace's equation for a box at 1 V on the top, 0 V on the sides
     # Exercise 9.2, over-relaxation
     from numpy import empty,zeros,max
     from pylab import imshow,colorbar,show
     import pylab as plt
     import time

     def runLaplaceOverRelax(omega = 0.9):
       L = 1.0
       M = 100
       V = 1.0
       target = 1e-6
       tstart = time.perf_counter()
       phi = zeros([M+1,M+1],float)
       phi[0,:] = V
       dphi = zeros([M+1,M+1],float)
       delta = 1.0
       while delta > target:
         for i in range(1,M):
           for j in range(1,M):
             dphi[i,j] = (1.+omega)*((phi[i+1,j] + phi[i-1,j] + phi[i,j+1] + phi[i,j-1]) / 4 - phi[i,j])
             phi[i,j] += dphi[i,j]
         delta = max(abs(dphi))
       imshow(phi,cmap=plt.get_cmap('cool'))
       colorbar()
       show()
       tend = time.perf_counter()
       print("Omega = ",omega," and it took",(tend - tstart)," seconds")
```

```
runLaplaceOverRelax(0.9)
runLaplaceOverRelax(0.8)
runLaplaceOverRelax(0.1)
runLaplaceOverRelax(0.0)
```

Overrelaxation example (9.2)




```
Omega =  0.9  and it took 10.56870855399984  seconds
```



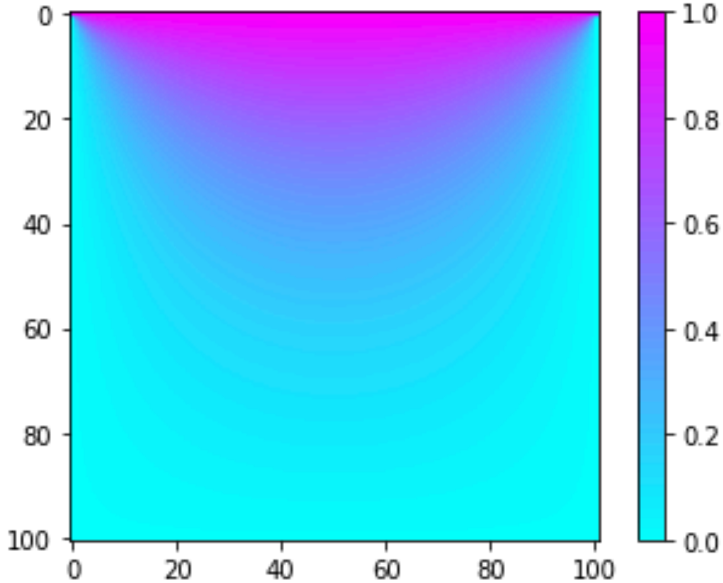

```
Omega =  0.8  and it took 22.417167475000042  seconds
```

MUCH faster! BUT:

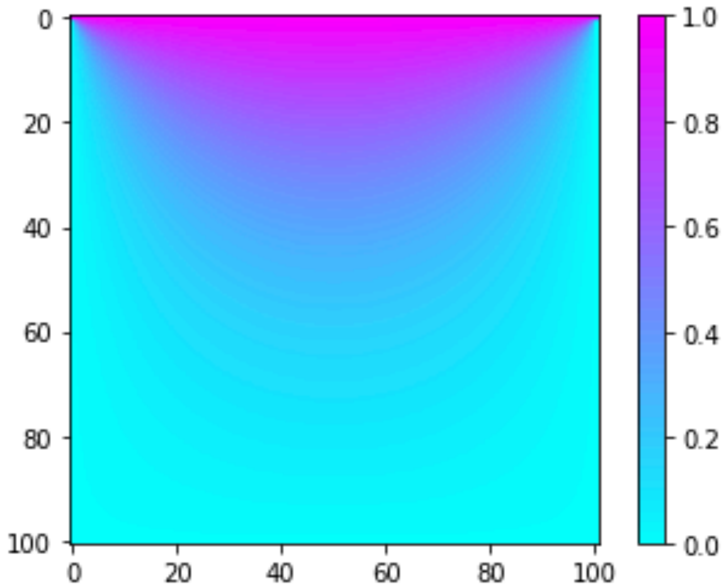
What do we think this does?

