$\omega \sim 1.7$ to 1.9 is usually used.

For complex grids use numerical experiments.

Parabolic equations

diffusion equation

$$\frac{\partial f}{\partial t} = \alpha \frac{\partial^2 f}{\partial x^2}$$

convection-diffusion

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = \alpha \frac{\partial^2 f}{\partial x^2}$$

reading → characteristics etc 10.2 – 10.3.3

consider $\dfrac{\partial \phi}{\partial t} = \alpha \dfrac{\partial^2 \phi}{\partial x^2}$, $\phi(0,t) = \phi(L,t) = 0$

$\phi(x,0) = g(x)$

$j = 1, 2, \ldots N$

Von-Neumann stability analysis:

→ does not take into account bcs

→ periodic bcs are assumed
i.e. soln & its derivatives are the same on both ends of the domain

→ It works for linear, constant coefficient pdes

→ uniform grid spacing

discretize the equation

Forward time (Euler) centered space (FTCS)

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \alpha \frac{\phi_{j+1}^n - 2\phi_j^{(n)} + \phi_{j-1}^n}{\Delta x^2}$$

$$\phi_j^{n+1} = \phi_j^n + \frac{\alpha \Delta t}{\Delta x^2}\left(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n\right)$$

Seek solutions that are periodic and of the form $\phi_j^n = \sigma^n e^{ikx_j}$

Note that periodic bcs are built into the sol^n the period is $\frac{2\pi}{k}$.

To see if the solution works we substitute the assumed form into the discretization

$$\sigma^{n+1} e^{ikx_j} = \sigma^n e^{ikx_j} + \frac{\alpha \Delta t}{\Delta x^2}\sigma^n\left(e^{ikx_{j+1}} - 2e^{ikx_j} + e^{ikx_{j-1}}\right)$$

$x_{j+1} = x_j + \Delta x$ & $x_{j-1} = x_j - \Delta x$.

Divide by σ^n

$$\sigma = 1 + \frac{\alpha \Delta t}{\Delta x^2}\frac{e^{ikx_j}}{e^{ikx_j}}\left[e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right]$$

$$= 1 + \frac{\alpha \Delta t}{\Delta x^2}\left[2\cos(k\Delta x) - 2\right]$$

$$\boxed{\sigma = 1 + \frac{2\alpha \Delta t}{\Delta x^2}\left[\cos(k\Delta x) - 1\right]}$$

For stability we must have

$|\sigma| \leq 1$ (or the sol^n would grow unbounded!)

$$\left| 1 + \frac{\alpha \Delta t}{\Delta x^2} \left(2\cos(k\Delta x) - 2 \right) \right| \leq 1$$

or

$$\underbrace{-1 \leq 1 + \frac{\alpha \Delta t}{\Delta x^2}}\ \underbrace{\left(2\cos(k\Delta x) - 2 \right) \leq 1}_{\text{always satisfied}}$$

always satisfied

as $2\cos(k\Delta x) \leq 2$

$\Rightarrow 2\cos(k\Delta x) - 2 \leq 0$

$$\frac{\alpha \Delta t}{\Delta x^2} \left[\cos(k\Delta x) - 1 \right] \geq -1$$

$$\boxed{\Delta t \leq \frac{\Delta x^2}{\alpha \left[1 - \cos(k\Delta x) \right]}}$$

The most restrictive Δt is obtained when the denominator is maximum

or $\cos(k\Delta x) = -1$

$$\Rightarrow \boxed{\Delta t \leq \frac{\Delta x^2}{2\alpha}}$$

Note that the analysis is not valid if α is a known function of x, or the meshes are non-uniform

However in such cases the minimum Δt obtained by maximum α and smallest Δx may still be used as a guideline for stability.

