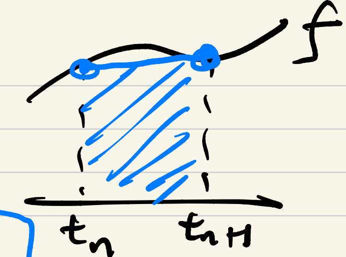
46 Trapezoidal method (TR)



$$y' = f(y,t) \rightarrow y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f(y,t)\,dt$$

$$\rightarrow \boxed{y_{n+1} = y_n + \frac{h}{2}\left[f(y_{n+1}, t_{n+1}) + f(y_n, t_n)\right]} \quad \text{TR}$$

implicit method

$$y' = f \Rightarrow \frac{y_{n+1} - y_n}{h} = \frac{1}{2}(f_{n+1} + f_n) \quad : \text{TR} \quad \text{implicit } O(h^2)$$

$$= f_n \quad : \text{EE} \quad \text{explicit } O(h)$$

$$= f_{n+1} \quad : \text{IE} \quad \text{implicit } O(h)$$

When TR is applied to PDE, it is called 'Crank-Nicolson' method

~~Nicholson~~

Model prob. $y' = \lambda y$

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

$$\rightarrow \quad y_{n+1} = \frac{1+\frac{1}{2}\lambda h}{1-\frac{1}{2}\lambda h} y_n = \sigma y_n \qquad \left(\frac{1}{1-\varepsilon} = 1+\varepsilon+\varepsilon^2+\cdots\right)$$

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

error

exact sol. $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \cdots$

$\therefore$ TR is 3rd-order accurate for one-time step

globally 2nd-order accurate.

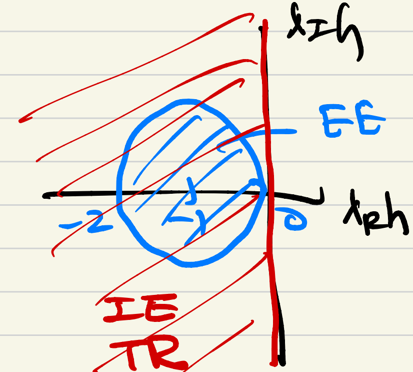
Stability : $\lambda = \lambda_R + i\lambda_I$

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

$$\theta = \tan^{-1}\frac{\frac{1}{2}\lambda_I h}{1+\frac{1}{2}\lambda_R h}, \quad \alpha = \tan^{-1}\frac{-\frac{1}{2}\lambda_I h}{1-\frac{1}{2}\lambda_R h}$$

$$|\sigma| = \frac{A}{B} = \frac{\sqrt{(1+\frac{1}{2}\lambda_R h)^2 + (\frac{1}{2}\lambda_I h)^2}}{\sqrt{(1-\frac{1}{2}\lambda_R h)^2 + (\frac{1}{2}\lambda_I h)^2}} \le 1 \quad \text{for } \lambda_R \le 0$$

$\therefore$ TR is unconditionally stable



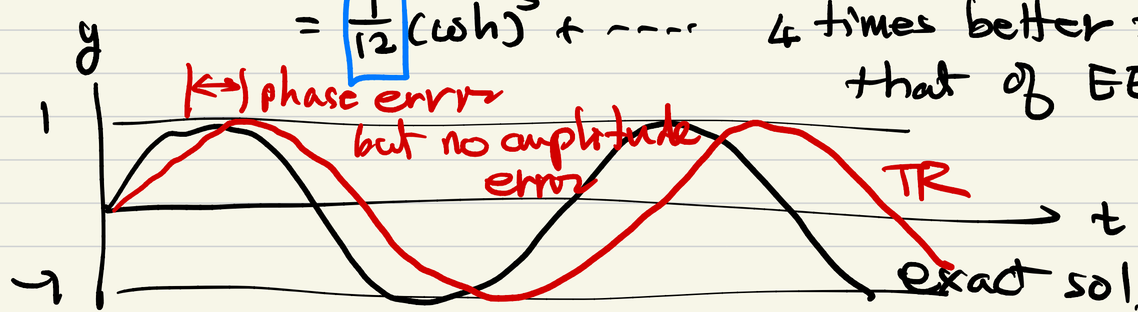
$\boxed{\text{For } \lambda_R = 0}$, $y' = i\omega y \quad (\lambda = i\omega)$

