Explicit Schemes – Matrix Form

Let's revisit the Diffusion equation from Chapter 6:

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

Where the discretized version is:

$$T_j^{n+1} = T_j^n + \frac{\tau\kappa}{h^2}(T_{j+1}^n \text{-} 2\, T_j^n + T_{j-1}^n)$$

As before, the label n is the time and j is the grid location. This can also be written in matrix form as

$$\boldsymbol{T}^{n+1} = \boldsymbol{T}^n + \frac{\tau\kappa}{h^2}\boldsymbol{D}\boldsymbol{T}^n$$
$$= \left(\boldsymbol{I} + \frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n}}$$

Where **I** is the identity matrix of size *NxN*, **D** is a matrix defined as

$$\boldsymbol{D} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & 0 & 1 & -2 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

And $\boldsymbol{T}^n$ is a vector

$$\boldsymbol{T}^n = \begin{bmatrix} T_1^n \\ T_2^n \\ T_3^n \\ \vdots \\ T_N^n \end{bmatrix}$$

This also includes the boundary conditions, in this case Dirichlet, setting T to 0 at the boundaries.

Implicit Schemes – Matrix Form

We can also discretize the diffusion equation so that the RHS uses the solution at the new time, n+1 as:

$$T_j^{n+1} = T_j^n + \frac{\tau\kappa}{h^2}(T_{j+1}^{n+1} \text{-} 2\, T_j^{n+1} + T_{j-1}^{n+1})$$

Again, the label n is the time and j is the grid location. In this case, the equation be written in matrix form as

$$\boldsymbol{T}^{n+1} = \boldsymbol{T}^n + \frac{\tau\kappa}{h^2}\boldsymbol{D}\boldsymbol{T}^{n+1}$$

Moving the (n+1) part of the solution to the LHS, we get

$$\left(\boldsymbol{I} - \frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n+1}} = \boldsymbol{T}^n$$

Using a matrix inversion, this becomes

$$\mathbf{T}^{\mathrm{n+1}} = \left(\boldsymbol{I} - \frac{\tau\kappa}{h^2}\mathbf{D}\right)^{-1}\boldsymbol{T}^n$$

In this case, in order to get the solution at the new time, one must invert a matrix. But since the matrix does not change, it only has to be done once.

Semi-Implicit Schemes – Matrix Form

We can also blend implicit and explicit scheme uses the solution at the new time, $n+1$ as:

$$T_j^{n+1} = T_j^n + \alpha \frac{\tau\kappa}{h^2}(T_{j+1}^{n+1} - 2\,T_j^{n+1} + T_{j-1}^{n+1}) + (1-\alpha)\frac{\tau\kappa}{h^2}(T_{j+1}^{n} - 2\,T_j^{n} + T_{j-1}^{n})$$

Where α is a number between 0 an 1, in matrix form

$$\mathbf{T}^{\mathrm{n+1}} = \mathbf{T}^{\mathrm{n}} + \alpha\frac{\tau\kappa}{h^2}\mathbf{D}\mathbf{T}^{\mathrm{n+1}} + (1-\alpha)\frac{\tau\kappa}{h^2}\mathbf{D}\mathbf{T}^{\mathrm{n}}$$

Moving the (n+1) part of the solution to the LHS, we get

$$\left(\boldsymbol{I} - \alpha\frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n+1}} = \left(\boldsymbol{I} + (1-\alpha)\frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n}}$$

Or as

$$\mathbf{T}^{\mathrm{n+1}} = \left(\boldsymbol{I} - \alpha\frac{\tau\kappa}{h^2}\mathbf{D}\right)^{-1}\left(\boldsymbol{I} + (1-\alpha)\frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n}}$$

When $\alpha = \frac{1}{2}$, the scheme is called the Crank-Nicholson Scheme that has some useful properties

Stability Analysis -Von Neumann Method

There are several ways to determine ahead of time whether a numerical scheme will be stable. As we have seen before, one way is to look what effect the numerical method has on a wave on the fourier compoents

$$a(x,t) = T(t)e^{ikx}$$

In a discretized form we write the above as

$$a(x_j, t_n) = a_j^n = T^n e^{ikjh}$$

Where $i = \sqrt{-1}$, h is the grid spacing, and k is the wave number. If we advance the solution by one step

$$a_j^{n+1} = T^{n+1}e^{ikjh} = AT^n e^{ikjh}$$

If the solution technique were exact that the amplification factor $|A|=1$

- if $|A|>1$, then the solution is unstable
- if $|A| < 1$ the the solution is stable, but the wave is diffused
- In general will be complex with some phase so $A = |A|e^{i\phi}$
  - A nonzero ϕ is an indicator of dispersion

Von Neumann Stability Analysis for the explicit FTCS method for the Diffusion Equation

Recall that the equation

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

in the FTCS approach is written as

$$T_j^{n+1} = T_j^n + \frac{\tau\kappa}{h^2}(T_{j+1}^n\text{-}2\,T_j^n + T_{j-1}^n)$$

Lets look at what effect this has on a wave of the form

$$T\left(x_j, t_n\right) = T_j^n = T^n e^{ikjh}$$

Plugging into the above we get

$$T^{n+1}e^{ikjh} = T^n e^{ikjh} + \frac{\tau\kappa}{h} T^n e^{ikjh}(\mathrm{e}^{\mathrm{ikh}} - 2 + \mathrm{e}^{-\mathrm{ikh}})$$