```
runLaplaceOverRelax(1.0)
```

Overrelaxation example (9.2)



Omega = 0.1 and it took 126.85352892300011 seconds



Omega = 0.0 and it took 145.62474876800025 seconds

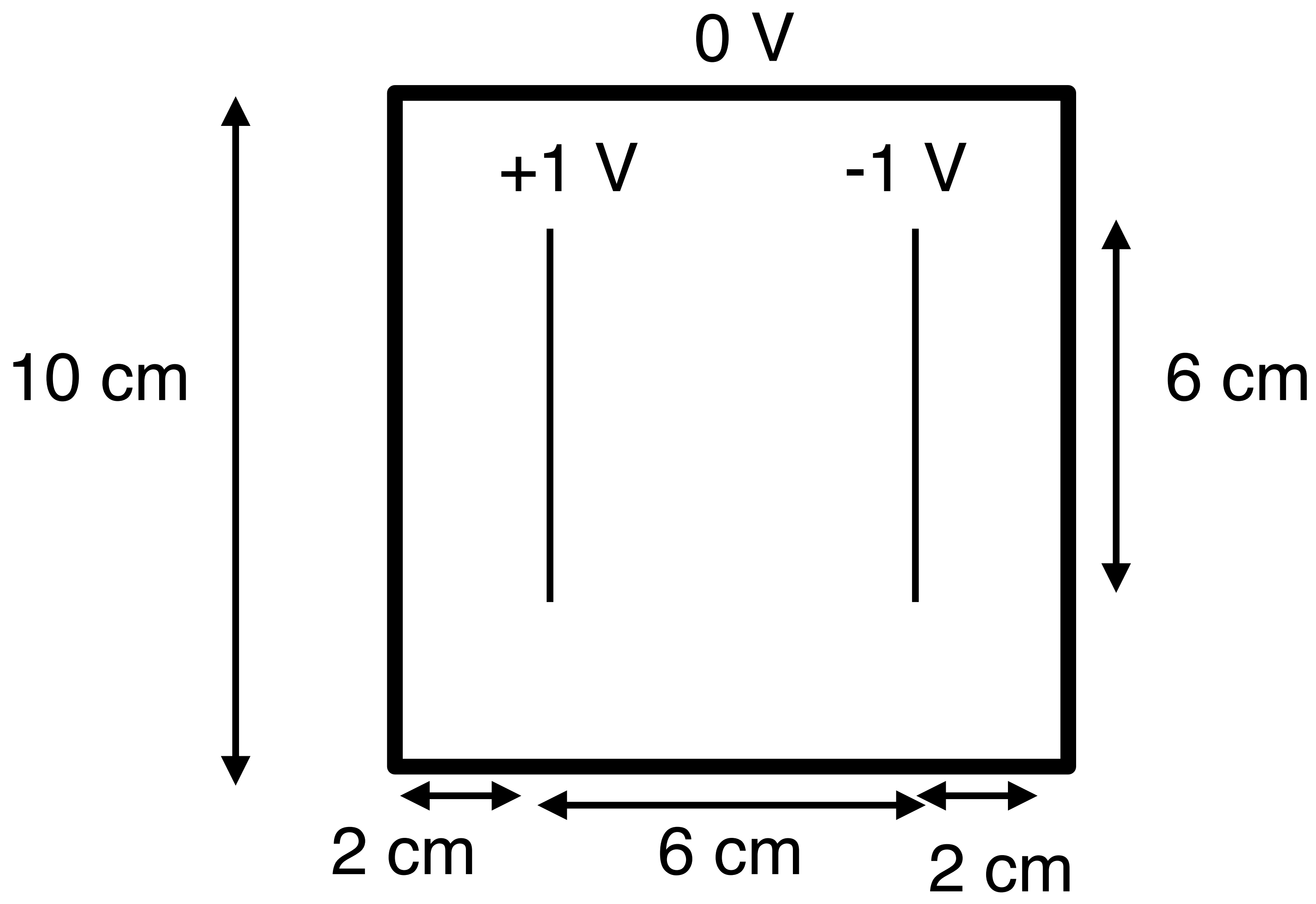
Gauss-Seidel method

In previous method, we used all the old values to compute our new values. And then we repeat. But in principle all the new values are better than the old ones, so we should just use them, even before we finish our next iteration

Only store one set of arrays ("best current guess"), not old and new. Saves on memory!

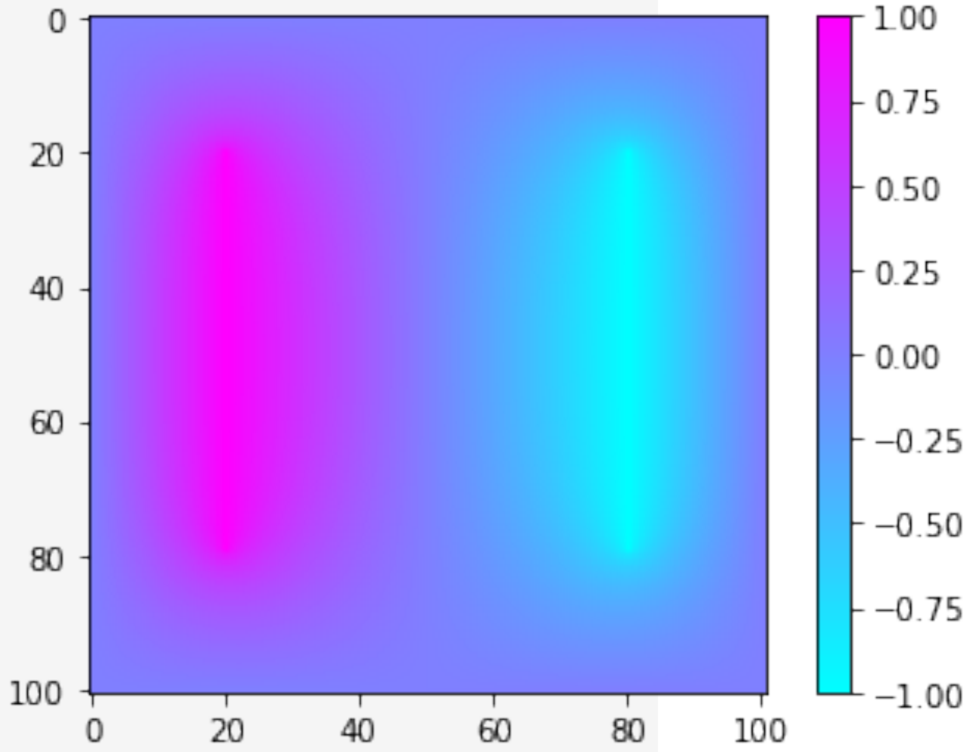
We will combine the Gauss-Seidel and over-relaxation methods. Book suggests a value of $\omega = 0.9$. Too big and results can be unstable

Gauss-Seidel method, Exercise 9.3



Gauss-Seidel method, Exercise 9.3

```
## Exercise 9.3, capacitor using Gauss-Seidel and over-relaxation

from numpy import zeros,max
from pylab import imshow, show, colorbar

L = 0.1
N = 100
a = L/N
clo = N//5
chi = 4*N//5
omega = 0.9

## Set up initial values and boundary array
phi = zeros([N+1,N+1],float)
phi[clo:chi,clo] = +1.0
phi[clo:chi,chi] = -1.0

# Store where plates are located
plates = zeros([N+1,N+1],int)
plates[clo:chi,clo] = 1
plates[clo:chi,chi] = 1

# Solve for phi
delta = 1.0
target = 1e-6
while delta > target:
  delta = 0.0
  for i in range(1,N):
    for j in range(1,N):
      if plates[i,j] == 0:
        oldphi = phi[i,j]
        phi[i,j] = (1+omega)*(phi[i+1,j] + phi[i-1,j] + phi[i,j+1] + phi[i,j-1])/4 - omega*phi[i,j]
        epsilon = abs(phi[i,j] - oldphi)
        if (epsilon > delta): delta = epsilon

