Multistage Methods – Runge Kutta

Butcher Table :

$$\begin{array}{c|c} \underline{c} & \underline{A} \\ \hline & \underline{b}^T \end{array}$$

F. Euler $O(\Delta t)$

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

$$k_1 = f(t_n, y_n)$$
$$y_{n+1} = y_n + \Delta t\, k_1$$

Midpoint $O(\Delta t^2)$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$

$$k_1 = f(t_n, y_n)$$
$$k_2 = f(t_n + 1/2\, \Delta t,\ y_n + 1/2\, \Delta t\, k_1)$$
$$y_{n+1} = y_n + \Delta t\, k_2$$

RK4 $O(\Delta t^4)$

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

$$k_1 = f(t_n, y_n)$$
$$k_2 = f(t_n + 1/2\, \Delta t,\ y_n + 1/2\, \Delta t\, k_1)$$
$$k_3 = f(t_n + 1/2\, \Delta t,\ y_n + 1/2\, \Delta t\, k_2)$$
$$k_4 = f(t_n + \Delta t,\ y_n + k_3)$$

$$y_{n+1} = y_n + \Delta t\left(1/6\, k_1 + 1/3\, k_2 + 1/3\, k_3 + 1/6\, k_4\right)$$

ex.) $\frac{dy}{dt} = 4e^{\frac{4t}{2}} - \frac{y}{2}$ $\qquad y(0) = 2$

$y(t) = \frac{40}{13}e^{4t/2} - \frac{14}{13}e^{-t/2}$

$y(3) \approx 33.6771717\ldots\ldots$

Show one step w/ $\Delta t = 1/2$

F. Euler $\quad k_1 = f(t_0, y_0) = 4e^0 - 2/2 = 3$

$y_1 = y_0 + \Delta t\, k_1 = 2 + (1/2)(3) = 3.5$

midpoint $\quad k_1 = 3$

$y_{1/2} = y_0 + 1/2\,\Delta t\, k_1 = 2.75$

$k_2 = f(t_0 + 1/2\,\Delta t,\ y_0 + 1/2\,\Delta t\, k_1) = f(1/2\,\Delta t,\ y_{1/2})$

$= 4e^{4(0.25)/2} - \frac{2.75}{2} \approx 3.51061$

$y_1 = y_0 + \Delta t\, k_2 = 2 + (1/2)(3.51061) \approx 3.75531$

RK-4 :

$k_1 = 3$

$k_2 = 3.51061$

$k_3 = 3.414678$

$k_4 = 4.1056$

$y_1 = 3.75517$

	$\Delta t = 1/2$ (6)		$\Delta t = 1/4$ (12)	
Method	Val	ε	Val	ε
F. Euler	~29.6	4.08	~31.64	2.03
Midpoint	~33.77	9.3×10^{-2}	~33.70	2.62×10^{-2}
RK4	~33.67	2.81×10^{-3}	~33.67	1.75×10^{-4}

Iterations need to have error $< 10^{-3}$,
(time steps)

RK4 : 9 $\xrightarrow{4 \text{ calc/step}}$ 36 K-evaluations

midpoint : 65 $\xrightarrow{2 \text{ calc/step}}$ 130 K-evals

F. Euler : 24271 $\xrightarrow{1 \text{ calc/step}}$ 24271 K-evals

Multi-step Methods

Multistage methods take many sub-steps in a single time step. → low memory but might be slow.

Multistep methods use the solution at multiple prior steps → higher memory but lower cost (less derivative evaluations).