Simplifying

$$A = 1 + \frac{\tau\kappa}{h^2}(\mathrm{e}^{\mathrm{ikh}} - 2 + \mathrm{e}^{-\mathrm{ikh}})$$

Explicit FTCS method for the Diffusion Equation

Since $\sin(x) = \frac{e^{ix}-e^{-ix}}{2i}$ and $\sin^2(x) = -\frac{e^{2ix}-2+e^{-2ix}}{4}$

We get

$$A = 1 - \frac{4\tau\kappa}{h^2}\sin^2\left(\frac{kh}{2}\right)$$

Since we want $|A| \leq 1$, we get the requirement that

$$\left|1 - \frac{4\tau\kappa}{h^2}\sin^2\left(\frac{kh}{2}\right)\right| \leq 1$$

Since the maximum value of sin is 1, this reduces to

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

This can be true if $\boxed{\tau \leq \frac{h^2}{2\kappa}}$

Von Neumann Stability Analysis for the implicit method for the Diffusion Equation

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

Lets look at what effect a method that uses the future value of the function, i.e.,

$$T_j^{n+1} = T_j^n + \frac{\tau\kappa}{h^2}(T_{j+1}^{n+1} \text{-} 2\, T_j^{n+1} + T_{j-1}^{n+1})$$

And looking the Fourier components

$$T\left(x_j, t_n\right) = T_j^n = T^n e^{ikjh}$$

We get

$$T^{n+1} e^{ikjh} = T^n e^{ikjh} + \frac{\tau\kappa}{h} T^{n+1} e^{ikjh} (\mathrm{e}^{\mathrm{ikh}} - 2 + \mathrm{e}^{-\mathrm{ikh}})$$

Gives and amplification factor of

$$\boxed{A = \frac{1}{1 + \frac{4\tau\kappa}{h^2} \sin^2 \frac{\kappa h}{2}}}$$

This scheme is unconditionally stable, but with significant damping.

Von Neumann Stability Analysis for the semi-implicit method for the Diffusion Equation

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

Lets look at what effect a method that uses the a weighted blend of the old and future value of the function, i.e.,

$$T_j^{n+1} = T_j^n + \alpha \frac{\tau\kappa}{h^2}(T_{j+1}^{n+1} - 2\,T_j^{n+1} + T_{j-1}^{n+1}) + (1-\alpha)\frac{\tau\kappa}{h^2}(T_{j+1}^n - 2\,T_j^n + T_{j-1}^n)$$

assuming $T(x_j, t_n) = T_j^n = T^n e^{ikjh}$

gives

$$T^{n+1}e^{ikjh} + \alpha\frac{\tau\kappa}{h}T^{n+1}e^{ikjh}\left(\mathrm{e}^{\mathrm{ikh}} - 2 + \mathrm{e}^{-\mathrm{ikh}}\right) = T^n e^{ikjh} + (1-\alpha)\frac{\tau\kappa}{h}T^n e^{ikjh}(\mathrm{e}^{\mathrm{ikh}} - 2 + \mathrm{e}^{-\mathrm{ikh}})$$

With an amplification factor

$$\boxed{A = \frac{1-(1-\alpha)\frac{4\tau\kappa}{h^2}\sin^2\frac{\kappa h}{2}}{1+\alpha\frac{4\tau\kappa}{h^2}\sin^2\frac{\kappa h}{2}}}$$

This scheme is *unconditionally stable when* $\alpha = ½$ (Crank Nicolson - see next page for derivation)

Crank Nicolson Stability

If we define D as $D^2 \equiv \frac{4\tau\kappa}{h^2} sin\frac{kh}{2}$, then A =$\frac{1-(1-\alpha)D^2}{1+\alpha D^2}$ and for the scheme to be stable we want $|A| \leq 1$ for all possible values of D, i.e., $\left|\frac{1-(1-\alpha)D^2}{1+\alpha D^2}\right| \leq 1$. For this to be true there are 2 conditions to be satisfied:

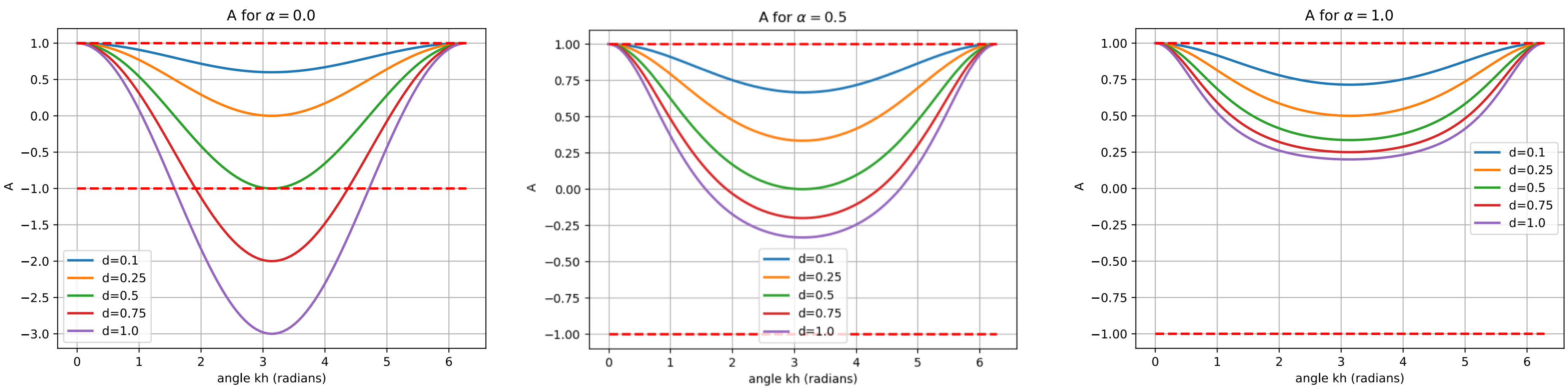
$$1-(1-\alpha)D^2 \leq 1+\alpha D^2$$
$$\Rightarrow 1-D^2+\alpha D^2 \leq 1+\alpha D^2$$
$$\Rightarrow -\mathrm{D}^2 \leq 0 \text{ which is always true}$$

