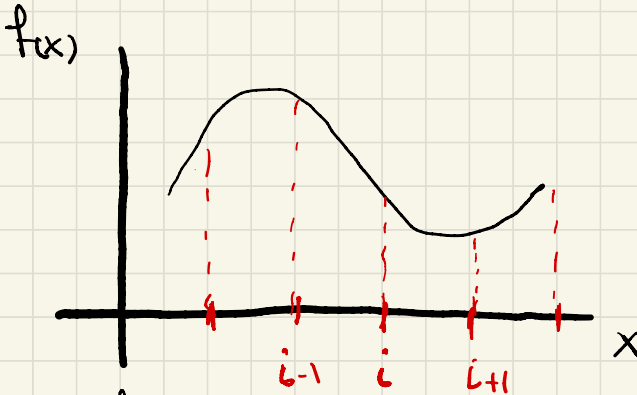
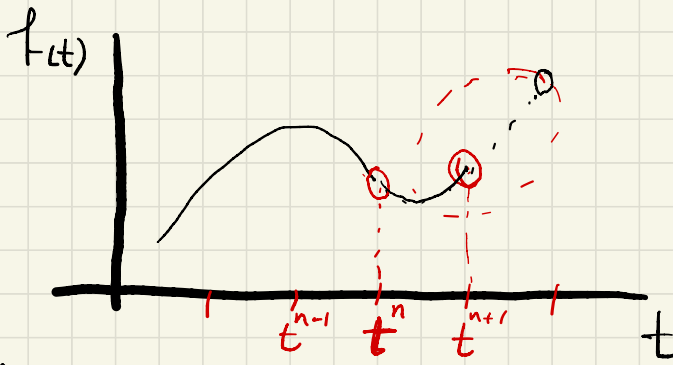



Solution of ordinary differential Equations (ODE)

- first order ODE's
- high order ODE can be converted to a system of first order ODE's
- Classes of ODE's :
 - Initial Value Problems
 - Boundary Value Problems
 - Eigenvalue Problems



$$f'_i \approx \alpha f_{(i-1)} + \beta f_i + \gamma f_{i+1} + \dots$$



$$f(t=0) \longrightarrow f(t=t_f)$$

first order ODE :

initial condition

$$\textcircled{*} \quad \frac{dy}{dt} = f(y, t) \quad ; \quad y(0) = y_0$$

find $y(t)$ for $0 < t \leq t_f$

Numerically: $t^{n+1} = t^n + \underline{\Delta t} \rightarrow 0 \leq t \leq t^n$

$$y^{n+1} = y(t^{n+1})$$

$$y^{n+2}$$

until

$$t_f$$

Taylor Series Method:

Expand the solution (a) t^{n+1} about the solution (a) t^n ($\Delta t = h$)

$$y_{n+1} = y_n + h y_n' + \frac{h^2}{2} y_n'' + \frac{h^3}{6} y_n''' + \dots$$

from (*) $\rightarrow y_n' = f(y_n, t_n)$

if \downarrow stop (a) \rightarrow Second order Method
(locally)

to approximate higher Order derivatives:

$$y'' = \frac{dy'}{dt} = \frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} \left(\frac{\partial y}{\partial t} \right) = \frac{f}{t} + \frac{f_y}{y}$$

Impractical \Rightarrow first two term

Euler Method:

$$y^{n+1} = y^n + h f(y^n, t^n)$$

Q: how does it work?

1. Start with initial conditions to
2. March forward $y_1 \rightarrow y_2 \rightarrow \dots \rightarrow y_n$

From Taylor Series Expansion: - 2nd order
One time Step

- 1st order
global error to $t^{\frac{1}{2}}$

Class of time Integrators:

* Multi-step

One-step Method

* Explicit / Implicit

Explicit Scheme

- Convergence \rightarrow accuracy

- NEW Concept in time Integration

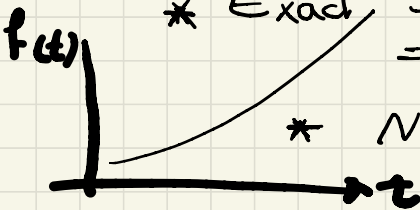
Numerical Stability :

* Critical property differential equations

* Exact Solution is well behaved
 \Rightarrow never grows unbounded

* Numerical Solution grows unbounded

\Rightarrow Numerical Instability



Given: $y' = f(y, t)$

\Rightarrow all dependant on the step size: $(h, \Delta t)$

Stable numerical schemes:

Solution will not grow unbounded (blow-up) with any choice of 'h'

Unstable numerical scheme:

Solution blows-up with any choice of 'h'

\Rightarrow does not depend on accuracy

Conditionally Stable numerical scheme:

Certain choice of h leads to stability

Stability Analysis:

Determine the stability Property

* Perform the analysis for \otimes assuming it has features of the general Eqn.

* Perform two-dimensional Taylor Series Expansion

$$f(y, t) = f(y_0, t_0) + (t-t_0) \frac{\partial f}{\partial t}(y_0, t_0) + (y-y_0) \frac{\partial f}{\partial y}(y_0, t_0) + \frac{1}{2!} \left[(t-t_0)^2 \frac{\partial^2 f}{\partial t^2} + 2(t-t_0)(y-y_0) \frac{\partial^2 f}{\partial t \partial y} + (y-y_0)^2 \frac{\partial^2 f}{\partial y^2} \right] + \dots$$

Collecting linear terms: $y' = \lambda y + \alpha_1 + \alpha_2 t + \dots$

$$y' = \lambda y \rightarrow \text{"model Problem"}$$

Exponential Soln & Worst case

It turns out \Rightarrow inhomogeneous terms do not significantly affect the results of stability analysis

$$\lambda \rightarrow \text{complex} \quad \underline{\lambda_R + i \lambda_I}$$

Stability Analysis for Explicit Euler (EE)

$$y^{n+1} = y^n + h f(y^n, t^n)$$

model
 \rightarrow
Problem

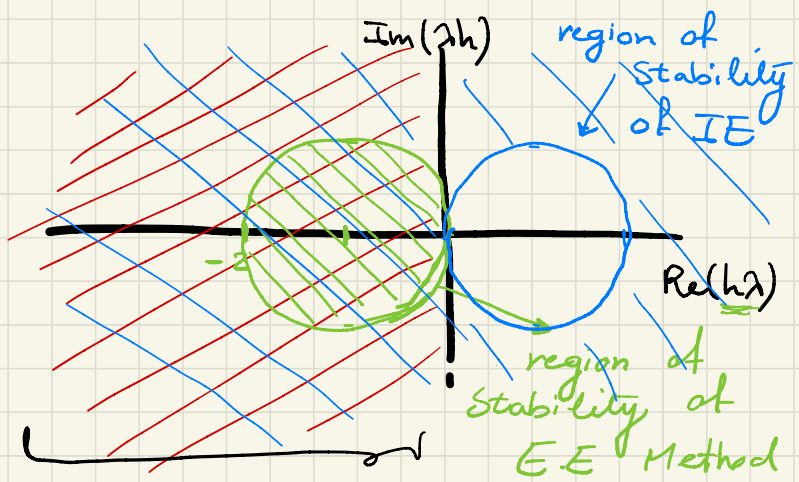
$$y^{n+1} = y^n + h \lambda y^n$$

$$= y^n (1 + \lambda h)$$

for complex λ , we have

$$y^n = y^0 \underbrace{(1 + \lambda h)^n}_{\text{amplification factor}} = y^0 \sigma^n$$

$$y' = \lambda y \rightarrow \underbrace{e^{\lambda t}}_{\text{exact}} \rightarrow \lambda_R < 0$$



Cond. Stable Scheme $\Rightarrow |\sigma| \leq 1$

$$(1 + \lambda_R h)^2 + \lambda_I^2 h^2 = 1$$

circle

for purely (λ_R) real : $h \leq \frac{2}{|\lambda_R|}$

for unstable soln :

$$|1 + \lambda h| > 1$$

negative with magnitude greater than 1 $\Rightarrow y^n = (1 + \lambda h)^n y_0$

\Rightarrow Oscillations with change of sign at every time step

Implicit or Backward Euler:

* One-step

* Implicit scheme

$$y^{n+1} = y^n + hf(y^{n+1}, t^{n+1})$$

if f nonlinear: solve a nonlinear algebraic Eqn.