Generically, look at $\frac{dy}{dt} = f(t,y)$

Then $\sum_i a_i = 0 \quad \sum_i b_i = 1$

$$a_0 y_{n+1} + a_1 y_n + a_2 y_{n-1} + \dots + a_s y_{n-s} =$$

$$\Delta t\left[b_0 f(t_{n+1}, y_{n+1}) + b_1 f(t_n, y_n) + \dots + b_s f(t_{n-s}, y_{n-s})\right]$$

for an s^{th}-order scheme.

$$\frac{y_{n+1} - y_n}{\Delta t} = f(t_n, y_n) \qquad \text{F. Euler}$$

$$\frac{1}{\Delta t} y_{n+1} - \frac{1}{\Delta t} y_n = f(t_n, y_n)$$

$$y_{n+1} - y_n = \Delta t f(t_n, y_n) \Rightarrow a_0 = 1,\ a_1 = -1,\ b_1 = 1$$

all others are 0

The values of $a_0 \to a_s$ & $b_0 \to b_s$ determine the particular scheme.

Note! Since you need y_{n+1}, $a_0 \neq 0$

If $b_0 = 0$, then the method is explicit.

If $b_0 \neq 0$, then it is implicit.

3 Main classes of Multistep

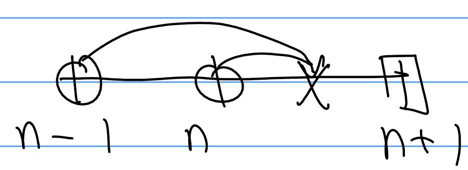
1. Adams-Bashforth (AB)
2. Adams-Moulton (AM)
3. Backward Finite Difference (BDF)

1. Adams-Bashforth: Explicit schemes with $a_0 = 1$, $a_1 = -1$, $b_0 = 0$, $b_{i>0} > 0$

$O(\Delta t)$: $b_1 = 1 \Rightarrow y_{n+1} - y_n = \Delta t\, f(t_n, y_n)$

$O(\Delta t^2)$: $b_1 = 3/2 \quad b_2 = -1/2$

$$y_{n+1} - y_n = \Delta t \left[\underbrace{\frac{3}{2} f(t_n, y_n) - \frac{1}{2} f(t_{n-1}, y_{n-1})}_{\simeq f(t_{n+1/2},\, y_{n+1/2})} \right]$$



$O(\Delta t^3)$: $b_1 = 23/12$, $b_2 = -4/3$, $b_3 = 5/12$

$O(\Delta t^4)$: $b_1 = 55/24$, $b_2 = -59/24$, $b_3 = 37/24$,
$b_4 = -3/8$

$\vdots$

Notes: Higher order schemes need to store more information.

You must have a bootstrap scheme,

How to compute Y_1 using $O(\Delta t^3)$?

You would need $Y_0, \underbrace{Y_{-1}, Y_{-2}}_{\text{Do not have.}}$

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② Adams - Moulton : Implicit Schemes
$a_0 = 1$, $a_1 = -1$, $b_0 \neq 0$

$O(\Delta t)$: $b_0 = 1$ $y_{n+1} - y_n = \Delta t f(t_{n+1}, y_{n+1})$
B. Euler

$O(\Delta t^2)$: $b_0 = 1/2$ $b_1 = 1/2$

$$y_{n+1} - y_n = \Delta t\left[\tfrac{1}{2} f(t_{n+1}, y_{n+1}) + \tfrac{1}{2} f(t_n, y_n)\right]$$

Called Crank - Nicholson.

$O(\Delta t^3)$: $b_0 = 5/12$, $b_1 = 2/3$, $b_2 = -1/12$

$O(\Delta t^4)$ = $b_0 = 3/8$, $b_1 = 19/24$, $b_2 = -5/24$
$b_3 = 1/24$

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(5) BDF : Implicit Schemes w/

$b_0 = 1$, $b_{i>0} = 0$

$O(\Delta t)$ $a_0 = 1$, $a_1 = -1$ (B. Euler)

$$y_{n+1} - y_n = \Delta t\, f(t_{n+1}, y_{n+1})$$

$O(\Delta t^2)$ $a_0 = 3/2$, $a_1 = -2$, $a_2 = 1/2$

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

$\downarrow$

$$\frac{\frac{3}{2} y_{n+1} - 2 y_n + \frac{1}{2} y_{n-1}}{\Delta t} = \frac{df}{dt} + O(\Delta t^2)$$