and

$$1-(1-\alpha)D^2 \geq -1-\alpha D^2$$
$$\Rightarrow 1-D^2+\alpha D^2 \geq -1-\alpha D^2$$
$$\Rightarrow 2 \geq D^2(1-2\alpha)$$

which is true if $\alpha \geq \frac{1}{2}$

Comparison plots for various α



Explicit | Crank Nicolson | Fully Implicit

For stability, require that: $|A| \leq 1$

Implicit method – Matrix Methods – Diffusion equation

If we assume a Dirichlet boundary where T_1 and T_N are specified and define $d = \frac{\tau\kappa}{h^2}$, then one gets a system of equations that can be written in matrix form as

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ -d & 1+2d & -d & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & -d & 1+2d & -d & & \vdots \\ \vdots & & & & \ddots & \ddots & 0 \\ \vdots & & & & -d & 1+2d & -d \\ 0 & & & & 0 & -d & 1 \end{bmatrix} \begin{pmatrix} T_1^{n+1} \\ T_2^{n+1} \\ \vdots \\ \vdots \\ T_j^{n+1} \\ \vdots \\ T_{N-1}^{n+1} \\ T_N^{n+1} \end{pmatrix} = \begin{pmatrix} T_1^n \\ T_2^n \\ \vdots \\ \vdots \\ T_j^n \\ \vdots \\ T_{N-1}^n \\ T_N^n \end{pmatrix}$$

This is a tridiagonal system of equations.

Semi-Implicit method

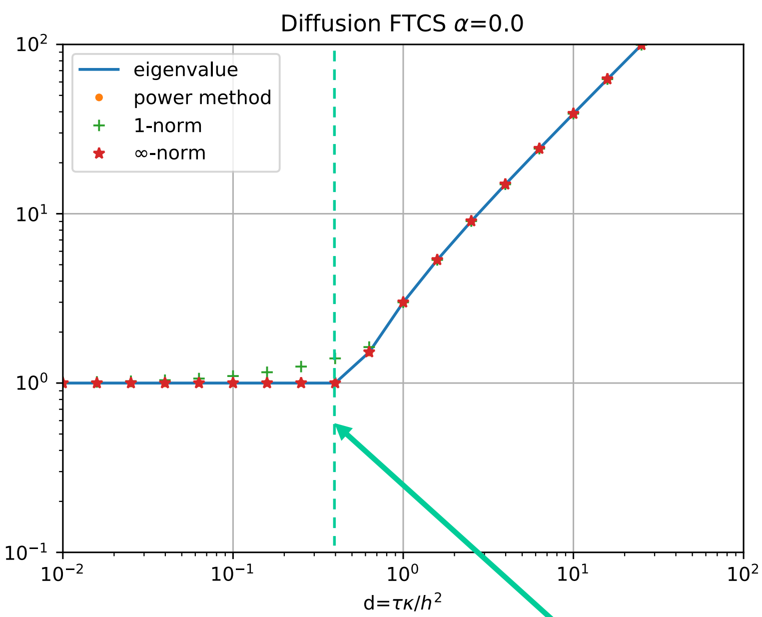
If we assume a Dirichlet boundary where T_1 and T_N are specified and define d = $\tau\kappa/h^2$, , then one gets a system of equations that can be written in matrix form as

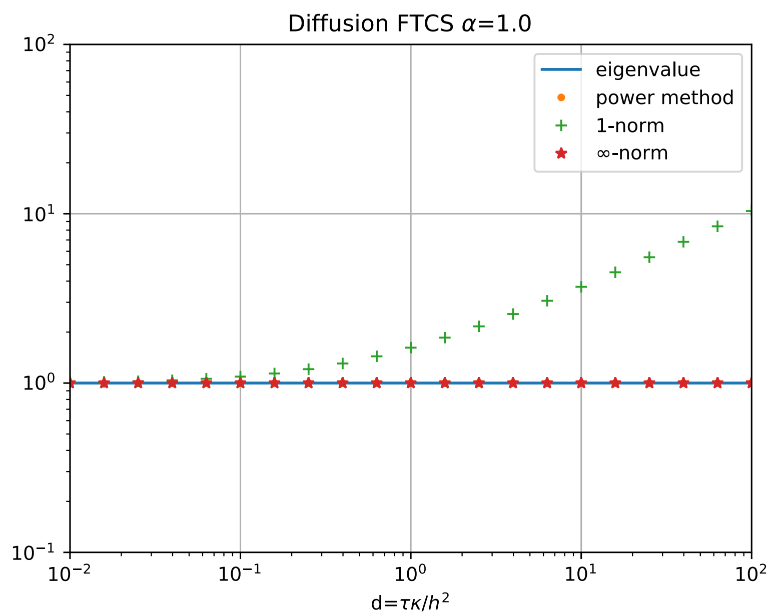
$$\begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ -\alpha d & 1+2\alpha d & -\alpha d & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & -\alpha d & 1+2\alpha d & -\alpha d & & \vdots \\ \vdots & & & & \ddots & \ddots & 0 \\ \vdots & & & & -\alpha d & 1+2\alpha d & -\alpha d \\ 0 & & & & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1^{n+1} \\ T_2^{n+1} \\ \vdots \\ \vdots \\ T_j^{n+1} \\ \vdots \\ T_{N-1}^{n+1} \\ T_N^{n+1} \end{bmatrix} =$$