Matrix method:

The other approach is to convert pde into a system of odes (semi-descritization).

consider the same problem

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \phi(0,t) = \phi(1,t) = 0$$

$$\phi(0,x) = \sin \pi x$$

domain is $[0,1]$. we do specify boundary conditions here. we consider $N+1$ points with uniform $\Delta x = 1/N$

Only discretizing in space

$$\frac{d\phi_j}{dt} = \alpha \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2} \qquad j = 1, 2, \cdots N-1$$

Thus $\frac{d\vec{\phi}}{dt} = A\vec{\phi}$ where A is a $N-1 \times N-1$ tri-diagonal matrix

$$A = \frac{\alpha}{\Delta x^2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -2 \end{bmatrix}$$

we applied bcs at $j=0$ & $j=N$

From odes we know that, for stability the eigenvalues of matrix A ≤ 1

In addition we know that

$$\Delta t_{max} \leq \frac{2}{|\lambda|_{max}} \longrightarrow \text{see stability of systems of ode}$$

In this case A is tridiagonal matrix. We can get its eigenvalues (analytically)

$$\lambda_j = \frac{\alpha}{\Delta x^2}\left(-2 + 2\cos\frac{\pi j}{N}\right), \quad j = 1, \cdots N-1$$

The largest magnitude of eigenvalue is when $\cos\frac{\pi j}{N} = -1$

$$\lambda_{max} = \frac{-4\alpha}{\Delta x^2}$$

Then $$\boxed{\Delta t_{max} \leq \frac{\Delta x^2}{2\alpha}}$$

Same as above.

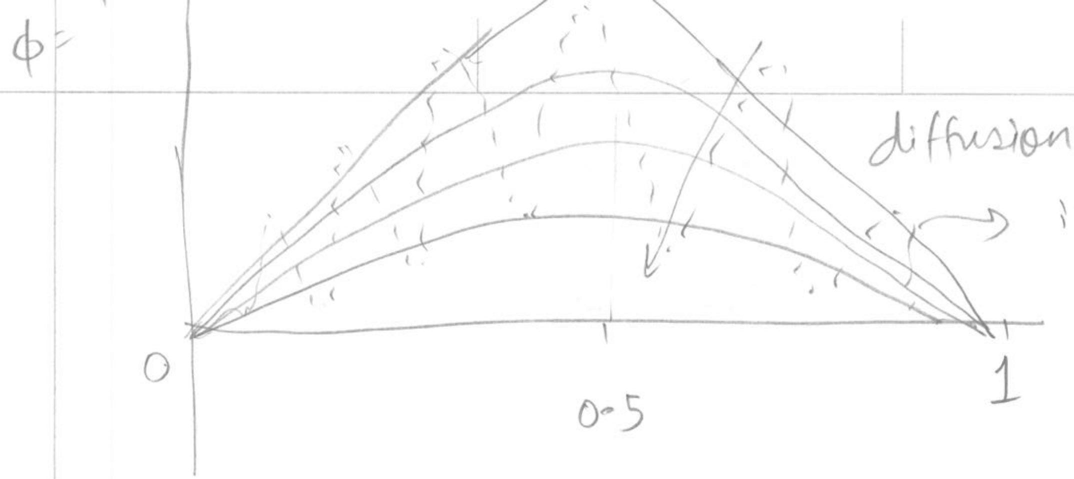
This is a more general technique. One may use non-uniform mesh & complex bcs, however seeking eigenvalues of A would be difficult $\Rightarrow$ will need numerical method for that

Let us consider our heat problem

with $\phi(x,0) = 200x \quad 0 \leq x \leq 0.5$

$\phi(x,0) = 200(1-x) \quad 0.5 \leq x \leq 1$

$\phi(0,t) = \phi(1,t) = 0 \qquad \underline{\alpha = 0.01}$



If $\Delta t > \dfrac{\Delta x^2}{2\alpha}$

No do it here

Do this after doing stability of RK4 & Leap frog & Implicit schemes

Accuracy / Consistency & modified Equation

What is a modified equation?

It is the equation we are "actually" solving in our numerical scheme.

This may not be "exactly" same as the original pde we started with. However, the numerical scheme is consistent if the "modified equation" approaches the continuous "exact pde" as Δt & $\Delta x \to 0$

$\rightarrow$ In general a numerical sol^n of a pde is a set of numbers (finite) defined at discrete set of space and time grid points.

$\rightarrow$ We can think of a continuous differentiable function that has same values as the numerical solution on the computational grid points.