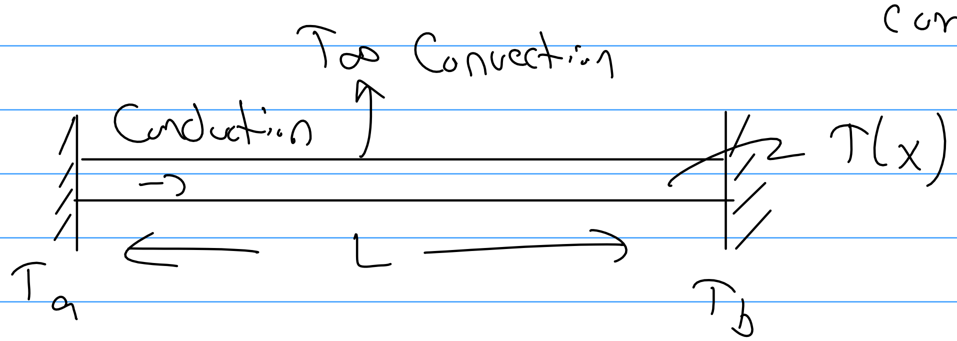
$O(\Delta t^3)$ $a_0 = 11/6$, $a_1 = -3$, $a_2 = 3/2$, $a_3 = -1/3$

Note: BDF of order > 6 is <u>not</u> stable.

Boundary Value Problems

Boundary value problems have conditions on the end states.

ex.) Temperature in a rod w/ convection & conduction

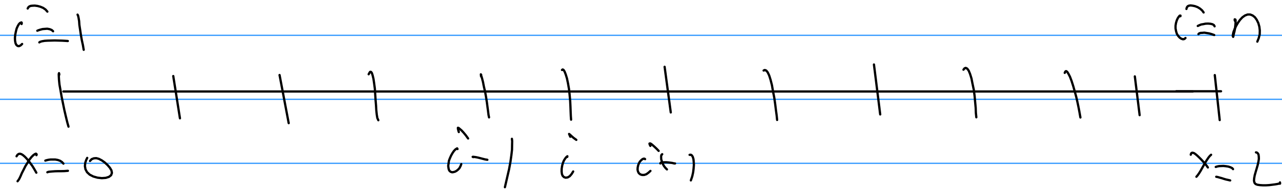


At steady-state $\quad \dfrac{d^2T}{dx^2} + h(T_\infty - T) = 0$

$$0 \le x \le L$$

$$\underbrace{T(0) = T_a \qquad T(L) = T_b}_{\text{Dirichlet B.C.}}$$

Discretize on a grid:



$$\frac{d^2T}{dx^2} + h(T_\infty - T) = \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} + h(T_\infty - T_i) = 0$$

with n grid points $\quad \Delta x = \dfrac{L}{n-1}$

Let $n = 16$, $\Delta x = \frac{L}{15}$

At $i = 1$ $(x = 0)$ $T_1 = T_a$

At $i = 2$ $\frac{T_1 - 2T_2 + T_3}{\Delta x^2} + h(T_\infty - T_2) = 0$

$$\Rightarrow -T_1 + (2 + \Delta x^2 h) T_2 - T_3 = \Delta x^2 h T_\infty$$

$$i = 3 \Rightarrow -T_2 + (2 + \Delta x^2 h) T_3 - T_4 = \Delta x^2 h T_\infty$$

$$\vdots$$

$$i = 15 \Rightarrow -T_{14} + (2 + \Delta x^2 h) T_{15} - T_{16} = \Delta x^2 h T_\infty$$

$$i = 16 \Rightarrow T_{16} = T_b$$

$$\Downarrow$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & & 0 \\ -1 & 2+\Delta x^2 h & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2+\Delta x^2 h & -1 & \cdots & 0 \\ & & & \ddots & & \\ & & & -1 & 2+\Delta x^2 h & -1 \\ 0 & \cdots & & & 0 & 1 \end{bmatrix}}_{\underline{A}} \underbrace{\begin{pmatrix} T_1 \\ T_2 \\ \vdots \\ \\ T_{15} \\ T_{16} \end{pmatrix}}_{\underline{T}} = \underbrace{\begin{bmatrix} T_a \\ \Delta x^2 h T_\infty \\ \vdots \\ \\ \Delta x^2 h T_\infty \\ T_b \end{bmatrix}}_{\underline{b}}$$