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ d(1-\alpha) & 1-2(1-\alpha)d & d(1-\alpha) & 0 & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & d(1-\alpha) & 1-2(1-\alpha)d & d(1-\alpha) & & \vdots \\ \vdots & & & & \ddots & \ddots & 0 \\ \vdots & & & & d(1-\alpha) & 1-2(1-\alpha)d & d(1-\alpha) \\ 0 & & & & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T_1^{n} \\ T_2^{n} \\ \vdots \\ \vdots \\ T_j^{n} \\ \vdots \\ T_{N-1}^{n} \\ T_N^{n} \end{bmatrix}$$

This also is a tridiagonal system of equations.

Diffusion equation effect of different α





Explicit

$$CFL\ \tau = \frac{h^2}{2\tau}$$

Implicit

(Not sure why the 1 norm disagrees)

Von Neumann Stability analysis of the advection equation for FTCS

Recall the advection equation

$$\frac{\partial a(x,t)}{\partial t} = -\frac{c\partial a(x,t)}{\partial x}$$

Assume the solution takes the form

$$a_j^n = T^n e^{ikjh}$$

So that the FTCS method becomes

$$T^{n+1}e^{ikjh} = T^n e^{ikjh} - \frac{c\tau}{2h}T^n\left(e^{ik(j+1)h} - e^{ik(j-1)h}\right)$$

$$A \equiv \frac{T^{n+1}}{T^n} = 1 - \frac{c\tau}{2h}\left(e^{ikh} - e^{-ikh}\right)$$

Or

$$A^2 = 1 + \left(\frac{c\tau}{h}\right)^2 \sin^2 kh$$

Which is <u>unconditionally</u> unstable.

Note that the fastest growing unstable mode is for when $kh = \pi/2$

Which corresponds to a wave of wavelength (since $k=2\pi/\lambda$) of $\lambda=4h$

Von Neumann Stability Analysis for the implicit method for the Advection Equation

In the implicit approach is written as

$$a_j^{n+1} = a_j^n - \frac{c\tau}{2h}\left(a_{j+1}^{n+1} - a_{j-1}^{n+1}\right)$$

Again, lets look at what effect this has on a wave of the form $a_j^n = T^n e^{ikjh}$

Plugging into the above we get

$$T^{n+1}e^{ikjh} = T^n e^{ikjh} - \frac{c\tau}{2h}T^{n+1}\left(e^{ik(j+1)h} - e^{ik(j-1)h}\right)$$

Simplifying

$$T^{n+1}e^{ikjh} + \frac{c\tau}{2h}T^{n+1}\left(e^{ik(j+1)h} - e^{ik(j-1)h}\right) = T^n e^{ikjh}$$

$$A = \frac{T^{n+1}}{T^n} = \frac{1}{1 + \frac{c\tau}{2h}\left(e^{ikh} - e^{-ikh}\right)} = \frac{1}{1 + \frac{ic\tau}{h}\sin kh}$$

Implicit Advection Equation (cont.)

Since we have $A = \frac{1}{1+\frac{ic\tau}{h}\sin kh}$ we get

$$|A| = \frac{1}{\sqrt{1 + \left(\frac{c\tau}{h}\right)^2 \sin^2 kh}}$$

In this case $|A|$ is always less than 1, and is therefore unconditionally stable. Note also in this case there is also significant amount of diffusion/damping - the larger the timestep the larger the amount of damping.

Von Neumann Stability Analysis for the semi-implicit method for the Advection Equation

In the semi-implicit approach is written as

$$a_j^{n+1} = a_j^n - (1-\alpha)\frac{c\tau}{2h}\left(a_{j+1}^n - a_{j-1}^n\right) - \alpha\frac{c\tau}{2h}\left(a_{j+1}^{n+1} - a_{j-1}^{n+1}\right)$$

Again, lets look at what effect this has on a wave of the form $a_j^n = T^n e^{ikjh}$

Plugging into the above we get

$$T^{n+1}e^{ikjh}\left[1+\alpha\frac{c\tau}{2h}\left(e^{ikh}-e^{-ikh}\right)\right] = T^n e^{ikjh}\left[1-(1-\alpha)\frac{c\tau}{2h}\left(e^{ikh}-e^{-ikh}\right)\right]$$

Simplifying

$$A \equiv \frac{T^{n+1}}{T^n} = \frac{1-(1-\alpha)i\frac{c\tau}{h}\sin kh}{1+\alpha i\frac{c\tau}{h}\sin kh}$$

Crank-Nicolson Method (α=1/2)

Better accuracy can be achieved, yielding second order in time accuracy, by time averaging the spatial derivatives.