\Rightarrow iteratively

\Rightarrow higher cost than Exp.

\Rightarrow Much better stability

Stability analysis: (model Problem)

$$y^{n+1} = y^n + \lambda h y^{n+1}$$

\rightarrow solve for y^{n+1}

$$y^{n+1} = \underbrace{(1 - \lambda h)^{-1}}_{\sigma} y^n \Rightarrow y^{n+1} = \sigma^n y_0$$

$$\sigma = \frac{1}{1 - \lambda h}$$

$$A = \sqrt{(1 - \lambda_R h)^2 + \lambda_I^2 h^2}$$

$$\sigma = \frac{1}{(1 - \lambda_R h) + i \lambda_I h}$$

modules
and
Phase factor

$$\sigma = \frac{1}{A e^{i\theta}}$$

$$\theta = -\tan^{-1} \frac{\lambda_I h}{1 - \lambda_R h}$$

For Stability: $|\sigma| \leq 1$

$$\frac{|e^{-i\theta}|}{A} = \frac{1}{A} \leq 1$$

For Stable exact Soln. λ_R is negative.

$$\Rightarrow A > 1 \Rightarrow \frac{1}{A} \leq 1 \Rightarrow \text{unconditionally stable}$$

Stability \neq accuracy

Numerical Accuracy:

take the model problem:

$$y' = \lambda y$$

$$y^n = (\sigma)^n y_0$$

$$\text{Exact solution: } y(t) = y_0 e^{\lambda t} = y_0 e^{\lambda n h} = y_0 (e^{\lambda h})^n$$

determine accuracy by comparing to the exact soln.

Exact : $e^{\lambda h} = 1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \dots$

E.E : $\sigma = 1 + \lambda h$

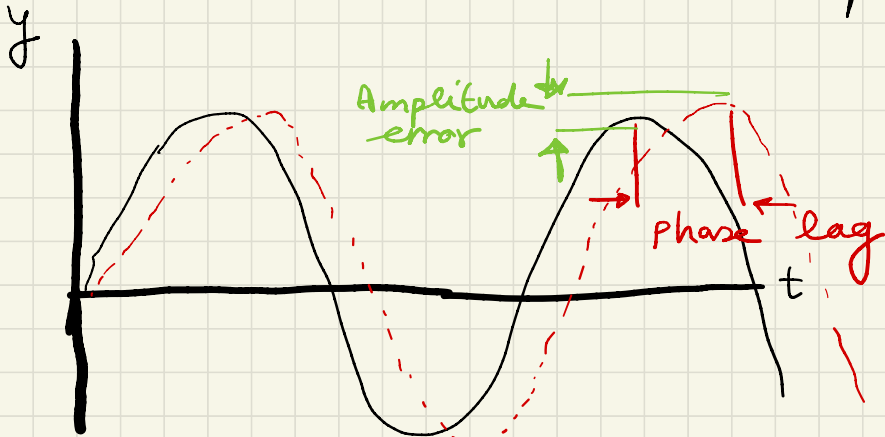
B.E : $\sigma = 1 + \lambda h + \lambda^2 h^2 + \lambda^3 h^3 + \dots$

↓
 $\frac{1}{1 - \lambda h}$

Both methods reproduce only up to " λh "

⇒ 2nd order locally
 1st order globally

⇒ linear analysis → upper limit
 → lower order for nonlinear eqns



for oscillatory soln. $\left. \begin{array}{l} * \text{accuracy not informative} \\ * \text{phase} \\ * \text{amplitude} \end{array} \right\} \lambda_{\pm}$

$y' = i\omega y$, $y(0) = 1$
 exact soln. $e^{i\omega t}$, which is oscillatory

$\left\{ \begin{array}{l} \text{frequency} : \omega \\ \text{Amplitude} : 1 \end{array} \right.$

Num Soln:

EE $y^n = \sigma^n y_0$, $\sigma = 1 + i\omega h$

Amplitude: $|\sigma| = \sqrt{1 + \omega^2 h^2} \geq 1$

\Rightarrow EE unstable for purely Imag. λ

phase:

$$\sigma = |\sigma| e^{i\theta}$$

$$\theta = \tan^{-1} \omega h = \tan^{-1} \frac{\text{Im}(\sigma)}{\text{Re}(\sigma)}$$

measure of the phase error (PE):

$$PE = \omega h - \theta = \omega h - \tan^{-1} \omega h$$

$$\tan^{-1}(\omega h) = \omega h - \frac{(\omega h)^3}{3} + \frac{(\omega h)^5}{5} + \dots$$

$$PE = \frac{(\omega h)^3}{3} \quad \text{in one time-step}$$

$$n(PE) \leftarrow n \text{ time steps}$$

Trapezoidal Method:

$$y(t) = y_n + \int_{t^n}^t f(y, t') dt'$$

$$(a) \quad t = t^{n+1}$$

$$y^{n+1} = y_n + \int_{t^n}^{t^{n+1}} f(y, t) dt$$

approximate the integral with trapezoidal rule:

$$y^{n+1} = y_n + \frac{h}{2} \left[f(y^{n+1}, t^{n+1}) + f(y^n, t^n) \right]$$

* Implicit scheme

* Crank-Nicolson scheme

A second order Equation:

$$y'' + \omega^2 y = 0 \quad t > 0$$

$$y(0) = y_0, \quad y'(0) = 0$$

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= -\omega^2 y_1 \end{aligned} \quad \text{in matrix form} \quad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}' = \begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$z_1' = i\omega z_1, \quad z_2' = -i\omega z_2$$

\Rightarrow eigenvalues \Rightarrow Both imaginary

$$Y' = AY$$

EE:

$$Y^{n+1} = Y^n + hAY^n = (I + hA)Y^n$$

IE

$$Y^{n+1} = Y^n + hAY^{n+1}$$

$$[I - hA] Y^{n+1} = Y^n \Rightarrow AX = b$$

$$\underbrace{\hspace{10em}}_B$$

$$BY^{n+1} = Y^n$$

Model Problem a ($y' = \lambda y$)

$$y_{n+1} - y_n = h/2 \left[\lambda y_{n+1} + \lambda y_n \right]$$

$$y_{n+1} = \underbrace{\frac{1 + \lambda h/2}{1 - \lambda h/2}}_{\sigma} y_n$$

$$\sigma = \frac{1 + \lambda h/2}{1 - \lambda h/2} = 1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{4} + \dots$$

Q: What is the order of accuracy?