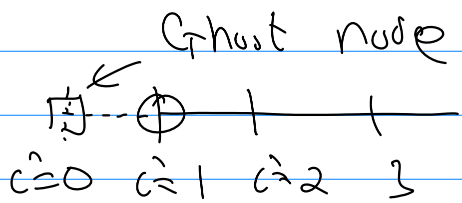
$$\Rightarrow \underline{T} = \underline{A}^{-1} \underline{b}$$

Neumann B.C.

Say that we have $\dfrac{\partial^2 T}{\partial x^2} + h(T_\infty - T) = 0$

w/ $\dfrac{dT(0)}{dx} = a$ & $T(L) = T_b$

Look at $i = 1$



$$\Rightarrow \quad -T_0 + (2 + \Delta x^2 h) T_1 - T_2 = \Delta x^2 h T_\infty$$

but, $\dfrac{dT(0)}{dx} \approx \dfrac{T_2 - T_0}{2\Delta x} = a$

$$\Rightarrow T_0 = T_2 - 2\Delta x a$$

$$-T_2 + 2\Delta x a + (2 + \Delta x^2 h) T_1 - T_2 = \Delta x^2 h T_\infty$$

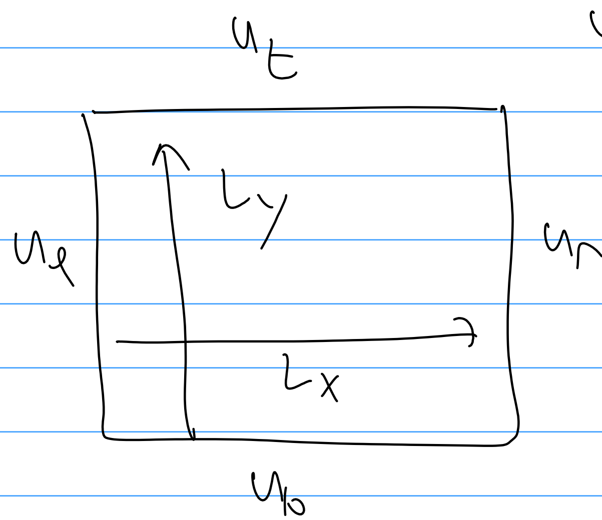
$$(2 + \Delta x^2 h) T_1 - 2 T_2 = \Delta x^2 h T_\infty - 2\Delta x a$$

$$\Rightarrow \begin{bmatrix} 2+\Delta x^2 h & -2 & 0 & \cdots \\ -1 & 2+\Delta x^2 h & -1 & \\ & & \ddots & -1 \\ 0 & \cdots & 0 & 1 \end{bmatrix} \begin{bmatrix} \underline{T} \end{bmatrix} = \begin{bmatrix} \underline{b} \end{bmatrix}$$

In 2D (& 3D, etc.)

In 2D, typical example is

$$\nabla^2 u = f \quad \text{w/} \quad \begin{aligned} u(0,y) &= u_l \\ u(L_x,y) &= u_r \\ u(x,0) &= u_b \\ u(x,L_y) &= u_t \end{aligned}$$