# Draw results
imshow(phi,cmap=plt.get_cmap('cool'))
colorbar()
show()
```



Diffusion equation

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2}$$

One-dimensional diffusion equation. Also the 1D heat equation where ϕ(x,t) is the temperature at some position and time

We typically can't use the relaxation method because we know the initial temperature at all x, but not the final temperature (at any, let alone all x). So we don't have the full boundary

Diffusion equation

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)}{a^2}$$

$$\frac{d\phi}{dt} = \frac{D}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

Euler:

$$\phi(t+h) = \phi(t) + h\frac{d\phi}{dt} = \phi(t) + hf(\phi,t)$$

Diffusion equation

$$\frac{d\phi}{dt} = \frac{D}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(t+h) = \phi(t) + h\frac{d\phi}{dt}$$

$$\phi(t+h) - \phi(t) = h\frac{d\phi}{dt}$$

Forward-time center-space method (FTCS), with h the spacing in time and a the spacing in position

$$\frac{hD}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right] = \phi(t+h) - \phi(t)$$

Following the textbook now closely, we try and solve the wave equation

$$\frac{\partial^2 \phi}{\partial t^2} = v^2 \frac{\partial^2 \phi}{\partial x^2}$$

$$\frac{d^2 \phi}{dt^2} = \frac{v^2}{a^2} \left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t) \right]$$

How to deal with a second-order equation? Remember from a few weeks ago, we can turn this into two first-order equations…

Wave equation

$$\frac{d^2\phi}{dt^2} = \frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\frac{d\psi}{dt} = \frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\frac{d\phi}{dt} = \psi(x,t)$$

Now we apply Euler's method twice, once for each of our two variables

Wave equation

$$\frac{d\psi}{dt} = \frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\frac{d\phi}{dt} = \psi(x,t)$$

Euler:

$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t)$$

Unfortunately, these two equations together are **numerically instable**. Let's continue to follow the book and do a von Neumann analysis to see why

von Neumann analysis

Let's go back and consider the solutions to the diffusion equation first, and look at them at one specific moment in time. If they are at one moment in time, we can do a Fourier decomposition:

$$\phi(x,t) = \sum_k c_k(t) e^{ikx}$$

$$\frac{hD}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right] = \phi(t+h) - \phi(t)$$

$$\phi(x,t+h) = \phi(x,t) + \frac{hD}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

von Neumann analysis

$$\phi(x,t) = \sum_k c_k(t) e^{ikx}$$

$$\phi(x,t+h) = \phi(x,t) + \frac{hD}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \sum_k c_k(t) e^{ikx} + \frac{hD}{a^2}\sum_k \left[c_k(t) e^{ik(x+a)} + c_k(t) e^{ik(x-a)} - 2c_k(t) e^{ikx}\right]$$

$$\phi(x,t+h) = \sum_k c_k(t) e^{ikx} + \frac{hD}{a^2}\sum_k c_k(t) e^{ikx}\left[e^{ika} + e^{-ika} - 2\right]$$

$$\phi(x,t+h) = \sum_k c_k(t) e^{ikx}\left[1 + \frac{hD}{a^2}\left(e^{ika} + e^{-ika} - 2\right)\right]$$

von Neumann analysis

$$\phi(x,t+h) = \sum_k c_k(t)e^{ikx}\left[1+\frac{hD}{a^2}\left(e^{ika}+e^{-ika}-2\right)\right]$$

$$\phi(x,t+h) = \sum_k c_k(t)e^{ikx}\left[1+\frac{hD}{a^2}\left(2\cos(ka)-2\right)\right]$$

$$\phi(x,t+h) = \sum_k c_k(t)e^{ikx}\left[1+\frac{hD}{a^2}\left(-4\sin^2 ka/2\right)\right]$$

$$\phi(x,t+h) = \sum_k c_k(t)e^{ikx}\left[1-\frac{4hD}{a^2}\sin^2\frac{ka}{2}\right]$$

von Neumann analysis

$$\phi(x, t+h) = \sum_k c_k(t) e^{ikx} \left[1 - \frac{4hD}{a^2} \sin^2 \frac{ka}{2} \right]$$

So we can read off the Fourier coefficients at some later time t+h:

$$c_k(t+h) = c_k(t) \left[1 - \frac{4hD}{a^2} \sin^2 \frac{ka}{2} \right]$$

Term in brackets can never be > 1 (sin^2 is always positive), but it can be < 1, which would imply exponential instability at t increases

von Neumann analysis

$$c_k(t+h) = c_k(t)\left[1 - \frac{4hD}{a^2}\sin^2\frac{ka}{2}\right]$$

Term in brackets can never be > 1 (sin^2 is always positive), but it can be < 1, which would imply exponential instability at t increases. Stable if:

$$\left[1 - \frac{4hD}{a^2}\sin^2\frac{ka}{2}\right] > -1$$

$$\frac{4hD}{a^2}\sin^2\frac{ka}{2} < 2$$

Largest possible value of sin^2 is 1, so…

von Neumann analysis

$$\frac{4hD}{a^2}\sin^2\frac{ka}{2} < 2$$

$$\frac{4hD}{a^2} < 2$$

Stability if: $$h < \frac{a^2}{2D}$$ (stable if step size small enough!)

Stability means the coefficients c_k all approach zero as time increases. Only term for which this is not true is the k = 0 piece:

$$c_k(t+h) = c_k(t)\left[1 - \frac{4hD}{a^2}\sin^2\frac{ka}{2}\right]$$

k = 0 component is the long-term remaining piece

von Neumann analysis of wave equation

Suppress the summation:

$$\begin{pmatrix} \phi(x,t) \\ \psi(x,t) \end{pmatrix} = \begin{pmatrix} c_\phi(t) \\ c_\psi(t) \end{pmatrix} e^{ikx}$$

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t)$$

$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

First equation is simpler:

$$c_\phi(t+h) = c_\phi(t) + hc_\psi(t)$$

Second equation:

$$c_\psi(t+h)e^{ikx} = c_\psi(t)e^{ikx} + h\frac{v^2}{a^2}\left[c_\phi(t)e^{ik(x+a)} + c_\phi(t)e^{ik(x-a)} - 2c_\phi e^{ikx}\right]$$

von Neumann analysis of wave equation

$$c_\phi(t+h) = c_\phi(t) + hc_\psi(t)$$

$$c_\psi(t+h)e^{ikx} = c_\psi(t)e^{ikx} + h\frac{v^2}{a^2}\left[c_\phi(t)e^{ik(x+a)} + c_\phi(t)e^{ik(x-a)} - 2c_\phi e^{ikx}\right]$$

Same rearrangement as before:

$$c_\psi(t+h)e^{ikx} = c_\psi(t)e^{ikx} + hc_\phi e^{ikx}\frac{v^2}{a^2}\left[e^{ika} + e^{-ika} - 2\right]$$

$$c_\psi(t+h) = c_\psi(t) + hc_\phi\frac{v^2}{a^2}\left[e^{ika} + e^{-ika} - 2\right]$$

$$c_\psi(t+h) = c_\psi(t) - hc_\phi\frac{4v^2}{a^2}\sin^2\frac{ka}{2}$$

von Neumann analysis of wave equation

$$c_\phi(t+h) = c_\phi(t) + hc_\psi(t)$$

$$c_\psi(t+h) = c_\psi(t) - hc_\phi \frac{4v^2}{a^2} \sin^2 \frac{ka}{2}$$

Write the two equations in vector form:

$\mathbf{c}(t+h) = \mathbf{A}\mathbf{c}(t)$

$\mathbf{c}(t) = (c_\Phi, c_\psi)$

$$\mathbf{A} = \begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix}$$

$$r = \frac{2v}{a} \sin \frac{ka}{2}$$

von Neumann analysis of wave equation

c(t+h) = **Ac**(t)

c(t) = (c_Φ,c_ψ)

$$\mathbf{A} = \begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix}$$

$$r = \frac{2v}{a} \sin \frac{ka}{2}$$

Any solution at time t can be written as a linear combination of the eigenvectors of the matrix **A**, which has eigenvalues λ_1 and λ_2

$$\mathbf{c}(t) = (\alpha_1 \mathbf{v_1} + \alpha_2 \mathbf{v_2})$$

$$\mathbf{c}(t+h) = \mathbf{Ac}(t) = (\alpha_1 \lambda_1 \mathbf{v_1} + \alpha_2 \lambda_2 \mathbf{v_2})$$

$$\mathbf{c}(t+2h) = \mathbf{Ac}(t+h) = (\alpha_1 \lambda_1^2 \mathbf{v_1} + \alpha_2 \lambda_2^2 \mathbf{v_2})$$

$$\mathbf{c}(t+nh) = \mathbf{Ac}(t+(n-1)h) = (\alpha_1 \lambda_1^n \mathbf{v_1} + \alpha_2 \lambda_2^n \mathbf{v_2})$$

von Neumann analysis of wave equation

c(t+h) = **Ac**(t)

c(t) = (c_Φ,c_ψ)

$$\mathbf{A} = \begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix}$$

$$r = \frac{2v}{a} \sin \frac{ka}{2}$$

Our solutions as time increases will only be stable if the eigenvalues have magnitude less than 1

$$\mathbf{c}(t) = (\alpha_1 \mathbf{v_1} + \alpha_2 \mathbf{v_2})$$

$$\mathbf{c}(t+h) = \mathbf{Ac}(t) = (\alpha_1 \lambda_1 \mathbf{v_1} + \alpha_2 \lambda_2 \mathbf{v_2})$$

$$\mathbf{c}(t+2h) = \mathbf{Ac}(t+h) = (\alpha_1 \lambda_1^2 \mathbf{v_1} + \alpha_2 \lambda_2^2 \mathbf{v_2})$$

$$\mathbf{c}(t+nh) = \mathbf{Ac}(t+(n-1)h) = (\alpha_1 \lambda_1^n \mathbf{v_1} + \alpha_2 \lambda_2^n \mathbf{v_2})$$

von Neumann analysis of wave equation

$$\mathbf{A} = \begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix}$$

$$r = \frac{2v}{a} \sin \frac{ka}{2}$$

$$(1-\lambda)^2 + h^2 r^2 = 0 \rightarrow \lambda = 1 \pm ihr$$

Magnitude of all but the k=0 component is always larger than 1, so this is not stable! We need to find a new approach

Crank-Nicolson method

Start with wave equation as before:

$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t)$$

Made the substitution h→-h:

$$\psi(x,t-h) = \psi(x,t) - h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t-h) = \phi(x,t) - h\psi(x,t)$$

And now t→t+h:

$$\psi(x,t) = \psi(x,t+h) - h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]$$

$$\phi(x,t) = \phi(x,t+h) - h\psi(x,t+h)$$

Crank-Nicolson method

Two sets of equations:

$$\psi(x, t+h) = \psi(x, t) + h\frac{v^2}{a^2}\left[\phi(x+a, t) + \phi(x-a, t) - 2\phi(x, t)\right]$$
$$\phi(x, t+h) = \phi(x, t) + h\psi(x, t)$$

$$\psi(x, t) = \psi(x, t+h) - h\frac{v^2}{a^2}\left[\phi(x+a, t+h) + \phi(x-a, t+h) - 2\phi(x, t+h)\right]$$
$$\phi(x, t) = \phi(x, t+h) - h\psi(x, t+h)$$

Let's rewrite the bottom ones to be in the same form as the other ones:

$$\psi(x, t+h) = \psi(x, t) + h\frac{v^2}{a^2}\left[\phi(x+a, t+h) + \phi(x-a, t+h) - 2\phi(x, t+h)\right]$$
$$\phi(x, t+h) = \phi(x, t) + h\psi(x, t+h)$$

Crank-Nicolson method

Two sets of equations:

$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t)$$

$$\psi(x,t+h) = \psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]$$

$$\phi(x,t+h) = \phi(x,t) + h\psi(x,t+h)$$

Two equations for our two variables at position x and time t+h. Which is right? Let's take the average of the two:

$$\psi(x,t+h) = \frac{1}{2}\left[\psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]\right] +$$

$$\frac{1}{2}\left[\psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]\right]$$