2nd order

$$\lambda = \lambda_R + i \lambda_I$$

$$\rightarrow \sigma = \frac{1 + \lambda_R h/2 + i \lambda_I h/2}{1 - \lambda_R h/2 - i \lambda_I h/2} = \frac{A e^{i\theta}}{B e^{i\alpha}}$$

$$\sigma = \frac{A}{B} e^{i(\theta - \alpha)}$$

$$|\sigma| = \frac{A}{B}$$

for $\lambda_R < 0$ (exact solution bounded)

$$\Rightarrow A < B \Rightarrow \underline{|\sigma|} < 1$$

\Rightarrow unconditionally stable
Implicit Scheme

$$\text{for } \lambda = i\omega \Rightarrow A = B \Rightarrow |\sigma| = 1$$

\Rightarrow no amplitude error

$$PE = \omega h - 2 \tan^{-1} \left(\frac{\omega h}{2} \right) = \frac{\omega h^3}{12} \rightarrow \dots$$

\hookrightarrow 4 times better!
EE

Apply to TD:

$$Y^{n+1} - Y^n = \frac{h}{2} \left[AY^{n+1} + AY^n \right]$$

$$\underbrace{\left[I - \frac{h}{2} A \right]}_{\sim} Y^{n+1} = \underbrace{\left[I + \frac{h}{2} A \right]}_{\sim} Y^n$$

$$A Y^{n+1} = b$$

Runge-Kutta Methods:

→ more information can be added by including terms

RK Methods →

- points between t^n & t^{n+1}
- evaluate f at intermediate points
- higher cost per time-step
- higher accuracy
- better stability properties

General form of (two-stage) 2nd Order RK formula for solving: $y' = f(y, t)$

Soln. at t^{n+1} is:

$$\textcircled{1} \quad y^{n+1} = y^n + \underline{\alpha_1 k_1} + \underline{\alpha_2 k_2}$$

k_1 & k_2 :

$$k_1 = h f(y_n, t_n)$$

$$k_2 = h f(y_n + \underline{\beta k_1}, t_n + \underline{\alpha h})$$

→ constants to be determined

⇒ ensure highest accuracy

Taylor Series expansion of $y(t^{n+1})$:

$$y^{n+1} = y^n + h y_n' + \frac{h^2}{2} y_n'' + \dots$$

$$y_n' = f(y_n, t_n)$$

using chain rule :

$$y_n'' = f_t + f f_y \rightarrow \begin{array}{l} \text{partial derivatives} \\ \text{of } f \\ \text{w.r.t. } t \text{ \& } y \end{array}$$

$$\Rightarrow \textcircled{2} \quad y_{n+1} = y_n + h f(y_n, t_n) + \frac{h^2}{2} \left(f_t + f f_y \right)$$

to establish the order of accuracy of

RK Method $\textcircled{1} \Rightarrow$ comparing its estimate for y^{n+1} $\textcircled{2}$

two-dimensional Taylor series expansion of k_2 leads to

$$k_2 = h \left[f(y_n, t_n) + \beta k_1 f_y + \alpha h f_{tt} + O(h^2) \right]$$

noting that $k_1 = h f(y_n, t_n)$, substituting in $\textcircled{1}$

$$y^{n+1} = y^n + (\delta_1 + \delta_2) h f_n + \frac{1}{2} \beta h^2 f_n' + \frac{1}{2} \alpha h^2 f_n'' + \dots$$

matching similar coefficients:

$$\left. \begin{array}{l} \delta_1 + \delta_2 = 1 \\ \delta_2 \alpha = \frac{1}{2} \\ \delta_2 \beta = \frac{1}{2} \end{array} \right\} \begin{array}{l} 3 \text{ equations} \\ 4 \text{ unknowns} \\ \Rightarrow \alpha = \text{free parameter} \end{array}$$

$$\Rightarrow \delta_2 = \frac{1}{2\alpha}, \quad \beta = \alpha, \quad \delta_1 = 1 - \frac{1}{2\alpha}$$

\Rightarrow One-parameter family of 2nd order RK formulas:

$$k_1 = h f(y_n, t_n)$$

$$k_2 = h f(y_n + \alpha k_1, t_n + \alpha h)$$

$$y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) k_1 + \frac{1}{2\alpha} k_2$$

usually: $\alpha = \frac{1}{2}$

predicted value $\leftarrow y_{n+1/2}^* = y_n + \frac{1}{2} f(y_n, t_n)$

corrected value $\leftarrow y_{n+1} = y_n + h f(y_{n+1/2}^*, t_{n+1/2})$

Stability analysis:

model eqn. $y' = \lambda y$, substitute in (1)

$$\Rightarrow k_1 = \lambda h y_n$$

$$k_2 = h(\lambda y_n + \alpha h k_1) = \lambda h(1 + \alpha \lambda h) y_n$$

$$y_{n+1} = y_n + (1 - \frac{1}{2\alpha}) \lambda h y_n + \frac{1}{2\alpha} \lambda h(1 + \alpha \lambda h) y_n$$

$$= y_n \left(1 + \lambda h + \frac{\lambda^2 h^2}{2} \right)$$

\Rightarrow 2nd order

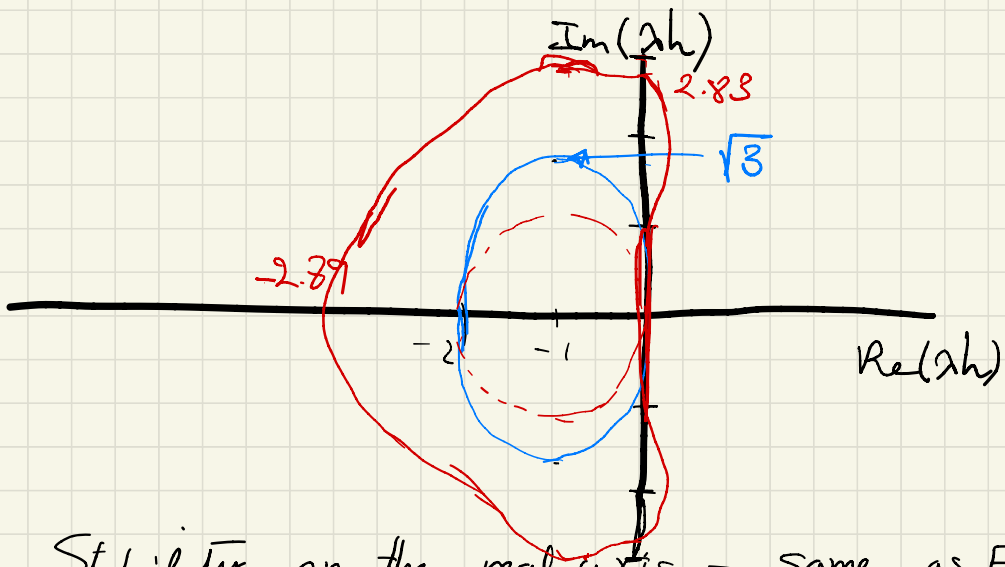
\Rightarrow for stability we must have

$$|\sigma| \leq 1$$

to find the stability region

$$\Rightarrow \sigma = e^{i\theta} = \left(1 + \lambda h + \frac{\lambda^2 h^2}{2} \right)$$

↓
find complex roots λh
for different values of θ



- Stability on the real axis = same as EE
- Significant improvement for complex λ
- for purely imaginary λ : $\boxed{|\lambda = i\omega|}$

unstable

$$\leftarrow |\sigma| = \sqrt{1 + \frac{\omega^4 h^2}{4}} > 1$$

for small values of $\omega h \Rightarrow$ less unstable than EE

Example: Amplification factor

consider $y' = i\omega y \quad y(0) = 1$

Use EE & RK2 schemes

Integration for 100 time-steps $\omega h = 0.2$

$$\Rightarrow t=0 \rightarrow 20/\omega$$

each numerical soln. after 100 iterations,

$$y = \sigma^{100} y_0$$

↓
amplification factor

$$EE: |\sigma| = \sqrt{1 + \omega^2 h^2} = 1.0198 \rightarrow |y| = 2.10$$

$$RK2: |\sigma| = 1.0002 \rightarrow |y| = 1.02$$

2% ↓

Phase Error:

real & imaginary parts of σ for $\lambda = i\omega$

$$PE = \omega h - \tan^{-1}\left(\frac{\omega h}{1 - \frac{\omega^2 h^2}{2}}\right)$$

$$PE = -\frac{\omega^3 h^3}{6} + \dots$$

only factor of 2 better than EE, but opposite sign

\Rightarrow negative phase error \Rightarrow phase lead

The most widely used RK Method is
the 4th order Formula:

$$y_{n+1} = y_n + \frac{1}{6}k_1 + \frac{1}{3}(k_2+k_3) + \frac{1}{6}k_4$$

where,

$$k_1 = hf(y_n, t_n)$$

$$k_2 = hf(y_n + \frac{1}{2}k_1, t_n + \frac{1}{2}h)$$

$$k_3 = hf(y_n + \frac{1}{2}k_2, t_n + \frac{1}{2}h)$$

$$k_4 = hf(y_n + k_3, t_n + h)$$

Stability Analysis (model eqn. $y' = \lambda y$)

$$y_{n+1} = \left(1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \frac{\lambda^4 h^4}{24} \right) y_n$$