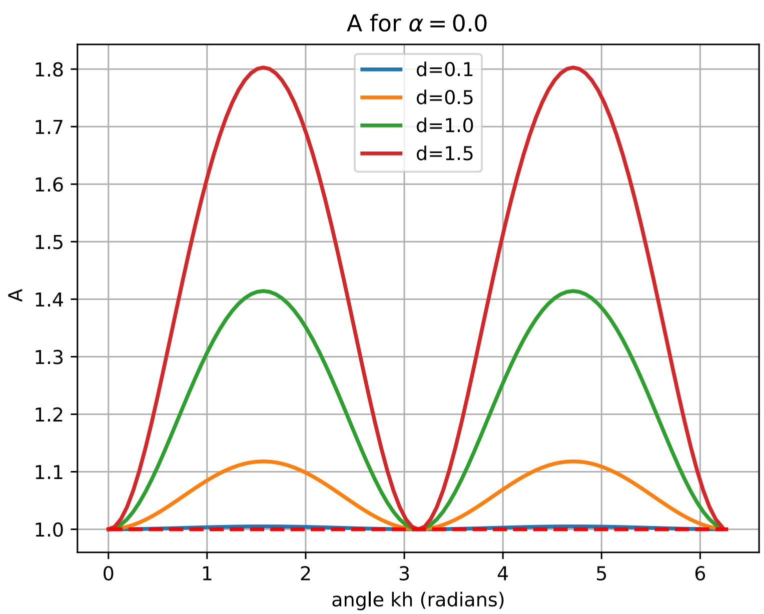
$$a_j^{n+1} = a_j^n - \frac{c\tau}{4h}\left(a_{j+1}^n - a_{j-1}^n\right) - \frac{c\tau}{4h}\left(a_{j+1}^{n+1} - a_{j-1}^{n+1}\right)$$

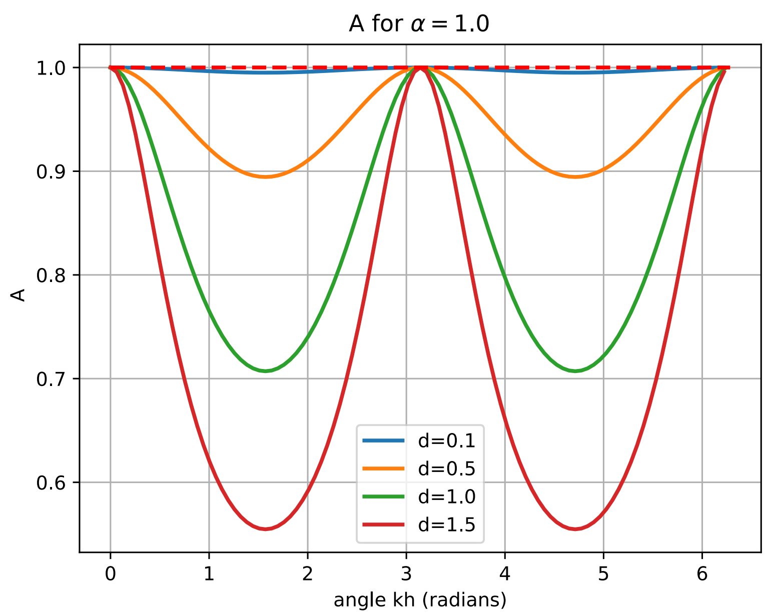
Stability analysis shows that

$$A = \frac{1 - i\frac{c\tau}{2h}\sin kh}{1 + i\frac{c\tau}{2h}\sin kh}$$

And note that |A| = 1 for all timesteps!

Comparison for |A| for different α





Explicit – always unstable

Fully implicit–always stable

Matrix form of the implicit advection equation

Since we have the equation

$$a_j^{n+1} = a_j^n - \frac{c\tau}{2h}\left(a_{j+1}^{n+1} - a_{j-1}^{n+1}\right)$$

We can rewrite this as

$$a_j^{n+1} + \frac{c\tau}{2h}\left(a_{j+1}^{n+1} - a_{j-1}^{n+1}\right) = a_j^n$$

In matrix/vector form it is

$$\left(I + \frac{c\tau}{2h}A\right)\vec{a}^{n+1} = \vec{a}^n$$

or

$$\vec{a}^{n+1} = \left(\boldsymbol{I} + \frac{c\tau}{2h}\boldsymbol{A}\right)^{-1}\vec{a}^n$$

Matrix form of advection equation

Where the matrix **A** takes the form

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 & 0 & \cdots & \cdots & -1 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 0 & 1 & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & 0 & -1 & 0 & 1 \\ 1 & 0 & \cdots & 0 & -1 & 0 \end{bmatrix}$$

And **I** is the identity matrix

Matrix form of the semi-implicit method for the advection equation

For this problem, we have the equation

$$a_i^{n+1} = a_i^n - (1-\alpha)\frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n) - \alpha\frac{c\tau}{2h}(a_{i+1}^{n+1} - a_{i-1}^{n+1})$$

or

$$a_i^{n+1} + \alpha\frac{c\tau}{2h}(a_{i+1}^{n+1} - a_{i-1}^{n+1}) = a_i^n - (1-\alpha)\frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n)$$