This "interpolant" is an approximation to the exact sol^n of the pde. and hence does not satisfy the exact pde. Instead it satisfies a "modified" equation.

Consider the heat equation

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \quad \text{with some bcs} \qquad \text{— (1)}$$

Let $\tilde{\phi}$ be the exact solution (say obtained analytically)

Let ϕ be the "interpolant f^n" of the numerical solution which is continuous & differentiable and which assumes same values on the space-time grid as the numerical solution.

$\tilde{\phi}$ satisfies the pde $\quad \frac{\partial \tilde{\phi}}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$

Let use use explicit Euler & second order centered finite difference to discretize (1)

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \alpha \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}$$

Let us define the operator

$$L[\phi^n] = \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} - \alpha \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}$$

If ϕ is the discrete sol^n, the $L[\phi] = 0$.

Let us expand each term in the operator using Taylor-series

$$\phi_j^{n+1} = \phi_j^n + \Delta t \frac{\partial \phi_j^n}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \phi_j^n}{\partial t^2} + \cdots$$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \frac{\partial \phi_j^n}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 \phi_j^n}{\partial t^2} + \cdots$$

||ly $\rightarrow$ Ask if you can derive?

$$\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} = \left.\frac{\partial^2 \phi^n}{\partial x^2}\right|_j + \frac{\Delta x^2}{12} \left.\frac{\partial^4 \phi^n}{\partial x^4}\right|_j + \cdots$$

We expand ϕ_{j+1}^n & ϕ_{j-1}^n in x

$$\phi_{j+1}^n = \phi_j^n + \cancel{\Delta x \left.\frac{\partial \phi^n}{\partial x}\right|_j} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 \phi^n}{\partial x^2}\right|_j + \cancel{\frac{\Delta x^3}{6} \left.\frac{\partial^3 \phi^n}{\partial x^2}\right|_j}$$
$$+ \frac{\Delta x^4}{24} \left.\frac{\partial^4 \phi^n}{\partial x^4}\right|_j + \cdots$$

$+$

$$\phi_{j-1}^n = \phi_j^n - \cancel{\Delta x \left.\frac{\partial \phi^n}{\partial x}\right|_j} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 \phi^n}{\partial x^2}\right|_j - \cancel{\frac{\Delta x^3}{6} \left.\frac{\partial^3 \phi^n}{\partial x^3}\right|_j}$$
$$+ \frac{\Delta x^4}{24} \left.\frac{\partial^4 \phi^n}{\partial x^4}\right|_j + \cdots$$

$$\frac{\phi_{j+1}^n + \phi_{j-1}^n - 2\phi_j^n}{\Delta x^2} = \left.\frac{\partial^2 \phi^n}{\partial x^2}\right|_j + \frac{\Delta x^2}{12} \left.\frac{\partial^4 \phi^n}{\partial x^4}\right|_j + \cdots$$

So we get

$$L[\phi] - \left(\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2}\right) = -\alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} + \frac{\Delta t}{2} \frac{\partial^2 \phi}{\partial t^2} + \cdots$$

$L[\phi] = 0$ for the numerical soln

$$\Rightarrow \boxed{\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = +\alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} - \frac{\Delta t}{2} \frac{\partial^2 \phi}{\partial t^2} + \cdots}$$

modified equation

as Δt & $\Delta x \to 0$, we obtain the exact pde

Also 1st order in time & 2nd order in space.

In order increase accuracy of the method we require

$$\frac{\alpha \Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} = \frac{\Delta t}{2} \frac{\partial^2 \phi}{\partial t^2}$$

This will be achieved by judicious choice of Δt & Δx

$$\frac{\partial^2 \phi}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial \phi}{\partial t}\right) = \frac{\partial}{\partial t}\left[\alpha \frac{\partial^2 \phi}{\partial x^2}\right] = \alpha \frac{\partial^2}{\partial x^2}\left(\frac{\partial \phi}{\partial t}\right)$$

$$= \alpha^2 \frac{\partial^4 \phi}{\partial x^4}$$

$$\Rightarrow \frac{\alpha \Delta x^2}{12} = \frac{\alpha^2 \Delta t}{2}$$

$$\Rightarrow \boxed{\frac{\alpha \Delta t}{\Delta x^2} = \frac{1}{6}}$$

This satisfies our von-Neumann stability criterion $\boxed{\alpha \Delta t / \Delta x^2 \le 1/2}$ However, more restrictive