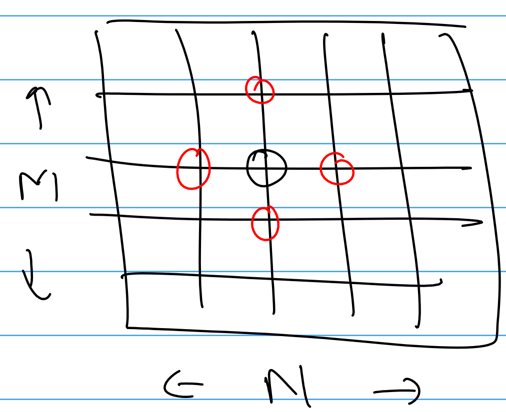


$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

$$\Rightarrow \frac{u_{i+1j} - 2u_{ij} + u_{i-1j}}{\Delta x^2} + \frac{u_{ij+1} - 2u_{ij} + u_{ij-1}}{\Delta y^2} = f_{ij}$$

w/ $\begin{aligned} U_{1,j} &= u_l \\ U_{N,j} &= u_r \end{aligned} \quad j = 1:M$

$\begin{aligned} U_{i,1} &= u_b \\ U_{i,M} &= u_t \end{aligned} \quad i = 1:N$



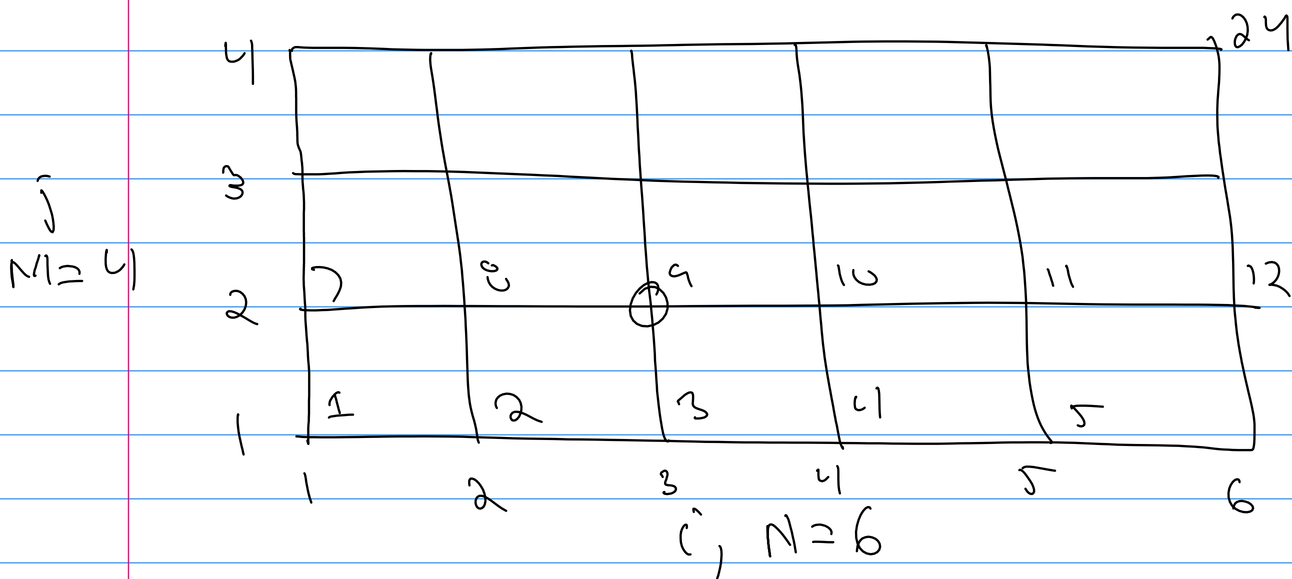
The linear system will be

$MN \times MN$

Method to organize the data:

Row or Column major ordering.

$$\text{index} = i + (j-1)N \leftarrow$$



i	j	$i + (j-1)N$
1	1	1
2	1	2
3	1	3
⋮		
6	1	6
1	2	7
2	2	8
⋮		
6	4	24

$\Rightarrow$ At $(3,2)$

$$\frac{u_8 - 2u_9 + u_{10}}{\Delta x^2} + \frac{u_{15} - 2u_9 + u_3}{\Delta y^2} = f_9$$