We can rewrite this as

$$\left(\boldsymbol{I} + \alpha\frac{c\tau}{2h}\boldsymbol{A}\right)\vec{a}^{n+1} = \left(\boldsymbol{I} - (1-\alpha)\frac{c\tau}{2h}\boldsymbol{A}\right)\vec{a}^n$$

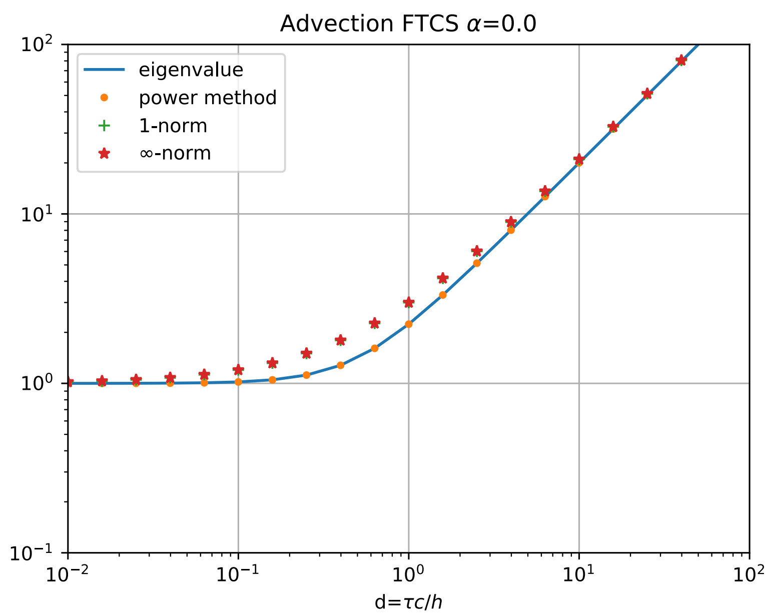
In matrix/vector form it is

$$\vec{a}^{n+1} = \left(\boldsymbol{I} + \alpha\frac{c\tau}{2h}\boldsymbol{A}\right)^{-1}\left(\boldsymbol{I} - (1-\alpha)\frac{c\tau}{4h}\boldsymbol{A}\right)\vec{a}^n$$

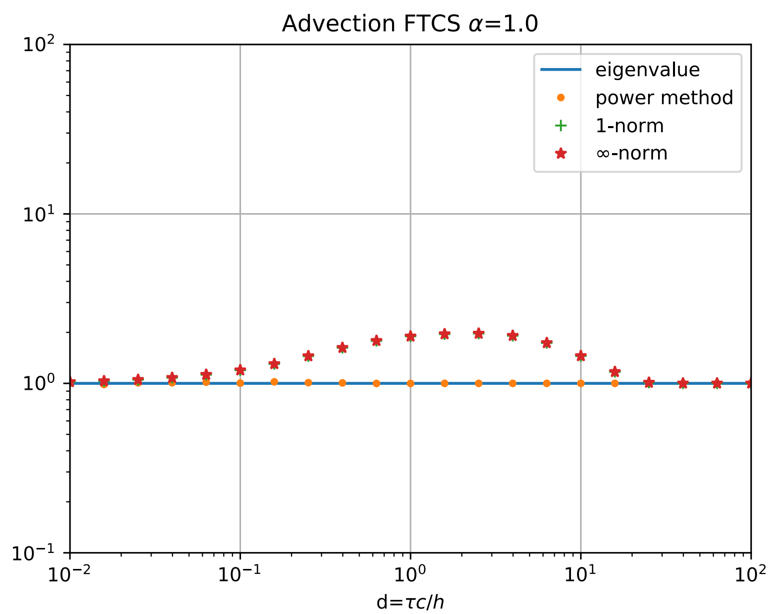
Where **A** is defined as on the previous slide.

Also, $\alpha = \frac{1}{2}$ for the Crank Nicolson Method

FTCS effect of different values of α



Explicit-Always unstable



Implicit
Norms don't work well as an estimate

Solution of Schrödinger's Equation

The standard 1D Schrödinger's equation is usually written in the form

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) = H\Psi(x,t)$$

Where $\Psi(x,t)$ is the wave function and V(x) is the potential and H is the Hamiltonian. The FTCS scheme for this equation, using the usual syntax

$$i\hbar\, \frac{\Psi_j^{n+1} - \Psi_j^n}{\tau} = -\frac{\hbar^2}{2m}\, \frac{\Psi_{j-1}^n - 2\Psi_j^n + \Psi_{j+1}^n}{h^2} + V_j^n \Psi_j^n$$

Which can be written in matrix form as

$$i\hbar \frac{\Psi_j^{n+1} - \Psi_j^n}{\tau} = \sum_{k=1}^{N} H_{jk}\Psi_k^n$$

Schrödinger's Equation - FTCS

This gives the numerical scheme to be

$$\boldsymbol{\Psi}^{n+1} = \left(\boldsymbol{I} - \frac{i\tau}{\hbar}\boldsymbol{H}\right)\Psi^{n}$$

Where Ψ is a column vector and $\mathbf{I}$ is the identity matrix.