Approximate Factorization and Alternating direction Implicit schemes:

Approximate Factorization:

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

Implicit scheme: $$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \alpha\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi^{n+1}$$

$$\Rightarrow \left[1 - \alpha \Delta t\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\right]\phi^{n+1} = \phi^n$$

$$A_x \phi = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} \quad ; \quad A_y \phi = \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2}$$

$$\left[I - \alpha \Delta t A_x - \alpha \Delta t A_y\right]\phi^{n+1} = \phi^n$$

$$\left[I - \alpha \Delta t A_x\right]\left[I - \alpha \Delta t A_y\right]\phi^{n+1} = \phi^n$$

$$\Rightarrow \left[I - \alpha \Delta t A_x \cancel{+ I} - \alpha \Delta t A_y + \underbrace{\alpha^2 \Delta t^2 A_x A_y}_{O(\Delta t^2)\ \text{error}}\right]\phi^{n+1} = \phi^n$$

$$\begin{cases} \left[I - \alpha \Delta t A_x\right] Z = \phi^n \\ \left[I - \alpha \Delta t A_y\right]\phi^{n+1} = Z \end{cases} \quad ; \quad Z = \left[I - \alpha \Delta t A_y\right]\phi^{n+1}$$

Two steps.

→ Boundary condition.

Stability of Leap-Frog:

$$\frac{\phi_j^{(n+1)} - \phi_j^{(n-1)}}{2\Delta t} = \alpha \frac{\phi_{j+1}^{(n)} - 2\phi_j^{(n)} + \phi_{j-1}^{(n)}}{\Delta x^2}$$

Use von-Neumann

here it is time level

$$\phi_j^{(n)} = \sigma^n e^{ikx_j}$$

Note σ^n is $\sigma \times \sigma \times \sigma \ldots$ n times

$$\frac{\sigma^{n+1} e^{ikx_j} - \sigma^{n-1} e^{ikx_j}}{2\Delta t} = \frac{\alpha}{\Delta x^2} \sigma^n e^{ikx_j} \left[e^{ik\Delta x} - 2 + e^{-ik\Delta x} \right]$$

Divide by $\sigma^n e^{ikx_j}$

$$\frac{\sigma - \frac{1}{\sigma}}{2\Delta t} = \frac{\alpha}{\Delta x^2} \left[2\cos(k\Delta x) - 2 \right]$$

$$\sigma^2 - \frac{2\alpha \Delta t}{\Delta x^2} \left[2\cos(k\Delta x) - 2 \right] \sigma - 1 = 0$$

$$\sigma^2 + \underbrace{\frac{4\alpha \Delta t}{\Delta x^2} \left[1 - \cos(k\Delta x) \right]}_{b} \sigma - 1 = 0$$

$$\sigma = \frac{-b \pm \sqrt{b^2 + 4}}{2}, \quad b = \frac{4\alpha \Delta t}{\Delta x^2} \left[1 - \cos(k\Delta x) \right]$$

Note that $0 \le b < 1$

when $b > 0$, $|\sigma| > 1$ & $b = 0 \Rightarrow |\sigma| = 1$

Thus Leap-frog for diffusion eqn is unconditionally unstable!

Implicit or Backward Euler

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \alpha \frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2}$$

$$\frac{\sigma^{n+1} e^{ikx_j} - \sigma^n e^{ikx_j}}{\Delta t} = \alpha \frac{\sigma^{n+1} e^{ikx_j}}{\Delta x^2}\left[e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right]$$

$$\frac{\sigma - 1}{\Delta t} = \frac{\alpha \sigma}{\Delta x^2}\left[2\cos(k\Delta x) - 2\right]$$

$$\sigma\left[1 + 2\frac{\alpha \Delta t}{\Delta x^2}\left[1 - \cos(k\Delta x)\right]\right] = 1$$

$$\boxed{\sigma = \frac{1}{1 + \frac{2\alpha\Delta t}{\Delta x^2}\left(1 - \cos(k\Delta x)\right)}}$$

$1 - \cos(k\Delta x) \leq 2$ and $1 - \cos(k\Delta x) \geq 0$

$\therefore |\sigma| \leq 1$ unconditionally stable!