\Rightarrow fourth Order accurate

\Rightarrow for plotting the stability diagram
find roots of the following 4th order
polynomial with complex Coefficients:

$$\lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \frac{\lambda^4 h^4}{24} + 1 - e^{i\theta} = 0 \text{ for } 0 \leq \theta \leq \pi$$

\Rightarrow Improvement over the stability region
of RK2 \Rightarrow larger time-steps
faster time to solution

\Rightarrow large stability region of Imaginary
axis

\Rightarrow Stability region in Positive $\text{Re}(\lambda)$
 \Rightarrow artificially stable

Multi-step Methods:

higher order accuracy achieved by
using data from prior to $t_n \rightarrow t_{n-1}, t_{n-2}$

\rightarrow Multi-step Methods

\rightarrow higher computer memory

\rightarrow not self starting \rightarrow usually another
method (EE, for example) start the
calculation.

leap-frog method

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h}$$

$$\textcircled{*} y_{n+1} = y_{n-1} + 2h f(y_n, t_n) + \textcircled{O(h^3)}$$

→ Central difference formula for y'

→ 2nd Order

→ y_0 (initial condition)

→ f_1 (EE)

Stability Analysis $\textcircled{8}$ ($y' = \lambda y$)

$$y_{n+1} - y_{n-1} = 2h\lambda y_n$$

to solve it, a solution of the form

$$y_n = \sigma^n y_0$$

in \textcircled{x} leads to

$$\sigma^{n+1} - \sigma^{n-1} = 2h\lambda \sigma^n$$

dividing by σ^{n-1} , we get a
quadratic eqn. for σ :

$$\sigma^2 - 2h\lambda\sigma - 1 = 0$$

$$\Rightarrow \sigma_{1,2} = h\lambda \pm \sqrt{h^2\lambda^2 + 1}$$

having more than one root is the characteristic of multi-step methods:

$$\sigma_1 = \lambda h + \sqrt{\lambda^2 h^2 + 1} = 1 + \lambda h + \frac{\lambda^2 h^2}{2} - \frac{\lambda^4 h^4}{8} + \dots$$

2nd order accurate

$$\sigma_2 = \lambda h - \sqrt{\lambda^2 h^2 + 1} = -1 + \lambda h - \frac{1}{2} \lambda^2 h^2 + \dots$$

spurious \rightarrow source of numerical problems.

- $h=0 \Rightarrow$ spurious root $\neq 1$

- for λ real and negative

$\Rightarrow |\sigma_2| > 1 \Rightarrow$ leads to instability

- linear problem: solution is a linear combination of σ_1, σ_2

$$y_n = c_1 \sigma_1^n + c_2 \sigma_2^n$$

starting conditions

$$y_0 \text{ \& } y_1 \\ n=0 \text{ \& } n=1$$

$$\begin{cases} y_0 = c_1 + c_2 \\ y_1 = c_1 \sigma_1 + c_2 \sigma_2 \end{cases}$$

for $i\omega = \lambda \rightarrow$ if $|\omega h| \leq 1 \Rightarrow |\sigma_{1,2}| = 1$
 \Rightarrow no amplitude errors

if $|\omega h| > 1 \Rightarrow |\sigma_{1,2}| = |\omega h \pm \sqrt{\omega^2 h^2 - 1}|$
 \Rightarrow unstable

Adams - Bashforth method :

Using Taylor Series Expansion :

$$y_{n+1} = y_n + h y'_n + \frac{h^2}{2} y''_n + \frac{h^3}{6} y'''_n + \dots$$

Substitute $y'_n = f(y_n, t_n)$

A first order finite difference approximation for y''_n :

$$y''_n = \frac{f(y_n, t_n) - f(y_{n-1}, t_{n-1})}{h} + o(h)$$

\Rightarrow

$$y_{n+1} = y_n + \frac{3h}{2} f(y_n, t_n) - \frac{h}{2} f(y_{n-1}, t_{n-1}) + o(h^3)$$

\hookrightarrow globally 2nd Order

Stability Analysis:

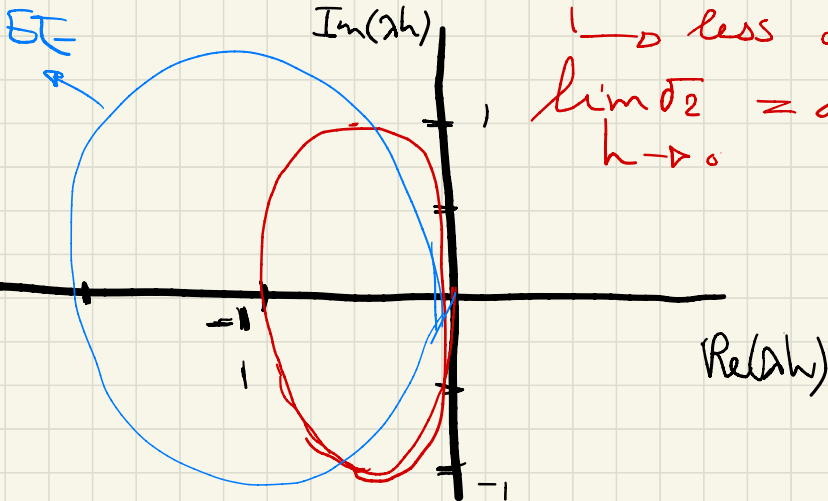
$$y_{n+1} - \left(1 + \frac{3\lambda h}{2}\right) y_n + \frac{\lambda h}{2} y_{n-1} = 0$$

\Rightarrow Quadratic eqn. for σ :

$$\sigma_{1,2} = \frac{1}{2} \left[1 + \frac{3}{2}\lambda h \pm \sqrt{1 + \lambda h + \frac{9}{4}\lambda^2 h^2} \right]$$

$$\sigma_1 = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + o(h^3)$$

$$\sigma_2 = \frac{1}{2}\lambda h - \frac{1}{2}\lambda^2 h^2 + o(h^3)$$



\hookrightarrow less dangerous
 $\lim_{h \rightarrow 0} \sigma_2 = 0$

- more limiting than EE & RK2
- unstable for pure imaginary λ s
- very mild instability
- for the problem at $j = -i\omega$
 $|\sigma_1|^{100} = 1.04$ 4% error
 slightly worse than RK2!