Schrödinger's Equation – Implicit and Crank Nicolson

The implicit scheme is then

$$i\hbar\,\frac{\Psi_j^{n+1}-\Psi_j^n}{\tau} = \sum_{k=1}^{N} H_{jk}\Psi_k^{n+1}$$

Which has the matrix form

$$\boldsymbol{\Psi}^{n+1} = \left(\boldsymbol{I} + \frac{i\tau}{\hbar}\boldsymbol{H}\right)^{-1}\Psi^n$$

While the Crank-Nicolson scheme is

$$\boldsymbol{\Psi}^{n+1} = \left(\boldsymbol{I} + \frac{i\tau}{2\hbar}\boldsymbol{H}\right)^{-1}\left(\boldsymbol{I} - \frac{i\tau}{2\hbar}\boldsymbol{H}\right)\Psi^n$$

Example Problem: Wave Packet of a Free Particle

The example code `schro` solves Schrödinger's equation for a free particle. The initial condition is a Gaussian wave packet

$$\psi(x,t=0) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}\mathrm{e}^{\mathrm{i}\mathrm{k}_0\mathrm{x}}\mathrm{e}^{-\frac{(x-x_0)^2}{2\sigma_0^2}}$$

The initial condition is normalized so that $\int_{-\infty}^{\infty}|\psi|^2 dx = 1$. In free space, where V(x)=0, the wave packet evolves as

$$\psi(x,t) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}\mathrm{e}^{\mathrm{i}\mathrm{k}_0\left(\mathrm{x}-\frac{\mathrm{p}_0\mathrm{t}}{2\mathrm{m}}\right)}\mathrm{e}^{-\frac{\left(x-x_0-\frac{p_0 t}{m}\right)^2}{2\alpha^2}}$$

Where $p_0 = \hbar k_0$is the momentum of the particle, and $\alpha^2 = \sigma_0^2 + \frac{i\hbar t}{m}$. The probability density $P(x,t) = |\psi(x,t)|^2$is then

$$P(x,t) = \frac{\sigma_0}{|\alpha|^2\sqrt{\pi}}\exp\left[-\left(\frac{\sigma_0}{|\alpha|}\right)^4\frac{\left(x-x_0-\frac{p_0 t}{m}\right)}{\sigma_0^2}\right]$$

Schro program

The example program solves the Schrödinger equation for a free particle assuming periodic boundary conditions.

The initial gaussian wave moves to the right and spreads out. The expected location of the particle $\langle x \rangle$ defined as $\langle x \rangle = \int_{-\infty}^{\infty} xP(x,t)dt$ moves as $\langle x \rangle = x_0 + p_0\, t/m$ and the gaussian spreads over time as

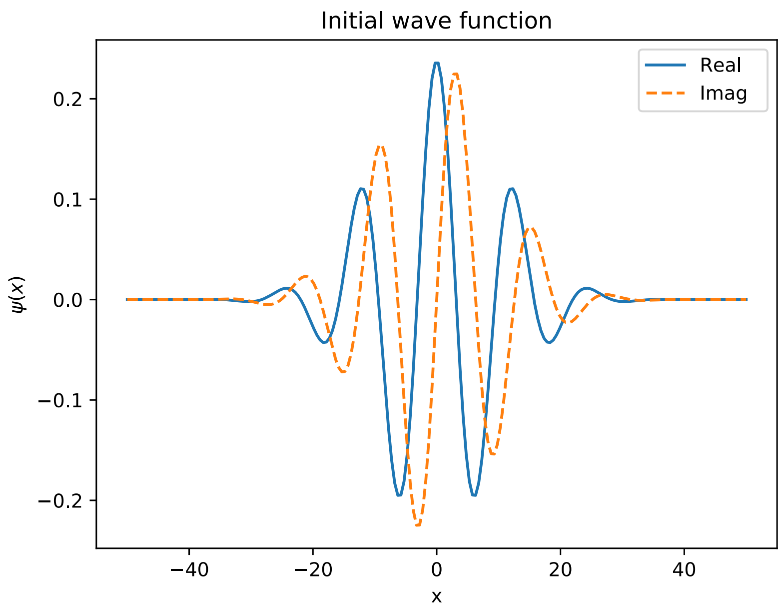
$$\sigma(t) = \sigma_0 \sqrt{\left(\frac{|\alpha|}{\sigma_0}\right)^4} = \sigma_0 \sqrt{1 + \frac{\hbar^2 t^2}{m^2 \sigma_0^4}}$$

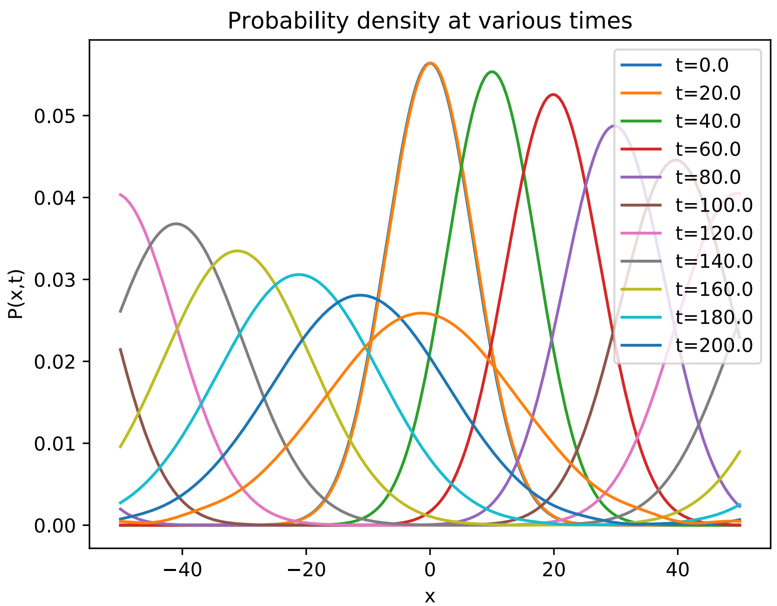
For the free particle, the Hamiltonian $V(x)=0$

For the assignment, the $V(x) = U\delta\left(x - \frac{L}{2}\right)$ where U will vary compared to $E = \frac{\hbar^2 k_0^2}{2m}$. In other words, do cases where U<E (quantum tunneling).