TR : $|\sigma| = 1 \quad \therefore$ no amplitude error

phase: $\sigma = \dfrac{1 + i\frac{1}{2}\omega h}{1 - i\frac{1}{2}\omega h} = e^{i \cdot 2\theta} \qquad \theta = \tan^{-1}\dfrac{\omega h}{2}$

phase error $= \omega h - 2\tan^{-1}\dfrac{\omega h}{2} = \omega h - 2\left[\dfrac{\omega h}{2} - \dfrac{1}{24}(\omega h)^3 + \cdots\right]$

$= \boxed{\frac{1}{12}}(\omega h)^3 + \cdots$ 4 times better than that of EE & IE.

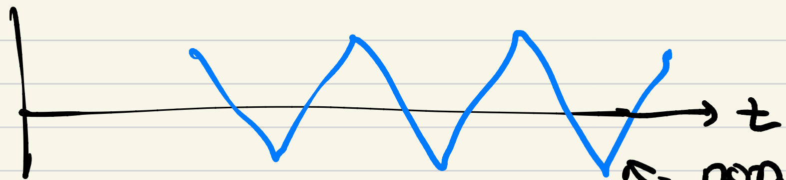


For $\lambda_I = 0$, λ is real & negative ($\lambda_R \leq 0$)

$$TR: \quad \sigma = \frac{1+\frac{1}{2}\lambda_R h}{1-\frac{1}{2}\lambda_R h} \qquad |\sigma| \leq 1$$

$y^n = \sigma^n y_0$ for large h, $\sigma \to -1$

σ^n oscillates between -1 and 1, but never blows up.

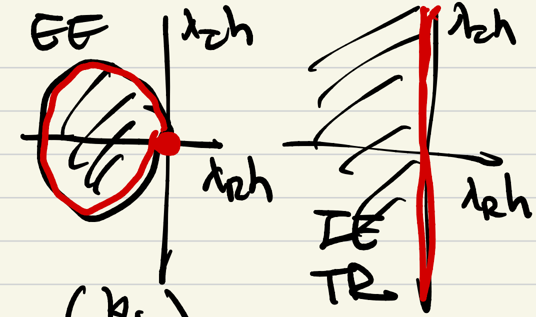


non-physical

should be careful!

try a different numerical method

- $y'' + \omega^2 y = 0 \qquad y(0) = y_0, \quad y'(0) = 0$



$y_1 = y$

$y_2 = y_1' \longrightarrow y_2' = y_1'' = -\omega^2 y_1$

$$\Rightarrow \begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & 1 \\ -\omega^2 & 0 \end{bmatrix}}_{A} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = S^{-1} \Lambda S \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

$$\det(A - \lambda I) = 0 = \begin{vmatrix} -\lambda & 1 \\ -\omega^2 & -\lambda \end{vmatrix} \rightarrow \lambda^2 = -\omega^2$$

$\lambda = \pm i\omega$

purely imaginary eigenvalues

$$\underbrace{S \begin{pmatrix} y_1' \\ y_2' \end{pmatrix}}_{z'} = \Lambda \underbrace{S \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}}_{z} \Rightarrow \begin{pmatrix} z_1' \\ z_2' \end{pmatrix} = \Lambda \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

$\rightarrow z_1' = \lambda_1 z_1$,

$z_2' = \lambda_2 z_2$

model prob.