TD :

$$y_{n+1} = y_n + 3\frac{h}{2} f(y_n, t_n) - \frac{h}{2} f(y_{n-1}, t_{n-1})$$

Example

$$Y' = AY$$

$$Y^{n+1} = Y^n + 3\frac{h}{2} AY^n - \frac{h}{2} AY^{n-1}$$

$$Y^{n+1} = \left[I + 3\frac{h}{2} A \right] Y^n - \frac{h}{2} AY^{n-1}$$

EE (first step)

$$Y^{n+1} = Y^n + hAY^n = [I + hA]Y^n$$

System of first order differential Eqn's :

- higher order ODE can be converted to a system of 1st order ODE's

→ Chemical reactions

→ Structure Vibration

- In generic form

$$y' = f(y, t); \quad y(0) = y_0$$

→ y is a vector with elements y_i

→ $f(y_1, y_2, \dots, y_m, t)$ is a vector function with elements

$$f_i(y_1, y_2, \dots, y_m, t), \quad i=1, 2, \dots, m$$

Application of time integration schemes are straight-forward

EE 1

$$y_i^{n+1} = y_i^n + h f_i(y_1^n, y_2^n, \dots, y_m^n, t_n)$$

$i = 1, 2, 3, \dots, m$

There is only one difference with one ODE,
Stiffness Property

lets discuss stiffness in connection with linear systems:

$$\frac{dy}{dt} = Ay$$

$m \times m$

constant matrix

model problem for a system of ODE's

All eigenvalues of A are real and negative \Rightarrow bounded Soln.

EE:

$$y^{n+1} = y^n + hAy^n = (I + hA)y^n$$

$$y^n = (I + hA)^n y^0$$

$$B = (I + hA)^n \rightarrow 0$$

for large n

\Rightarrow from linear Algebra \Rightarrow magnitude of its eigenvalues (α_i) < 1

$$\Rightarrow \alpha_i = 1 + h\lambda_i$$

↓ eigenvalues of A

$$\Rightarrow |1 + \lambda_i h| \leq 1 \Rightarrow h \leq \frac{2}{|\lambda|_{\max}}$$

if the range of the magnitudes of eigenvalues is large

$$\left(\frac{|\lambda|_{\max}}{|\lambda|_{\min}} \gg 1 \right) \Rightarrow \text{Stiff system}$$

Since the step size is limited by the part of the soln with the "fastest" response time (largest λ) \Rightarrow large # of steps.

long time behavior \Rightarrow small time-steps

\rightarrow implicit scheme

Numerical Soln. of Partial differential equations (PDEs)

* Solid Mechanics

- vibrations
- elasticity
- - - -

* Acoustics (waves)

* heat & mass transfer

faster computer \Rightarrow numerical soln.

\rightarrow More challenging than ODE's

Semi-Discretization

PDE \rightarrow converted easily to a system of ODEs

\rightarrow finite difference approximation for derivatives in all but one of the dimensions.

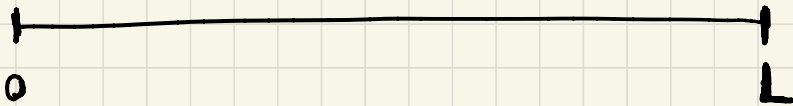
Example: One-dimensional diffusion equation (heat equation) for $\varphi(x, t)$

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

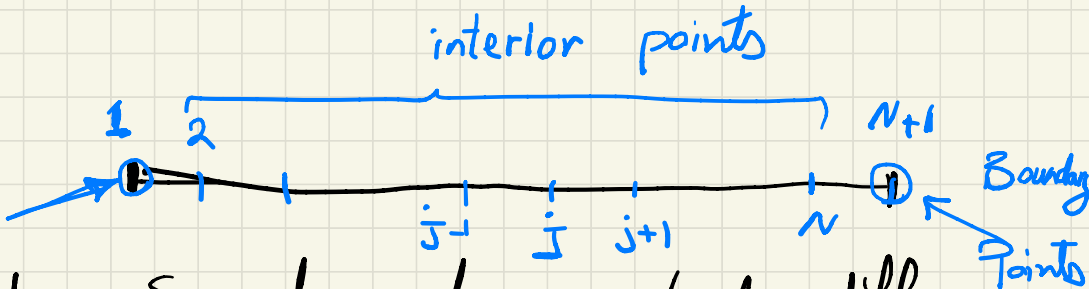
↓ diffusion coefficient

Suppose the boundary and initial conditions are:

$$\varphi(0, t) = \varphi(L, t) = 0 \quad \& \quad \varphi(x, 0) = g(x)$$

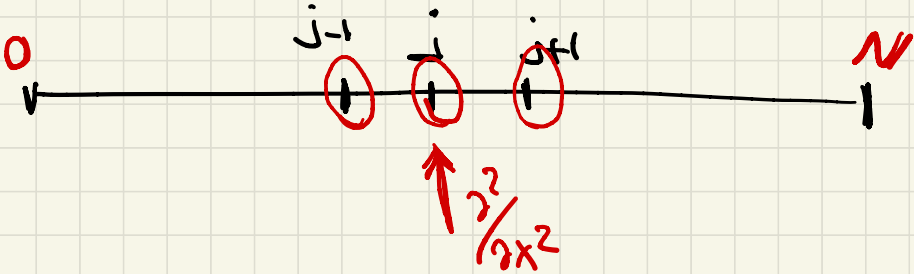


We discretize the coordinate "x" with $N+1$ uniformly spaced grid points



Use second order central difference scheme to approximate the second derivative $\ddot{\varphi}$

$$\frac{\partial^2 \varphi_j}{\partial x^2} = \frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{\Delta x^2}$$



$$\underbrace{\frac{\partial \varphi_j}{\partial t}}_{\text{PDE}} = \alpha \underbrace{\frac{\partial^2 \varphi_j}{\partial x^2}}_{\text{System of ODE}} = \alpha \frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{\Delta x^2}$$

where $\varphi_j \equiv \varphi(x_j, t)$.

In matrix form

$$\frac{d}{dt} \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{N-1} \\ \varphi_N \end{bmatrix} = \frac{\alpha}{\Delta x^2} \begin{bmatrix} & & & & \\ 1 & -2 & 1 & \dots & \\ 0 & 1 & -2 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & \dots & 1 & -2 & 1 \\ & & & & \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \vdots \\ \varphi_{N-2} \\ \varphi_{N-1} \\ \varphi_N \end{bmatrix}$$

$$\frac{d}{dt} (\varphi_j) = \alpha \frac{\varphi_{j+1} - 2\varphi_j + \varphi_{j-1}}{\Delta x^2}$$

$$j=2 \rightarrow \frac{d}{dt} [\varphi_2] = \frac{\alpha}{\Delta x^2} (\varphi_3 - 2\varphi_2 + \varphi_1)$$

$$j=N-1 \rightarrow \frac{d}{dt} [\varphi_{N-1}] = \frac{\alpha}{\Delta x^2} (\varphi_N - 2\varphi_{N-1} + \varphi_{N-2})$$

$$j=1 \rightarrow \frac{d}{dt} [\varphi_1] = \frac{\alpha}{\Delta x^2} (\varphi_2 - 2\varphi_1 + \varphi_0)$$

$$j=N \rightarrow \frac{d}{dt} [\varphi_N] = \frac{\alpha}{\Delta x^2} (\varphi_{N+1} - 2\varphi_N + \varphi_{N-1})$$

A is a banded matrix, compact notation

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

lower diagonal diagonal upper diagonal

ODE system solve using any of the numerical methods introduced ODEs

⇒ RK Methods

⇒ Multi-step methods

→ consider the notion of stiffness

$$A^{(n-1) \times (n-1)} \xrightarrow{\neq} \text{eigenvalues}^{(n-1)}$$

Range of eigenvalues of A determine whether the system is stiff or not.