$$\phi(x,t+h) = \frac{1}{2}\left[\phi(x,t) + h\psi(x,t+h) + \phi(x,t) + h\psi(x,t)\right]$$

Crank-Nicolson method

$$\psi(x,t+h) = \frac{1}{2}\left[\psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]\right] +$$

$$\frac{1}{2}\left[\psi(x,t) + h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]\right]$$

$$\phi(x,t+h) = \frac{1}{2}\left[\phi(x,t) + h\psi(x,t+h) + \phi(x,t) + h\psi(x,t)\right]$$

$$\psi(x,t+h) = \psi(x,t) +$$

$$h\frac{v^2}{2a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h) + \phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \phi(x,t) + \frac{h}{2}\left[\psi(x,t+h) + \psi(x,t)\right]$$

Again look at plane wave solutions:

$$\begin{pmatrix} \phi(x,t) \\ \psi(x,t) \end{pmatrix} = \begin{pmatrix} c_\phi(t) \\ c_\psi(t) \end{pmatrix} e^{ikx}$$

Crank-Nicolson method

$$\psi(x,t+h) = \psi(x,t) +$$

$$h\frac{v^2}{2a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h) + \phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

$$\phi(x,t+h) = \phi(x,t) + \frac{h}{2}\left[\psi(x,t+h) + \psi(x,t)\right]$$

$$\begin{pmatrix} \phi(x,t) \\ \psi(x,t) \end{pmatrix} = \begin{pmatrix} c_\phi(t) \\ c_\psi(t) \end{pmatrix} e^{ikx}$$

Second equation is the easier one, again:

$$c_\phi(t+h) = c_\phi(t) + \frac{h}{2}(c_\psi(t+h) + c_\psi(t))$$

First equation:

$$c_\psi(t+h) = c_\psi(t) + \frac{hv^2}{2a^2}\left(e^{ika}c_\phi(t+h) + e^{-ika}c_\phi(t+h) - 2c_\phi(t+h) + e^{ika}c_\phi(t) + e^{-ika}c_\phi(t) - 2c_\phi(t)\right)$$

Crank-Nicolson method

$$c_\phi(t+h) = c_\phi(t) + \frac{h}{2}\left(c_\psi(t+h) + c_\psi(t)\right)$$

$$c_\psi(t+h) = c_\psi(t) + \frac{hv^2}{2a^2}\left(e^{ika}c_\phi(t+h) + e^{-ika}c_\phi(t+h) - 2c_\phi(t+h) + e^{ika}c_\phi(t) + e^{-ika}c_\phi(t) - 2c_\phi(t)\right)$$

$$c_\phi(t+h) - \frac{h}{2}c_\psi(t+h) = c_\phi(t) + \frac{h}{2}c_\psi(t)$$

$$c_\psi(t+h) - \frac{hv^2}{2a^2}\left(e^{ika}c_\phi(t+h) + e^{-ika}c_\phi(t+h) - 2c_\phi(t+h)\right) = c_\psi(t) + \frac{hv^2}{2a^2}\left(e^{ika}c_\phi(t) + e^{-ika}c_\phi(t) - 2c_\phi(t)\right)$$

$$c_\psi(t+h) + \frac{2hv^2}{a^2}c_\phi(t+h)\sin^2\frac{ka}{2} = c_\psi(t) - \frac{2hv^2}{a^2}\sin^2\frac{ka}{2}c_\phi(t)$$

Crank-Nicolson method

$$c_\phi(t+h) - \frac{h}{2} c_\psi(t+h) = c_\phi(t) + \frac{h}{2} c_\psi(t)$$

$$c_\psi(t+h) + \frac{2hv^2}{a^2} c_\phi(t+h) \sin^2 \frac{ka}{2} = c_\psi(t) - \frac{2hv^2}{a^2} \sin^2 \frac{ka}{2} c_\phi(t)$$

Put in the form we need for matrices:

$$c_\phi(t+h) = h \frac{c_\psi(t)}{\frac{h^2 v^2}{a^2} \sin^2 \frac{ka}{2} + 1} + c_\phi(t) \frac{1 - \frac{h^2 v^2}{a^2} \sin^2 \frac{ka}{2}}{1 + \frac{h^2 v^2}{a^2} \sin^2 \frac{ka}{2}}$$

Crank-Nicolson method

$$c_\phi(t+h) - \frac{h}{2}c_\psi(t+h) = c_\phi(t) + \frac{h}{2}c_\psi(t)$$

$$c_\psi(t+h) + \frac{2hv^2}{a^2}c_\phi(t+h)\sin^2\frac{ka}{2} = c_\psi(t) + \frac{2hv^2}{a^2}\sin^2\frac{ka}{2}c_\phi(t)$$

Put in the form we need for matrices:

$$c_\psi(t+h) = \frac{1-\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}{1+\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}c_\psi(t) - \frac{\frac{4hv^2}{a^2}\sin^2\frac{ka}{2}}{1+\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}c_\phi(t)$$

Crank-Nicolson method

$$c_\phi(t+h) = h\frac{c_\psi(t)}{\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}+1} + c_\phi(t)\frac{1-\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}{1+\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}$$

$$c_\psi(t+h) = \frac{1-\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}{1+\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}c_\psi(t) - \frac{\frac{4hv^2}{a^2}\sin^2\frac{ka}{2}}{1+\frac{h^2v^2}{a^2}\sin^2\frac{ka}{2}}c_\phi(t)$$

$$r = \frac{v}{a}\sin ka/2$$

$$c_\phi(t+h) = hc_\psi(t)\frac{1}{h^2r^2+1} + c_\phi(t)\frac{1-h^2r^2}{1+h^2r^2}$$

$$c_\psi(t+h) = c_\psi(t)\frac{1-h^2r^2}{1+h^2r^2} - c_\phi(t)\frac{4hr^2}{1+h^2r^2}$$

Crank-Nicolson method

$$r = \frac{v}{a}\sin ka/2$$

$$c_\phi(t+h) = hc_\psi(t)\frac{1}{h^2r^2+1} + c_\phi(t)\frac{1-h^2r^2}{1+h^2r^2}$$

$$c_\psi(t+h) = c_\psi(t)\frac{1-h^2r^2}{1+h^2r^2} - c_\phi(t)\frac{4hr^2}{1+h^2r^2}$$

$$\mathbf{A} = \begin{pmatrix} \frac{1-h^2r^2}{1+h^2r^2} & \frac{h}{1+h^2r^2} \\ \frac{-4hr^2}{1+h^2r^2} & \frac{1-h^2r^2}{1+h^2r^2} \end{pmatrix}$$

$$\mathbf{A} = \frac{1}{1+h^2r^2}\begin{pmatrix} 1-h^2r^2 & h \\ -4hr^2 & 1-h^2r^2 \end{pmatrix}$$

Crank-Nicolson method

$$\mathbf{A} = \frac{1}{1+h^2r^2}\begin{pmatrix} 1-h^2r^2 & h \\ -4hr^2 & 1-h^2r^2 \end{pmatrix}$$

$$\mathbf{A} = k\begin{pmatrix} 1-h^2r^2 & h \\ -4hr^2 & 1-h^2r^2 \end{pmatrix} k = \frac{1}{1+h^2r^2}$$

$$(k - kh^2r^2 - \lambda)^2 + 4k^2h^2r^2 = 0$$

$$\lambda^2 + k^2 + k^2h^4r^4 - 2k^2h^2r^2 - 2\lambda k + 2\lambda kh^2r^2 + 4k^2h^2r^2 = 0$$

$$\lambda^2 + \lambda(2kh^2r^2 - 2k) + k^2 + k^2h^4r^4 + 2k^2h^2r^2 = 0$$