4.7 Linearization for implicit methods

TR : $y' = f(y,t) \rightarrow y_{n+1} = y_n + \frac{h}{2}\left[\boxed{f(y_{n+1}, t_{n+1})} + f(y_n, t_n)\right] + O(h^3)$

→ solve a nonlinear algebraic eq.

→ require iterative solution procedure

→ can be avoided by a linearization technique

$$f(y_{n+1}, t_{n+1}) = f(y_n, t_n) + (y_{n+1} - y_n)\frac{\partial f}{\partial y}\Big|_{y_n, t_{n+1}} + \frac{1}{2}(y_{n+1} - y_n)^2 \frac{\partial^2 f}{\partial y^2}\Big|_{y_n, t_{n+1}} + \cdots$$

$O(h^2)$

$O(h^3)$

$$h\frac{\partial y}{\partial t}\Big|_n + \frac{1}{2}h^2\frac{\partial^2 y}{\partial t^2}\Big|_n + \cdots$$

neglect this term w/o losing any accuracy.

$$\Rightarrow y_{n+1} = y_n + \frac{h}{2}\left[f(y_n, t_n) + (y_{n+1} - y_n)\frac{\partial f}{\partial y}\Big|_{y_n, t_{n+1}} + f(y_n, t_n)\right] + O(h^3)$$

$$\rightarrow \boxed{y_{n+1} = y_n + \frac{h}{2}\,\frac{f(y_n, t_{n+1}) + f(y_n, t_n)}{1 - \frac{h}{2}\left.\frac{\partial f}{\partial y}\right|_{y_n, t_{n+1}}}} + O(h^3)$$

linearized TR (LTR)

this formula does not require iteration, while retaining global second-order accuracy.

Linear stability analysis ($y' = \lambda y$)

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

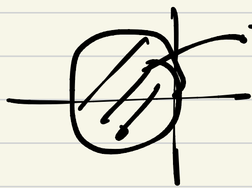
same as TR
unconditionally stable.

Linearization may lead to some loss of total stability for nonlinear f.

4.8 Runge-Kutta method (RK)

① Predictor-corrector method (PC)

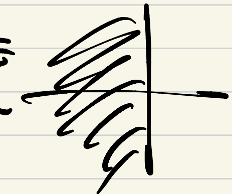
explicit method



timestep limit

implicit method

IE
TR



iterative sol. → LTR

predictor-corrector method

↳ explicit method

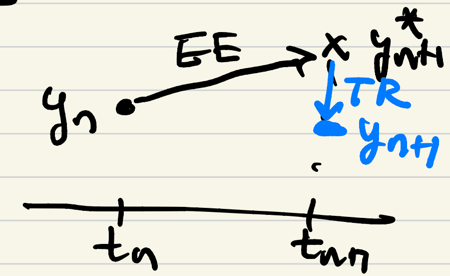
PC & RK methods provide better stability than explicit method like EE

but require less work/timestep than implicit method

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

① $y^*_{n+1} = y_n + h f(y_n, t_n)$: EE as predictor

② $y_{n+1} = y_n + \frac{h}{2}\left[f(y^*_{n+1}, t_{n+1}) + f(y_n, t_n)\right]$: TR as corrector



model prob. $y' = \lambda y$

① $y^*_{n+1} = y_n + h\lambda y_n = (1+\lambda h) y_n$

② $y_{n+1} = y_n + \frac{h}{2}\left[\lambda(1+\lambda h) y_n + \lambda y_n\right]$

$= y_n \left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right) = \sigma y_n$ $\quad O(h^3)$

exact sol. $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \cdots$

$\therefore$ PC is 2nd-order accurate.