→ Analytical expression are not always available

→ for A eigenvalues are

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

The eigenvalue with smallest magnitude is 0

$$\lambda_1 = \frac{\alpha}{\Delta x^2} \left(-2 + 2 \cos \frac{\pi}{N} \right)$$

for large N :

$$\cos \frac{\pi}{N} = 1 - \frac{1}{2!} \left(\frac{\pi}{N} \right)^2 + \frac{1}{4!} \left(\frac{\pi}{N} \right)^4 - \dots$$

converges rapidly: Retain the first 2 terms

$$\lambda_1 \approx -\frac{\pi^2 \alpha}{N^2 \Delta x^2}$$

& for large N we get 0

$$\lambda_{N-1} \approx -4\alpha / \Delta x^2$$

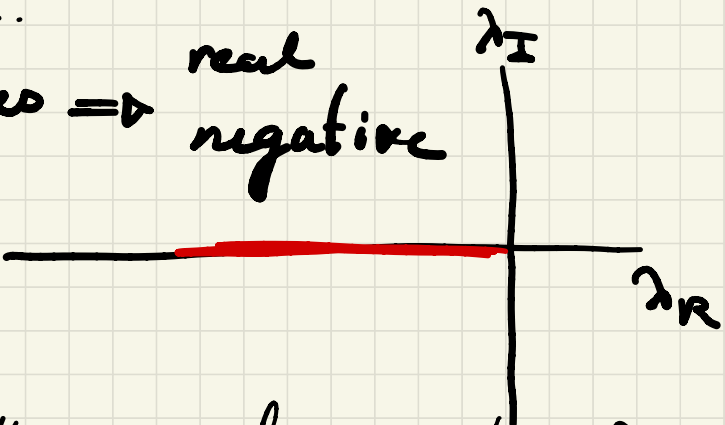
Therefore, the ratio of the eigenvalues:

$$\left| \frac{\lambda_{N-1}}{\lambda_1} \right| \approx \frac{4N^2}{\pi^2} \sim N^2$$

$$\boxed{N=20} \rightarrow N^2 = 400$$

As insight into the physical behavior of the soln.

eigenvalues \Rightarrow real negative



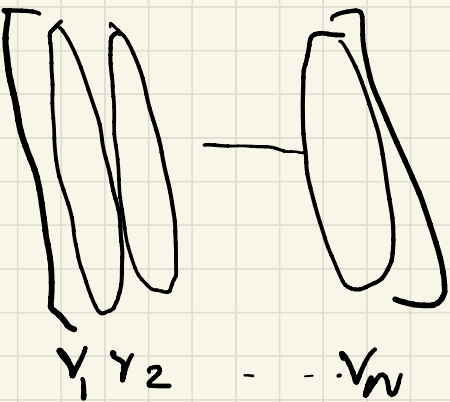
to see the role of eigenvalues \circ

Diagonalize A (linear Algebra)

$$A = S \Lambda S^{-1}$$

$$\Lambda = S^{-1} A S$$

$$\Lambda = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_{N-1} \end{bmatrix}$$



$\Lambda \rightarrow$ eigenvalues
 $\leftarrow S \rightarrow$ eigenvectors

Substitute A with $S \Lambda S^{-1}$

$$\text{in } \frac{\partial \varphi}{\partial t} = A \varphi$$

$$\underbrace{S^{-1}} \frac{d}{dt} \varphi = \underbrace{S^{-1} S}_{I} \Lambda \underbrace{S^{-1} \varphi}_{\psi} \rightarrow \frac{d}{dt} \underbrace{\psi}_{\psi} = \Lambda \underbrace{\psi}_{\psi}$$

$$\frac{d}{dt} \psi = \Lambda \psi$$

\hookrightarrow diagonal \Rightarrow equations are decoupled

$$\psi_j(t) = \psi_j(0) e^{\lambda_j t}$$

$$\varphi = S \psi = \psi_1 s^{(1)} + \psi_2 s^{(2)} + \dots + \psi_n s^{(n)}$$

$A = \begin{cases} \text{eigenvalues} \Rightarrow \text{Temporal behavior of} \\ \text{The Soln.} \\ \text{eigenvectors} \Rightarrow \text{Spatial behavior} \\ \text{of the Soln.} \end{cases}$

$$A = [1 \quad -2 \quad 1]$$

negative & real eigenvalues
 \Rightarrow decaying soln. in time

\Rightarrow Rate of decay: magnitude
at the eigenvalues

Solve the system of ODEs:

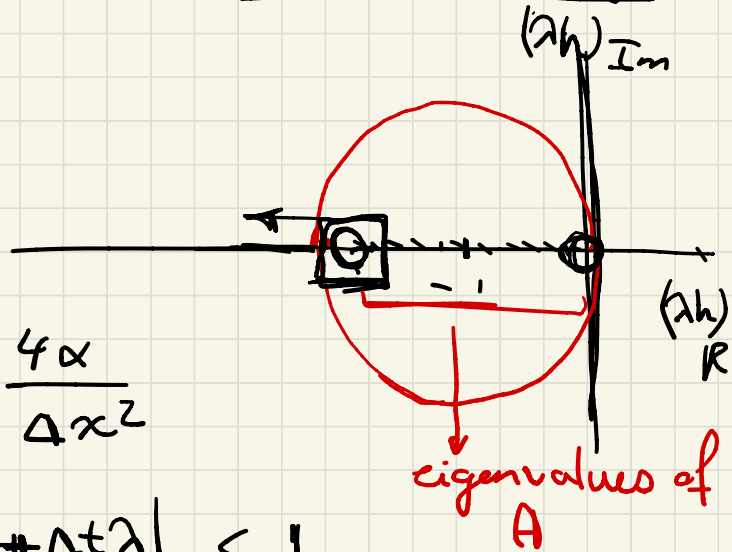
EE for time advancement

\rightarrow Conditionally Stable

Q. Estimate Δt_{\max} ?

$$\frac{d\phi}{dt} = \frac{\alpha}{\Delta x^2} A [1, -2, 1] \phi$$

The stability depends on the eigenvalues of the system. having the largest mag^e



$$\lambda_{n-1} \approx -\frac{4\alpha}{\Delta x^2}$$

model

Problem EE: $|1 + \Delta t \lambda|_{\max} \leq 1$

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

$$\alpha = 1, \quad \Delta x = 0.05 \rightarrow \Delta t_{\max} = 0.00125$$

$$\Delta t < 0.00125 \quad \text{Stable}$$

$$\Delta t > 0.00125 \quad \text{unstable}$$

$$\Delta t = 0.001$$

$$\Delta t = 0.0015$$

$$\frac{d\varphi}{dt} = \frac{\alpha}{\Delta x^2} \mathbb{A} [1, -2, 1] + \varphi$$

$\varphi_0 = 0$
 $\varphi_n = 0$

EE :

$$\frac{dy}{dt} = Ay \quad (\text{model Problem})$$

$$\frac{y^{n+1} - y^n}{\Delta t} = Ay^n \rightarrow y^{n+1} = y^n + \Delta t Ay^n$$

$$\Rightarrow y^{n+1} = \left(\overset{(n \times (n-1))}{\mathbb{I}} + \Delta t A \right) y^n$$

$$\begin{pmatrix} \mathbb{I} \\ \text{or} \end{pmatrix} \varphi^{n+1} = \left(\mathbb{I} + \frac{\Delta t \alpha}{\Delta x^2} \mathbb{A} \right) \varphi^n$$

\downarrow
 (step+1)

 \downarrow
 tstep

Von-Neuman Stability Analysis

Matrix Stability analysis \rightarrow
look at the Matrix and
extract eigenvalues

\rightarrow B.C is included.
disadvantage \rightarrow

Diagonalize A and
extract the eigenvalues
 \Rightarrow not possible always.

\rightarrow Simplifies the B.C. \rightarrow periodic B.C.

B.C commonly do not influence
Stability criteria.

\rightarrow Constant coeff differential
eqn.

\rightarrow uniformly spaced grid.