Crank-Nicolson method

$$\lambda^2 + \lambda(2kh^2r^2 - 2k) + k^2 + k^2h^4r^4 + 2k^2h^2r^2 = 0$$

$$\lambda = \frac{1}{2}\left(2k - 2kh^2r^2 \pm \sqrt{4k^2h^4r^4 + 4k^2 - 8k^2h^2r^2 - 4k^2 - 4k^2h^4r^4 - 8k^2h^2r^2}\right)$$

$$\lambda = \frac{1}{2}\left(2k - 2kh^2r^2 \pm \sqrt{-16k^2h^2r^2}\right)$$

$$\lambda = k - kh^2r^2 \pm 2ikrh \qquad k = \frac{1}{1 + h^2r^2}$$

These have an imaginary and real component. What are the magnitudes of the eigenvalues?

$$|\lambda| = k(\sqrt{(1 - h^2r^2)^2 + (2rh)^2})$$

Crank-Nicolson method

$$|\lambda| = k(\sqrt{(1-h^2r^2)^2 + (2rh)^2}) \qquad k = \frac{1}{1+h^2r^2}$$

$$|\lambda| = \frac{\sqrt{(1-h^2r^2)^2 + (2rh)^2}}{1+h^2r^2}$$

$$|\lambda| = \frac{\sqrt{1+h^4r^4 - 2h^2r^2 + 4h^2r^2}}{1+h^2r^2}$$

$$|\lambda| = \frac{\sqrt{1+h^4r^4 + 2h^2r^2}}{1+h^2r^2}$$

Crank-Nicolson method

$$|\lambda| = \frac{\sqrt{1 + h^4 r^4 + 2h^2 r^2}}{1 + h^2 r^2}$$

$$|\lambda| = \frac{\sqrt{(1 + h^2 r^2)^2}}{1 + h^2 r^2}$$

$$|\lambda| = 1$$

Phew! So we have shown here that our eigenvalues have magnitude 1, which is what we want. Waves that are in the initial conditions never damp or die out (or grow!) If eigenvalue was larger than 1, any initial waves would grow exponentially, if less than 1 they would die out (we have no damping conditions!)

Schrödinger (Example 9.8)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial dt}$$

Recall FTCS equation:

$$\frac{\partial^2\phi}{\partial t^2} = v^2\frac{\partial^2\phi}{\partial x^2}$$

$$\frac{d^2\phi}{dt^2} = \frac{v^2}{a^2}\left[\phi(x+a,t)+\phi(x-a,t)-2\phi(x,t)\right]$$

where a is the grid point spacing

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = -\frac{\hbar^2}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

Schrödinger (Example 9.8)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial dt}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = -\frac{\hbar^2}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$-\frac{\hbar^2}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right] = i\hbar\frac{\partial\psi}{\partial t}$$

$$\frac{i\hbar}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right] = \frac{\partial\psi}{\partial t}$$

Schrödinger (Example 9.8)

$$\frac{i\hbar}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]=\frac{\partial\psi}{\partial t}$$

Now apply Euler's method:

$$\psi(x,t+h)=\psi(x,t)+h\frac{\partial\psi}{\partial t}$$

$$\psi(x,t+h)=\psi(x,t)+h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

Now let h→ -h as we saw

$$\psi(x,t-h)=\psi(x,t)-h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

And as before let t→ t+h as we saw

$$\psi(x,t)=\psi(x,t+h)-h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$

Schrödinger (Example 9.8)

$$\psi(x,t+h) = \psi(x,t) + h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)\right]$$

$$\psi(x,t) = \psi(x,t+h) - h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h)\right]$$

Rewriting the second equation

$$\psi(x,t+h) = \psi(x,t) + h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h)\right]$$

Two equations for the wave function at position x, time t+h, we can average the two

$$\psi(x,t+h) = \frac{1}{2}\left(2\psi(x,t)\right) +$$

$$\frac{1}{2}\left(h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h) + \psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)\right]\right)$$

Schrödinger (Example 9.8)

$$\psi(x,t+h) = \frac{1}{2}\left(2\psi(x,t)\right) +$$

$$\frac{1}{2}\left(h\frac{i\hbar}{2ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)+\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]\right)$$

$$\psi(x,t+h) = \psi(x,t) +$$

$$h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)+\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$
$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

This is a simultaneous set of equations, one at each of our grid points in space (with grid spacing a)

Schrödinger (Example 9.8)

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$
$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$\psi(t) = \begin{pmatrix} \psi(0,t) \\ \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ \cdot \\ \cdot \\ \cdot \\ \psi(L-a,t) \\ \psi(L,t) \end{pmatrix}$$

Let's put our particle in a box of infinitely high walls at x=0 and x=L, so that the wave function there is zero. Our equation above tells us how to find the wave function at time t+h given the wave function at time t. Note that the "wave function" is a vector along the grid spacing!

Schrödinger (Example 9.8)

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$
$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ . \\ . \\ . \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