<u>But</u>, <u>costly</u> <u>iterations</u> <u>necessary</u>!

tridiagonal system of linear algebraic eqn's

$$\boxed{-\frac{\alpha \Delta t}{\Delta x^2}\phi_{j-1}^{n+1} + \left(1 + 2\frac{\alpha\Delta t}{\Delta x^2}\right)\phi_j^{n} - \frac{\alpha \Delta t}{\Delta x^2}\phi_{j+1}^{n+1} = \phi_j^n}$$

reading 10.6.2

<u>Du-Fort Frankel</u> <u>An inconsistent scheme</u>:

$$\frac{\phi_j^{n+1} - \phi_j^{n-1}}{2\Delta t} = \frac{\alpha}{\Delta x^2}\left[\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n\right]$$

Leap-frog → unconditionally unstable

Replace ϕ_j^n on RHS by $\phi_j^n = \dfrac{\phi_j^{n+1} + \phi_j^{n-1}}{2}$

$$\Rightarrow \boxed{(1+2\gamma)\,\phi_j^{n+1} = (1-2\gamma)\,\phi_j^{n-1} + 2\gamma\,\phi_{j+1}^n + 2\gamma\,\phi_{j-1}^n}$$

$$\gamma = \frac{\alpha\Delta t}{\Delta x^2}$$

This method is unconditionally stable!

→ HW show that this is.

→ Derive modified equation

→ see example 5.5

Using Taylor series expansions for ϕ_j^{n+1}, ϕ_j^{n-1}, ϕ_{j+1}^n & ϕ_{j-1}^n and substituting above

$$\boxed{\frac{\partial\phi}{\partial t} - \alpha\frac{\partial^2\phi}{\partial x^2} = -\frac{\Delta t^2}{6}\frac{\partial^3\phi}{\partial t^3} + \frac{\alpha\Delta x^2}{12}\frac{\partial^4\phi}{\partial x^4} \underbrace{- \frac{\alpha\Delta t^2}{\Delta x^2}\frac{\partial^2\phi}{\partial t^2}}_{3} \underbrace{- \frac{\alpha\Delta t^4}{12\Delta x^2}\frac{\partial^4\phi}{\partial x^4}}_{4} + \cdots}$$

As $\Delta t \to 0$, $\Delta x \to 0$ consider 3 & 4

If for a given Δt, $\Delta x \downarrow$, the error increases!

Third term $\to 0$ iff $\Delta t \to 0$ faster than $\Delta x \to 0$

Inconsistent scheme!

Put Crank-Nicolson as HW.

Convection - Diffusion

$$f_t + u f_x = \alpha f_{xx}$$

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + u \frac{f_{j+1}^n - f_{j-1}^n}{2\Delta x} = \alpha \frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{\Delta x^2}$$

$$f_j^{n+1} = f_j^n\left(1 - 2\alpha \frac{\Delta t}{\Delta x^2}\right) - \frac{u\Delta t}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{\alpha \Delta t}{\Delta x^2}\left[f_{j+1}^n + f_{j-1}^n\right]$$

Again seek sol^n

$$f_j^n = \sigma^n e^{ikx_j}$$

$$\sigma^{n+1} e^{ikx_j} = \sigma^n e^{ikx_j}\left(1 - 2\frac{\alpha\Delta t}{\Delta x^2}\right) - \frac{u\Delta t}{2\Delta x}\left[e^{ik\Delta x} - e^{-ik\Delta x}\right]\sigma^n e^{ikx_j} + \frac{\alpha\Delta t}{\Delta x^2}\left[e^{ik\Delta x} + e^{-ik\Delta x}\right]\sigma^n e^{ikx_j}$$

$$\sigma = 1 - 2d - \frac{\lambda}{2}\left[2 \sin k\Delta x\right] + d\left(2\cos k\Delta x\right]$$