Heat eqn. 8

- EE time advancement
- 2nd order central difference

time counter

$(n+1)$
 Φ_j

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

(*)

grid index

Key Part

Assume soln. of the form:

$$\Phi_j^{(n)} = \sigma^n e^{ikx_j}$$
$$\Phi = \sum_i \beta_i e^{ikx_j}$$

Substitute in (*)

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

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

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

divide
→

$$\sigma e^{ikx_j} = e^{ikx_{j+1}} - 2e^{ikx_j} + e^{ikx_{j-1}}$$

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

bounded exact Soln: $|\sigma| \leq 1$

↓
for stability

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

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

always satisfied $\left[2 \cos(k \Delta x) - 2 \right] \leq 0$

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

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

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

← worst case: $\cos(k \Delta x) = -1$
 → They match.

Modified wavenumber analysis

Very Similar to von-Neumann analysis.

→ more straight forward

$$\text{take } \frac{d\phi}{dt} = A\phi \quad (1)$$

Assume a soln. $\phi(x,t) = \psi(t) e^{ikx}$ Periodic BC

substitute in (1)

$$\frac{d\psi}{dt} = -\alpha k^2 \psi \quad \equiv \quad y' = \lambda y$$

↖
wave-number

→ in practice instead of analytical expression we use discretisation to approximate the derivative

Heat eqn. → 2nd order central diff.

$$\frac{\partial^2}{\partial x^2}$$

$$\frac{d\phi_j}{dt} = \alpha \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta x^2}, \quad j = 1, 2, 3, \dots, N-1$$

Assume : $\varphi_j = \psi(t) e^{ikx_j}$
 soln to the (semi-) discrete equation

\Rightarrow substituting and dividing by $e^{ikx_j} = 0$

$$\frac{d\psi}{dt} = -\frac{2\alpha}{\Delta x^2} [1 - \cos(k\Delta x)] \psi$$

or

$$\text{FD} : \frac{d\psi}{dt} = -\alpha k^2 \psi(t)$$

$$\text{exact} : \frac{d\psi}{dt} = -\alpha k^2 \psi(t)$$

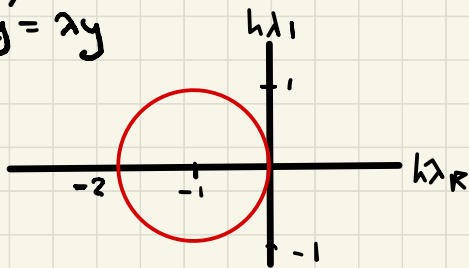
$$\text{2nd FD} : \frac{2}{k^2} = \frac{+2}{\Delta x^2} [1 - \cos(k\Delta x)]$$

↓
 modified wave-number

eqn. decoupled \Rightarrow we can directly compare to the result of $y' = \lambda y$ with $\lambda = -\alpha k^2$

Example: EG. from $y' = \lambda y$
 (Heat eqn.)

$$\Delta t \leq \frac{2}{|\lambda|}$$



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

worst case scenario \Rightarrow max limitation $\rightarrow \cos(k\Delta x) = -1$
on Δt

$$\Rightarrow \Delta t \leq \frac{\Delta x^2}{2\alpha} \Rightarrow \text{von-Neumann analysis.}$$

Wave equations:

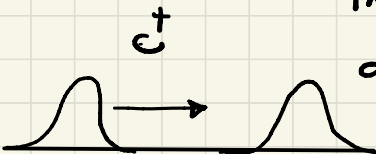
Consider the following eqn:

$$\frac{\partial u}{\partial t} + \underbrace{c}_{\text{wave speed}} \frac{\partial u}{\partial x} = 0 \quad a \leq x \leq L, \quad t \geq 0$$

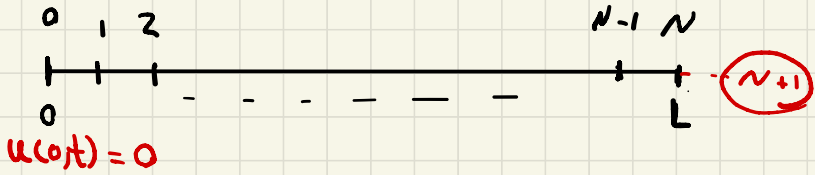
with the boundary condition $u(0, t) = 0$

\Rightarrow model equation for the convection phenomenon.

\rightarrow exact soln: A wave that propagates with constant convection speed (c)
in positive direction c^+
or negative direction c^-



Semi-discrete form \Rightarrow discretise in space (2)



2nd order FD scheme: $\frac{\partial}{\partial x}$

interior points: $\frac{\partial u_j}{\partial x} = \frac{u_{j+1} - u_{j-1}}{2\Delta x} + O(\Delta x^2)$

$u = [u_1, u_2, \dots, u_N]$

$$\frac{d}{dt} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} = \frac{c}{2\Delta x} \begin{bmatrix} 0 & 1 & \dots & \dots \\ -1 & 0 & 1 & 0 & \dots \\ 0 & -1 & 0 & 1 & \dots \\ \dots & \dots & \dots & -1 & 0 & 1 \\ \dots & \dots & \dots & \dots & -2 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_N \end{bmatrix} - \frac{c}{2\Delta x} \begin{bmatrix} u_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

$\underbrace{\hspace{10em}}_{bc.}$

(a) $j=1$: $\frac{\partial u_1}{\partial x} = \frac{u_2 - u_0}{2\Delta x}$ BC

(a) $j=N$: $\frac{\partial u_N}{\partial x} = \frac{u_{N+1} - u_{N-1}}{2\Delta x}$

$\frac{\partial}{\partial x} \rightarrow$ 2nd FD ~~X~~ apply to (u)

$$u' = \frac{\partial u}{\partial x} = \alpha u_N + \beta u_{N-1}$$

$$u'_N - \alpha u_N - \beta u_{N-1} = 0$$

	u_N	u'_N	u''_N	u'''_N
u'_N	0	1	0	0
$-\alpha u_N$	$-\alpha$	0	0	0
$-\beta u_{N-1}$	$-\beta$	$+\beta \Delta x$	$-\beta \frac{\Delta x^2}{2}$	
$-\gamma u_{N-2}$	$-\gamma$	$+\gamma (2\Delta x)$	$-\gamma \frac{(2\Delta x)^2}{2}$...
0				

3 eqn. 3 unknowns \rightarrow 2nd order

Taylor

$$\text{Series expansion } -\beta u_{N-1} = -\beta u_N + \beta \Delta x u'_N - \beta \frac{\Delta x^2}{2} u''_N + \dots$$

expansion

$$\begin{cases} 2 \text{ eqn.} \\ 2 \text{ unknowns} \end{cases} \begin{cases} -\alpha - \beta = 0 \\ +\beta \Delta x + 1 = 0 \end{cases} \Rightarrow \begin{cases} \alpha = -\beta = +\frac{1}{\Delta x} \\ \beta = -\frac{1}{\Delta x} \end{cases}$$

1st order

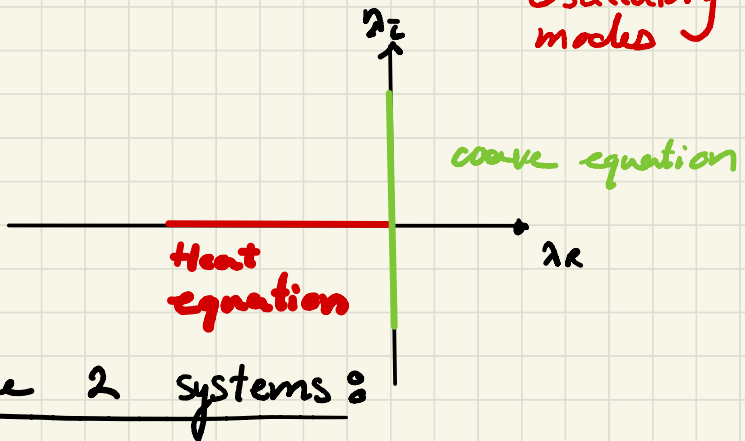
$$O(\text{scheme}) = -\beta \frac{\Delta x^2}{2} u'' = O(\Delta x)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{-u_{N-1} + u_N}{\Delta x}$$