Rewrite things as a matrix equation, removing the boundaries where the wave function is constant (and zero)

Schrödinger (Example 9.8)

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$

$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ . \\ . \\ . \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

Work out some of the terms, x=a

$$\psi(a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(2a,t+h)+\psi(0,t+h)-2\psi(a,t+h)\right]$$

$$= \psi(a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(2a,t)+\psi(0,t)-2\psi(a,t)\right]$$

$$\psi(a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(2a,t+h)-2\psi(a,t+h)\right] = \psi(a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(2a,t)-2\psi(a,t)\right]$$

Schrödinger (Example 9.8)

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h)\right]$$
$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)\right]$$

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ \cdot \\ \cdot \\ \cdot \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

Work out some of the terms, x=2a

$$\psi(2a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(3a,t+h) + \psi(a,t+h) - 2\psi(2a,t+h)\right]$$
$$= \psi(2a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(3a,t) + \psi(a,t) - 2\psi(2a,t)\right]$$

Schrödinger (Example 9.8)

$$\psi(x,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)\right]$$

$$= \psi(x,t) + h\frac{i\hbar}{4ma^2}\left[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)\right]$$

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ \cdot \\ \cdot \\ \cdot \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

Work out some of the terms, x=3a

$$\psi(3a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(4a,t+h)+\psi(2a,t+h)-2\psi(3a,t+h)\right]$$

$$= \psi(3a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(4a,t)+\psi(2a,t)-2\psi(3a,t)\right]$$

Schrödinger (Example 9.8)

Let's check this!

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ . \\ . \\ . \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & & & & \\ a_2 & a_1 & a_2 & & & \\ & a_2 & a_1 & a_2 & & \\ & & a_2 & a_1 & a_2 & \\ & & & a_2 & a_1 & a_2 \\ & & & \cdots & & \end{pmatrix}$$

$$a_1 = 1 + h\frac{i\hbar}{2ma^2}$$

$$a_2 = -h\frac{i\hbar}{4ma^2}$$

$$\psi(a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(2a,t+h) - 2\psi(a,t+h)\right] = \psi(a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(2a,t) - 2\psi(a,t)\right]$$

$$\psi(2a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(3a,t+h) + \psi(a,t+h) - 2\psi(2a,t+h)\right]$$

$$= \psi(2a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(3a,t) + \psi(a,t) - 2\psi(2a,t)\right]$$

$$\psi(3a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(4a,t+h) + \psi(2a,t+h) - 2\psi(3a,t+h)\right]$$

$$= \psi(3a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(4a,t) + \psi(2a,t) - 2\psi(3a,t)\right]$$

Schrödinger (Example 9.8)

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ . \\ . \\ . \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

Let's check this!

$$\mathbf{B} = \begin{pmatrix} b_1 & b_2 & & & & \\ b_2 & b_1 & b_2 & & & \\ & b_2 & b_1 & b_2 & & \\ & & b_2 & b_1 & b_2 & \\ & & & b_2 & b_1 & b_2 \\ & & & \cdots & & \end{pmatrix}$$

$$b_1 = 1 - h\frac{i\hbar}{2ma^2}$$

$$b_2 = h\frac{i\hbar}{4ma^2}$$

$$\psi(a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(2a,t+h) - 2\psi(a,t+h)\right] = \psi(a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(2a,t) - 2\psi(a,t)\right]$$

$$\psi(2a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(3a,t+h) + \psi(a,t+h) - 2\psi(2a,t+h)\right]$$

$$= \psi(2a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(3a,t) + \psi(a,t) - 2\psi(2a,t)\right]$$

$$\psi(3a,t+h) - h\frac{i\hbar}{4ma^2}\left[\psi(4a,t+h) + \psi(2a,t+h) - 2\psi(3a,t+h)\right]$$

$$= \psi(3a,t) + h\frac{i\hbar}{4ma^2}\left[\psi(4a,t) + \psi(2a,t) - 2\psi(3a,t)\right]$$

Schrödinger (Example 9.8)

$$\psi(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ . \\ . \\ . \\ \psi(L-a,t) \end{pmatrix}$$

$$\mathbf{A}\psi(t+h) = \mathbf{B}\psi(t)$$

$$\mathbf{B} = \begin{pmatrix} b_1 & b_2 & & & & \\ b_2 & b_1 & b_2 & & & \\ & b_2 & b_1 & b_2 & & \\ & & b_2 & b_1 & b_2 & \\ & & & b_2 & b_1 & b_2 \\ & & & \cdots & & \end{pmatrix}$$

$$b_1 = 1 - h\frac{i\hbar}{2ma^2}$$

$$b_2 = h\frac{i\hbar}{4ma^2}$$

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & & & & \\ a_2 & a_1 & a_2 & & & \\ & a_2 & a_1 & a_2 & & \\ & & a_2 & a_1 & a_2 & \\ & & & a_2 & a_1 & a_2 \\ & & & \cdots & & \end{pmatrix}$$

$$a_1 = 1 + h\frac{i\hbar}{2ma^2}$$

$$a_2 = -h\frac{i\hbar}{4ma^2}$$

Can easily solve using the tools from Chapter 6! What do we get if we start out with a nicely Gaussian wave function?

Schrödinger (Example 9.8)