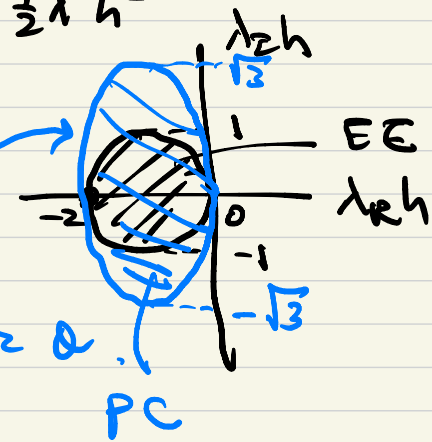
Stability: $y_n = \sigma^n y_0$, $\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2$

$|\sigma| \le 1$ to be stable

$$|1 + \lambda h + \frac{1}{2}\lambda^2 h^2| \le 1$$

$$1 + \lambda h + \frac{1}{2}\lambda^2 h^2 = e^{i\theta}$$

find λh for different trials for θ.

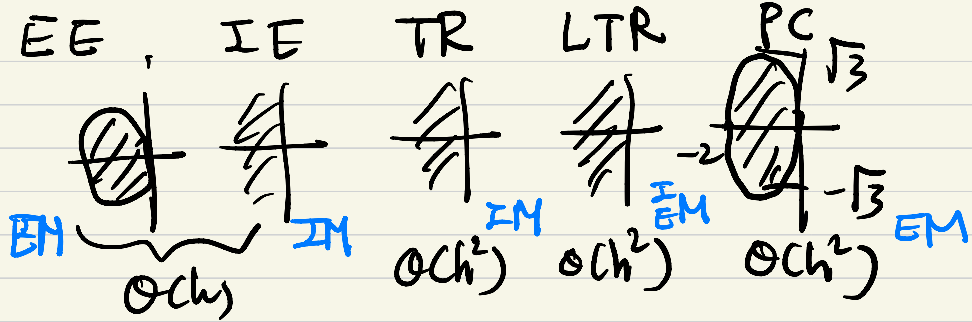


$\therefore$ PC is conditionally stable.

For $\lambda = i\omega$, $\sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 = 1 + i\omega h - \frac{1}{2}\omega^2 h^2$

$$|\sigma|^2 = (1 - \frac{1}{2}\omega^2 h^2)^2 + (\omega h)^2 = 1 + \frac{1}{4}\omega^4 h^4 > 1$$

unstable for purely imaginary λ.



$y' = f(y, t)$

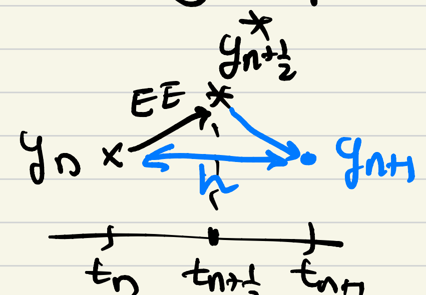
- Runge-Kutta methods – explicit methods

advantages : ① good stability properties

② timesteps can be changed during computation

③ self starting

2nd-order Runge-Kutta method (RK2)

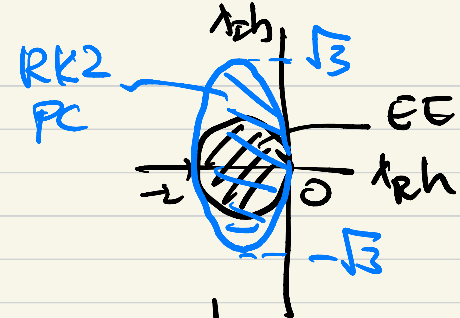


① $y^*_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(y_n, t_n)$: EE

② $y_{n+1} = y_n + h f(y^*_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})$: midpoint rule model prob. $y' = \lambda y$

$$\xrightarrow{①②} \quad y_{n+1} = y_n\left(1 + \lambda h + \frac{1}{2}\lambda^2 h^2\right)$$