Wave equation (eigenvalues)

$$\lambda_j = -\frac{c}{\Delta x} \left(i \cos \frac{\pi j}{N} \right), \quad j = 1, 2, \dots, N$$

eigenvalues are purely imaginary $\lambda_j = i\omega_j$



Oscillatory modes

wave equation

Heat equation

Compare the 2 systems:

examples of two limiting cases

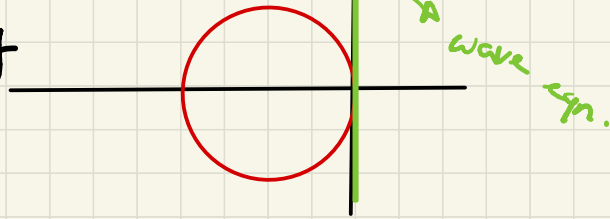
diffusive * decaying soln. (negative real λ_s)

convective * Oscillatory behavior (imaginary λ_s)

Q: what will be the result of EE applied to a wave eqn.?

After 2nd order FD

→ purely imaginary eigenvalues



→ EE unstable.

EE applied to wave eqn. with 2nd order central diff:

$$\underbrace{\frac{du}{dt} = -\frac{c}{2\Delta x} B u}_{u_0=0} + \vec{b} = 0$$

$$EE: \frac{y^{n+1} - y^n}{\Delta t} = f(y^n, t^n)$$

$$u^{n+1} = u^n - \frac{c}{2\Delta x} B u^n = \begin{pmatrix} \text{I} & \text{B} \\ \text{N} \times \text{N} & \text{N} \times \text{N} \end{pmatrix} u^n$$

$$c=1$$

$u_0 = \text{known.}$

Modified wave number applied to wave eqn.

* Second order central difference

$$\Rightarrow \varphi_j = \psi(t) e^{ikx_j}$$

in semi-discrete form:

$$\frac{d\varphi}{dt} = -ik'c\varphi$$

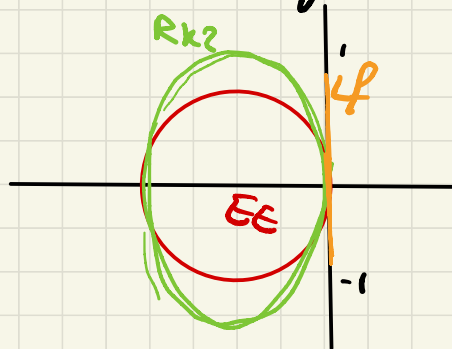
$$\text{and } k' = \frac{\sin(k\Delta x)}{\Delta x}$$

modified wave number
for second order central
diff. scheme \rightarrow

$$j' = \lambda y$$

replace: $\lambda = -ik'c$

EE & RK2 = numerically unstable



but leap-frog $\rightarrow \Delta t = \frac{1}{|\lambda_i|}$

$$\Delta t_{\max} = \frac{1}{k'c} = \frac{\Delta x}{C \sin(k\Delta x)}$$

The worst case scenario:

$$\Delta t_{\max} = \frac{\Delta x}{c}$$

or $\boxed{\frac{c\Delta t}{\Delta x}} \leq 1$ CFL number

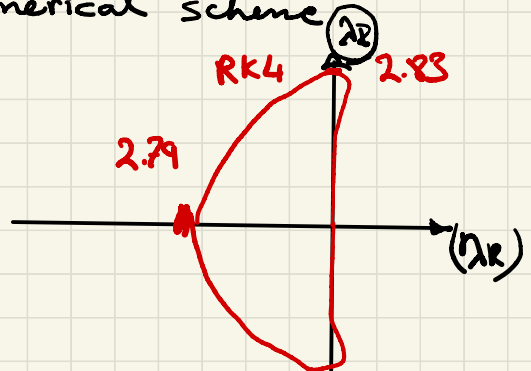
this non-dimensional quantity is called CFL number

\rightarrow Courant, Friedrich and Leay

In wave (convection-type) problems, the term "CFL number" is used as an indicator of stability of a numerical scheme.

Q: if apply RK4 with 2nd order FD

CFL ? $CFL \leq 2.83$



$$\text{leap frog} : y_{n+1} = y_{n-1} + 2h f(y_n, t_n)$$

$$\frac{du}{dt} = Bu$$

$$u^{n+1} = u^{n-1} + 2\Delta t B u^n$$

$u_1 \rightarrow$ starter scheme : EE

u_0

$$\textcircled{u_1} = (\mathbb{I} + \Delta t B) u_0$$

\rightarrow leap frog

$$u^2 = u^0 + 2\Delta t B u^1$$

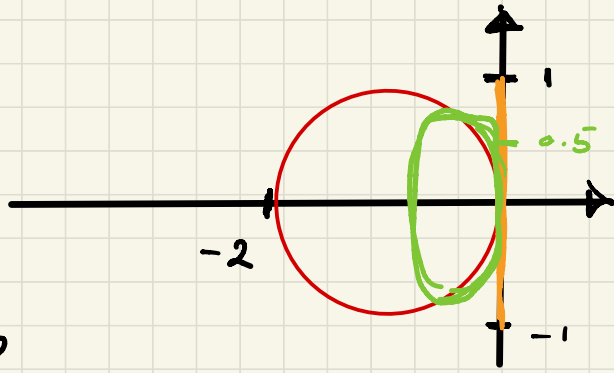
⋮

Adams-Bashforth

$$y_{n+1} = y_n + 3h/2 f(y_n, t_n) - h/2 f(y_{n-1}, t_{n-1})$$

$$u^{n+1} = u^n + \frac{3\Delta t}{2} B u^n - \frac{\Delta t}{2} B u^{n-1}$$

$$\textcircled{u^{n+1} = \left(\mathbb{I} + \frac{3\Delta t}{2} B\right) u^n - \frac{\Delta t}{2} B u^{n-1}}$$



CFL ?

AB

2nd order Central scheme? $\Delta x = 0.5$

Example

Modifed wave number
analysis

heat & wave eqn.

Apply modifed wave number to heat-eqn.

$$\frac{d\psi}{dt} = -\alpha k^2 \psi$$

for 2nd order Central diff. scheme,
the worst case scenario:

$$k^2 = \frac{4}{\Delta x^2}$$

We can now predict the stability of various marching methods.

$$EG: \Delta t \leq \frac{\Delta x^2}{2\alpha} = \frac{0.00125}{1} = 0.00125$$

$\Delta t_{\max} = \frac{2}{(1\lambda)}$

$$RK4: \Delta t \leq \frac{2.79 \Delta x^2}{4\alpha} = 0.00174$$

leap-frog is unstable

Similarly for convection equation:

$$\frac{d\psi}{dt} = -i c k' \psi$$

Second order central diff the worst case

$$k' = \frac{1}{\Delta x}$$

Since ick' purely imaginary

EE: unstable

$$\text{Rk4} : \quad \Delta t \leq \frac{2.83 \Delta x}{c}$$
$$\Rightarrow \text{CFL} \leq 2.83$$

for $\Delta x = 0.01$, $c = 1$
 TD^\dagger

Rk4	$\rightarrow 0.028 = \Delta t$	$\text{CFL} \approx 2.83$
leapfrog	$\rightarrow 0.01 = \Delta t$	$\text{CFL} \approx 1$
AB	$\rightarrow 0.005 = \Delta t$	$\text{CFL} \approx 0.5$

$\text{CFL} \uparrow \rightarrow \Delta t \uparrow$
faster time to soln.