```
from numpy import empty, arange, linspace, exp, real, full
import matplotlib.pyplot as plt
import matplotlib.animation as animation
from banded import banded

#constants
L = 1.0e-8
N = 1000
a = L/N
m = 9.109e-31
hbar = 1.055e-34
x0 = L/2
sigma = 1.0e-10
kappa = 5.0e10

tmax = 1.0e-12
yscale = 1e-9
h = 5e-19

C = 1j*hbar/(4*m*a*a)
a1 = 1 + 2*h*C
a2 = -h*C
b1 = 1 - 2*h*C
b2 = h*C
```

Schrödinger (Example 9.8)

```
# Create the initial arrays of x and psi values
x = linspace(0,L,N+1)
psi = exp(-(x-x0)**2/(2*sigma**2))*exp(1j*kappa*x)
psi[0] = psi[N] = 0
# Create the tridiagonal array A
A = empty([3,N-1],complex)
A[0,:] = a2
A[1,:] = a1
A[2,:] = a2

def init():
    line.set_data([], [])
    return line,


def animate(i):
    ## main loop for the Crank-Nicolson method
    v = b2*psi[0:N-1] + b1*psi[1:N] + b2*psi[2:N+1]
    psi[1:N] = banded(A,v,1,1)
    ys = yscale*real(psi)
    line.set_data(x,ys)
    return line,
```

Schrödinger (Example 9.8)


```
def animate(i):
    ## main loop for the Crank-Nicolson method
    v = b2*psi[0:N-1] + b1*psi[1:N] + b2*psi[2:N+1]
    psi[1:N] = banded(A,v,1,1)
    ys = yscale*real(psi)
    line.set_data(x,ys)
    return line,


fig = plt.figure()
ax = plt.axes(xlim=(0, L), ylim=(-yscale,yscale))
line, = ax.plot([], [], lw=3)

ani = animation.FuncAnimation(fig, animate, interval=15, frames = 5000, init_func=init)
ani.save('schrodinger.mp4', fps=60, extra_args=['-vcodec', 'libx264'])
```

Let’s watch the output together

Consider wave equation in 1D with wave fixed at both ends of a string, $\phi(x=0) = \phi(x=L) = 0$. And consider a plane wave solution:

$$\phi_k(x,t) = \sin(\frac{\pi k x}{L})e^{i\omega t}$$

$$\frac{\partial^2 \phi}{\partial t^2} = v^2 \frac{\partial^2 \phi}{\partial x^2}$$

Solution iff: $\omega = \dfrac{\pi k v}{L}$

$$\phi_k(x,t) = \sin(\frac{\pi k x}{L})e^{\frac{i\pi k v t}{L}}$$

Divide our string into N equally spaced intervals, with N+1 grid points (need the +1 to have two-sided bounds for all intervals), so that the nth grid point is given by:

$$x_n = \frac{n}{N} L$$

We know: $$\phi_k(x,t) = \sin(\frac{\pi k x}{L}) e^{\frac{i \pi k v t}{L}}$$

$$\phi_k(x_n,t) = \sin(\frac{\pi k n}{N}) e^{\frac{i \pi k v t}{L}}$$

But we know that we can combine any of our solutions to the wave equation to get another solution (it is a linear differential equation)

So another equally valid, more general solution is:

$$\phi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1} b_k \sin(\frac{\pi k n}{N}) e^{\frac{i\pi k v t}{L}}$$

$$\phi(x_n,0) = \frac{1}{N}\sum_{k=1}^{N-1} \alpha_k \sin(\frac{\pi k n}{N})$$

where α_k is the real component of $b_k = \alpha_k + i\eta_k$

If our solution at any time is:

$$\phi(x_n, t) = \frac{1}{N}\sum_{k=1}^{N-1} b_k \sin(\frac{\pi k n}{N}) e^{\frac{i\pi k v t}{L}}$$

Then we can compute the time derivative:

$$\frac{\partial \phi(x_n, t)}{\partial t} = \frac{1}{N}\sum_{k=1}^{N-1} b_k \frac{i\pi k v}{L} \sin(\frac{\pi k n}{N}) e^{\frac{i\pi k v t}{L}}$$

And then:

$$\frac{\partial \phi(x_n, 0)}{\partial t} = \frac{1}{N}\sum_{k=1}^{N-1} b_k \frac{i\pi k v}{L} \sin(\frac{\pi k n}{N})$$

$$\frac{\partial\phi(x_n,0)}{\partial t} = \frac{1}{N}\sum_{k=1}^{N-1} b_k \frac{i\pi k v}{L}\sin(\frac{\pi k n}{N})$$

The real part of this is then given by the complex part of $b_k = \alpha_k + i\eta_k$

$$\frac{\partial\phi(x_n,0)}{\partial t} = \frac{1}{N}\sum_{k=1}^{N-1} b_k \frac{i\pi k v}{L}\sin(\frac{\pi k n}{N})$$

$$\frac{\partial\phi(x_n,0)}{\partial t} = -\frac{1}{N}\frac{\pi v}{L}\sum_{k=1}^{N-1} k\eta_k \sin(\frac{\pi k n}{N})$$

$$\phi(x_n, 0) = \frac{1}{N} \sum_{k=1}^{N-1} \alpha_k \sin(\frac{\pi k n}{N})$$

$$\frac{\partial \phi(x_n, 0)}{\partial t} = -\frac{1}{N} \frac{\pi v}{L} \sum_{k=1}^{N-1} k \eta_k \sin(\frac{\pi k n}{N})$$

So if we have the initial values and initial derivatives at all of our grid points, then our coefficients for the Fourier sine series are fully defined, and our solution is fully determined at all times

$$\phi(x_n, t) = \frac{1}{N} \sum_{k=1}^{N-1} (\alpha_k + i\eta_k) \sin(\frac{\pi k n}{N}) e^{\frac{i\pi k v t}{L}}$$

Spectral methods

$$\phi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1}(\alpha_k + i\eta_k)\sin(\frac{\pi k n}{N})e^{\frac{i\pi k v t}{L}}$$

Evaluating the real pieces:

$$\phi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1}(\alpha_k + i\eta_k)\sin(\frac{\pi k n}{N})\left(\cos\frac{\pi k v t}{L} + i\sin\frac{\pi k v t}{L}\right)$$

$$\phi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1}(\alpha_k\cos\frac{\pi k v t}{L} - \eta_k\sin\frac{\pi k v t}{L})\sin(\frac{\pi k n}{N})$$

Note that this is another sine series! Easy to evaluate coefficients at any arbitrary later times, with no need to "step" through time. Only works though for nice boundary conditions like we defined, and for linear differential equations

Homework #7

9.4,9.5 (For 9.5, use matplotlib for the animation). And if you can run on your local laptop or desktop, save a video for a larger period of time!)