2nd-order accurate



For $\lambda = i\omega$,

$$\sigma = 1 + i\omega h - \frac{1}{2}\omega^2 h^2 \qquad |\sigma| > 1, \qquad \theta = \tan^{-1}\frac{\omega h}{1 - \frac{1}{2}\omega^2 h^2}$$

$$\text{phase error} = \omega h - \theta = -\frac{1}{6}\omega^3 h^3 + \cdots$$

- RK4 (most popular scheme) — explicit

$y' = f(y, t)$

① $y^{*}_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(y_n, t_n)$

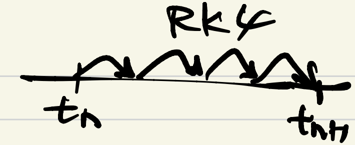
② $y^{**}_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(y^{*}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})$

③ $y^{***}_{n+1} = y_n + h f(y^{**}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})$

④ $y_{n+1} = y_n + h\left[\frac{1}{6} f(y_n, t_n) + \frac{1}{3} f(y^{*}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) + \frac{1}{3} f(y^{**}_{n+\frac{1}{2}}, t_{n+\frac{1}{2}}) + \frac{1}{6} f(y^{***}_{n+1}, t_{n+1})\right]$

$\Rightarrow$ requires 4 function evaluations/timestep

$\Rightarrow$ expansive



$y' = \lambda y$: $y_{n+1} = \sigma y_n$

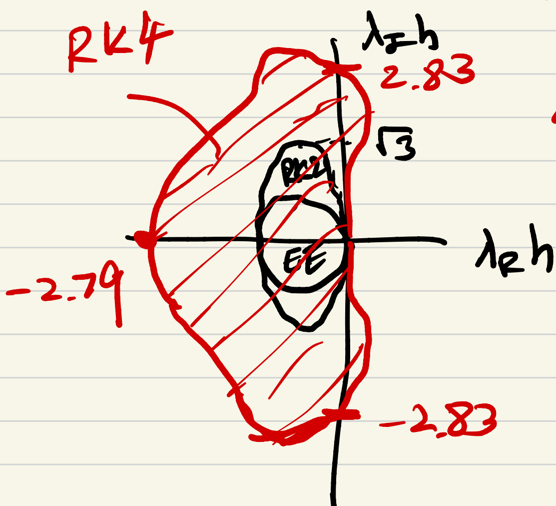
$$\to \sigma = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4$$

exact sol : $e^{\lambda h} = 1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4 + \cdots$

$\therefore$ RK4 is fourth-order accurate.

stability : $|\sigma| \le 1$ to be stable

$$1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3 + \frac{1}{24}\lambda^4 h^4 = e^{i\theta}$$



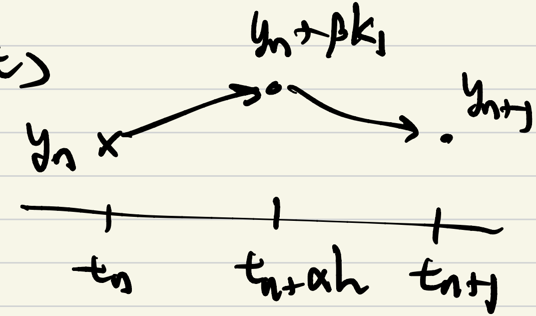
conditionally stable

for $\lambda = i\omega$, $|\lambda_I h| \le 2.83$ conditionally stable

for $\lambda_I = 0$, $|\lambda_R h| \le 2.79$ 〃 〃

<u>RK3</u>

- How to construct RK2? $\quad y' = f(y,t)$



$$\begin{cases} k_1 = h f(y_n, t_n) \\ k_2 = h f(y_n + \beta k_1, t_n + \alpha h) \\ y_{n+1} = y_n + \gamma_1 k_1 + \gamma_2 k_2 \end{cases}$$

Find $\alpha, \beta, \gamma_1, \gamma_2$ to ensure the highest order of accuracy for the method.