Example result from the Schro program for a free particle

code uses Crank-Nicolson method





N=200 grid points, $\tau = 0.25$ *sec*

Notes on Matrix Stability Analysis

Matrix Stability

Another way to look at stability, that also includes the effects of boundary conditions is via Matrix Stability Analysis. Lets go back to the diffusion problem

We can write this as $T_j^{n+1} = T_j^n + \frac{\tau\kappa}{h^2}(T_{j+1}^n$-2 T_j^n+ T_{j-1}^n) and in matrix form

$$\boldsymbol{T}^{n+1} = \boldsymbol{T}^n + \frac{\tau\kappa}{h^2}\boldsymbol{D}\boldsymbol{T}^n$$

$$= \left(\boldsymbol{I} + \frac{\tau\kappa}{h^2}\mathbf{D}\right)\mathbf{T}^{\mathrm{n}} = \boldsymbol{A}\mathbf{T}^{\mathrm{n}}$$

Where $\boldsymbol{D} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & 0 & 1 & -2 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}$ and $\boldsymbol{T}^n = \begin{bmatrix} T_1^n \\ T_2^n \\ T_3^n \\ \vdots \\ T_N^n \end{bmatrix}$

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Stability is determined by looking at the eigenvalues of the Matrix **A**, i.e., lets look at

$$\boldsymbol{A}\boldsymbol{v}_k = \lambda_k \boldsymbol{v}_k$$

where $\mathbf{v}_k$ is the eigenvector for eigenvalue λ_k. The eigenvalues are labeled in decreasing order so that $|\lambda_1| > |\lambda_2| > |\lambda_3| \ldots |\lambda_N|$

We can use these eigenvectors to form a basis so that the initial condition can be written as $\boldsymbol{T}^1 = \sum_{k=1}^{N} b_k \boldsymbol{v}_k$

so that $\boldsymbol{T}^{n+1} = \boldsymbol{A}\boldsymbol{T}^n = \boldsymbol{A}^n \boldsymbol{T}^1$

This means that

$$\boldsymbol{T}^{n+1} = \sum_{k=1}^{N} \boldsymbol{A}^n b_k \boldsymbol{v}_k = \sum_{k=1}^{N} (\boldsymbol{\lambda}_k)^n b_k \boldsymbol{v}_k$$

If $|\lambda_k| > 1$ for any eigenvalue, then $\mathbf{T}^{\mathrm{n}} \rightarrow \infty$ as $n \rightarrow \infty$.

The spectral radius of **A** is $|\lambda_1|$ so the scheme is stable if $|\lambda_1| \leq 1$.

The Power Method

A reasonably quick way of determining the largest eigenvalue and eigenvector of a matrix is through the power method. Take any vector $\mathbf{x}_0$ and write it as

$$\boldsymbol{x}_0 = \sum_{k=1}^{N} c_k \boldsymbol{v}_k$$

where $\mathbf{v}_k$ are the normalized eigenvectors of the matrix $\mathbf{M}$ and $\forall c_k \neq 0$ If we then compute $\boldsymbol{M}^{\boldsymbol{n}}\boldsymbol{x}_0 = \boldsymbol{M}^{\boldsymbol{n}} \sum_{k=1}^{N} c_k \boldsymbol{v}_k = \sum_{k=1}^{N} c_k \boldsymbol{M}^{\boldsymbol{n}} \boldsymbol{v}_k = \sum_{k=1}^{N} \mathrm{c}_k \lambda_k^n \boldsymbol{v}_k$.

If $n \to \infty$ and then $\boldsymbol{M}^{\boldsymbol{n}}\boldsymbol{x}_0 \to c_1 \lambda_1^n \boldsymbol{v}_1$ where λ_1 is the dominant eigenvalue.

A more efficient approach is the following, is to iterate, so that at the $k+1$-th step we have $\mathbf{M}^{\mathrm{n}}\boldsymbol{x} \approx c_1 \lambda_1^n \boldsymbol{v}_1$ and the vectors $\boldsymbol{v}_{\mathbf{1}}$ are normalized so that $\boldsymbol{v}_{\mathbf{1}} = \frac{\boldsymbol{M}^{\boldsymbol{n}}\boldsymbol{x}}{|\boldsymbol{M}^{\boldsymbol{n}}\boldsymbol{x}|}$

Other Norms that can be used to estimate stability

Other norms that can be used include the 1-norm

$$\|A\|_1 \equiv max\left\{\sum_{j=1}^{N} \left|A_{i,j}\right|\right\}$$

and the infinity norm

$$\|A\|_\infty \equiv max\left\{\sum_{\mathrm{i}=1}^{N} \left|A_{i,j}\right|\right\}$$