Taylor series for k_2

$$k_2 = h\left[f(y_n, t_n) + \beta k_1 \frac{\partial f}{\partial y}\Big|_n + \alpha h \frac{\partial f}{\partial t}\Big|_n + \cdots \right]$$

$$\rightarrow y_{n+1} = y_n + \gamma_1 h f_n + \gamma_2 h (f_n + \beta h f_n f_{y_n} + \alpha h f_{t_n} + \cdots)$$

$$= y_n + (\gamma_1 + \gamma_2) h f_n + \gamma_2 \beta h^2 f_n f_{y_n} + \gamma_2 \alpha h^2 f_{t_n} + \cdots$$

$$y(t_{n+1}) = y(t_n) + h y'(t_n) + \frac{1}{2} h^2 y''(t_n) + \cdots$$

$$= y_n + h f_n + \frac{1}{2} h^2 (f_{t_n} + f_{y_n} f_n) + \cdots$$

match the coeffs.

$$\begin{cases} \gamma_1 + \gamma_2 = 1 \\ \gamma_2 \beta = \frac{1}{2} \\ \gamma_2 \alpha = \frac{1}{2} \end{cases}$$

3 eqs for 4 unknowns

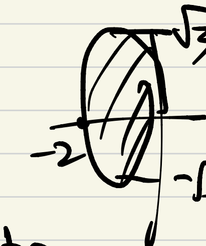
$\downarrow$

α as a free parameter

$$\rightarrow \gamma_2 = \frac{1}{2\alpha}, \quad \beta = \alpha, \quad \gamma_1 = 1 - \frac{1}{2\alpha}$$

$$\Rightarrow \text{RK2}: \quad \begin{cases} k_1 = h f(y_n, t_n) \\ k_2 = h f(y_n + \alpha k_1, t_n + \alpha h) \\ y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) k_1 + \frac{1}{2\alpha} k_2 \end{cases}$$

$0 < \alpha < 1$

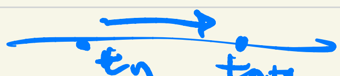


model prob: $y' = \lambda y \rightarrow y_{n+1} = y_n \left(1 + \lambda h + \frac{1}{2} \lambda^2 h^2\right)$

2nd-order accurate

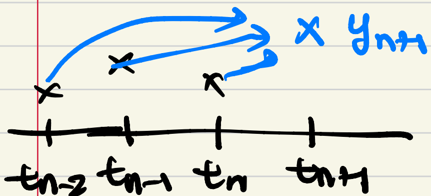
$y' = f(y,t)$ EE, IE, TR, LTR, PC, RK2, RK4

$\uparrow$



4.9 Multistep methods

Higher-order accuracy is achieved by using data at previous timesteps, $t_{n-1}, t_{n-2}, t_{n-3}, \ldots$ & t_n.

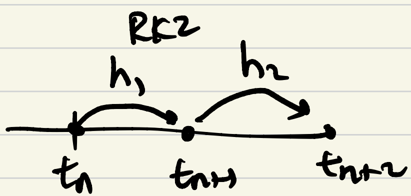


price: storage & memory ↑

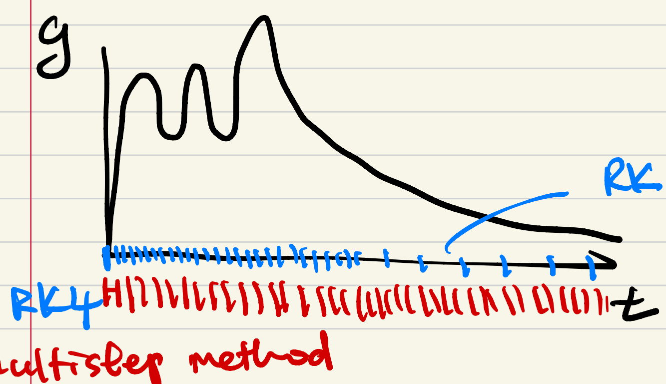
not self-starting

$y_0 \longrightarrow y_1$ needs another method to start (like FE)

~~y_{-1}~~
~~y_{-2}~~



cannot change timestep size h during computation (h is fixed)



RK can change Δt during computation (or h)

- Leapfrog method (LF) $\qquad y' = \lim_{h\to 0} \frac{y_{n+1}-y_n}{h}$

$y' = f(y,t)$

$\frac{y_{n+1}-y_n}{h} = f_n$ EE $O(h)$ 1

$= f_{n+1}$ IE $O(h)$ 1

$= \frac{1}{2}(f_n + f_{n+1})$ TR $O(h^2)$ 2

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

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

leapfrog method

not self-starting (get y_1 using EE or RK2, ...)

1 fn. evaluation $\Rightarrow$ 2nd-order accurate

$\downarrow$

too good to be true!

model prob. $y' = \lambda y$

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

$y_{n+1} - 2\lambda h y_n - y_{n-1} = 0$

Assume $y_n = \sigma^n y_0 \rightarrow \sigma^{n+1} y_0 - 2\lambda h \sigma^n y_0 - \sigma^{n-1} y_0 = 0$

$\rightarrow \sigma^2 - 2\lambda h \sigma - 1 = 0 \rightarrow \sigma = \lambda h \pm \sqrt{\lambda^2 h^2 + 1}$

two roots! $\rightarrow y_n = c_1 \sigma_1^n + c_2 \sigma_2^n$

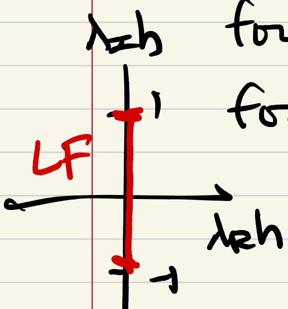
$$\sigma_1 = \lambda h + \sqrt{\lambda^2 h^2 + 1} \simeq \underline{1 + \lambda h + \tfrac{1}{2}\lambda^2 h^2} - \tfrac{1}{8}\lambda^4 h^4 + \cdots,$$ $O(h^2)$ second-order accurate.

$$\left(e^{\lambda h} = \underline{1 + \lambda h + \tfrac{1}{2}\lambda^2 h^2} + \tfrac{1}{6}\lambda^3 h^3 + \cdots \right)$$

$$\sigma_2 = \lambda h - \sqrt{\lambda^2 h^2 + 1} = -1 + \lambda h - \tfrac{1}{2}\lambda^2 h^2 + \tfrac{1}{8}\lambda^4 h^4 + \cdots$$

$\Rightarrow$ σ_1 shows that the method is 2nd-order accurate

σ_2 is the spurious root and has no physical meaning.



for real & negative λ, $|\sigma_2| > 1 \rightarrow$ LF is unstable.

for $\lambda = i\omega$, $\sigma = \lambda h \pm \sqrt{\lambda^2 h^2 + 1} = i\omega h \pm \sqrt{1 - \omega^2 h^2}$

if $|\omega h| < 1$, $|\sigma|^2 = (\omega h)^2 + (1 - \omega^2 h^2) = 1 \Rightarrow$ no amplitude error!

$|\omega h| > 1$, $|\sigma|^2 = |\omega h \pm \sqrt{\omega^2 h^2 - 1}|^2 > 1 \rightarrow$ unstable

General sol. $y_n = c_1 \sigma_1^n + c_2 \sigma_2^n$

Find c_1 & c_2 $\quad n=0: \quad y_0 = c_1 + c_2$

let y_1 be the sol. @ $n=1$ obtained by some other num. method.

$n=1: \quad y_1 = c_1 \sigma_1 + c_2 \sigma_2$

$$c_1 = \frac{y_1 - y_0 \sigma_2}{\sigma_1 - \sigma_2}, \quad c_2 = \frac{-y_1 + y_0 \sigma_1}{\sigma_1 - \sigma_2}$$

If we choose $y_1 = y_0 \sigma_1$, $c_2 = 0$

Then, the spurious root is completely suppressed

In general, the starting scheme plays a role in determining the level of contribution of the spurious root.

However, even if the spurious root is suppressed initially, the round-off error can restart it.