Integration of Ordinary Differential Equations

- An Ordinary Differential Equation (ODE) is a relation between one or several derivatives with respect to x of an unknown scalar function $u(x)$.

- A 1^{st} order ODE is of the general implicit form

$$\boxed{F(x, u, u') = 0} \qquad (1)$$

- In most cases, one can solve explicitly for u' as

$$\boxed{u' = f(x, u)} \qquad (2)$$

- Several techniques exist for solving (2) analytically depending on existence & uniqueness of general & particular solutions. Equation (2) becomes a well posed problem when complemented by a initial condition

$$\boxed{u(x_0) = u_0} \tag{3}$$

- Then we refer to an initial value problem. In general, an ODE of order n requires n initial conditions.

- Definition: An ODE is said to be of order n if the highest derivative in the equation is $\frac{d^n u}{dx^n}$. Any ODE of order n can be transformed into a system of n ODEs of 1st order by introducing $n-1$ new unknowns which are successive derivatives of $u_1 = u$; $u_2 = u'$; $u_3 = u''$; etc. and the associated equations.

- Remark: If x is time-like, then one must solve an initial value problem. $\Rightarrow$ If x is space-like, the boundary conditions can be split between both ends of the domain. This would be a boundary value problem.

Also note that a nonlinear 1st order ODE may require more than one condition, i.e. more conditions than the order of the equations.

Example: Consider the following ODE

$$\boxed{\frac{d}{dx}\left(\frac{u^2}{2}\right) = u \quad ; \quad 0 \le x \le 1} \qquad (4)$$

- Equation (4) is a 1st order ODE, however it is nonlinear, as

$$\underbrace{\frac{d}{dx}\left(\frac{u^2}{2}\right)}_{A} = \underbrace{u\frac{du}{dx}}_{B}$$

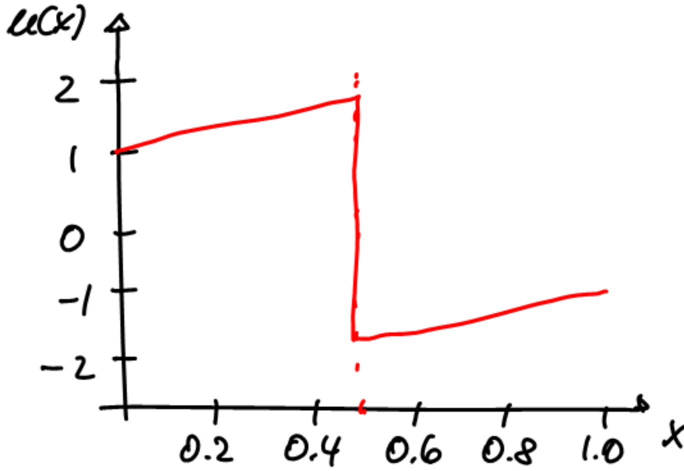
, where A is written in conservation form and B is referred to as the non-conservative form.

- Equation (4) has the following two boundary conditions

$$\boxed{u(0) = 1 \quad ; \quad u(1) = -1} \qquad (5)$$

and the exact solution

$$\boxed{\begin{cases} u(x) = x+1 & ; \ 0 \le x < \frac{1}{2} \\ u(x) = x-2 & ; \ \frac{1}{2} < x \le 1 \end{cases}} \qquad (6)$$



- Note the jump @ $x = \frac{1}{2}$
- The jump could be a "shock" in transonic flow.

- Rule-of-Thumb

  "Jump" conditions can only be solved numerically, if the governing equation is written in conservation form.

The Euler-Cauchy Method

- Consider equation (2) and represent the derivative on the L.H.S. by a FD scheme and the R.H.S. at the initial values of the step. The initial condition is (3).

- Let $x_i = x_0 + (i-1)h$ where h is the constant integration (or discretization) step.
- The "Euler - Cauchy" method reads:

$$\begin{cases} \dfrac{u_1 - u_0}{h} = f(x_0, u_0) \\ \qquad \cdots \\ \dfrac{u_{i+1} - u_i}{h} = f(x_i, u_i) \end{cases} \qquad (7)$$

- In update form, the general formula is

$$\boxed{u_{i+1} = u_i + h \cdot f(x_i, u_i) \ ; \quad i = 0, 1, \dots} \qquad (8)$$

- What is the truncation error (TE) for the "Euler - Cauchy" method?

$$\begin{aligned} \varepsilon_i &= \frac{u_{i+1} - u_i}{h} - f(x_i, u_i) \\ &= \cancel{u_i'} + \frac{h}{2} u_i'' + O(h^2) - \cancel{f(x_i, u_i)} \qquad (9) \\ &= \frac{h}{2} u_i'' + O(h^2) \end{aligned}$$

$\Longrightarrow$ The "Euler-Cauchy" method is 1st order accurate.

Improved Euler Method

- This is a two-step method $\Longrightarrow$ Higher accuracy than Euler-Cauchy.
- At first, a 1st order estimate is computed using the Euler-Cauchy method.

$$\boxed{\tilde{u}_{i+1} = u_i + h f(x_i, u_i)} \qquad (10a)$$

- The final value is obtained by

$$\boxed{u_{i+1} = u_i + \frac{h}{2}\left(f(x_i, u_i) + f(x_{i+1}, \tilde{u}_{i+1})\right)} \qquad (10b)$$

- How about the truncation error (TE) ?

$$\varepsilon_i = \frac{\overbrace{u_{i+1} - u_i}^{A}}{h} \qquad (11)$$

$$\underbrace{-\frac{1}{2}\left(f(x_i, u_i) + f[x_i + h, u_i + h f(x_i, u_i)]\right)}_{B}$$

- Say that

$$f(x_i, u_i) = f_i$$

$$f(x_i+h, u_i+hf_i) = f_i + h\frac{\partial f_i}{\partial x_i} + hf_i\frac{\partial f_i}{\partial u_i} + O(h^2)$$

- Thus, the TE in (11) becomes

$$\varepsilon_i = \cancel{u_i'} + \frac{h}{2}u_i'' + \frac{h^2}{3!}u_i''' + O(h^3) \quad \Big\} \text{ A}$$

$$- \cancel{\frac{1}{2}f_i} - \frac{1}{2}f_i - \frac{h}{2}\frac{\partial f_i}{\partial x_i} - \frac{hf_i}{2}\frac{\partial f_i}{\partial u_i} + O(h^2) \quad \Big\} \text{ B}$$

$$\varepsilon_i = \frac{h}{2}\underbrace{\left(u_i'' - \frac{\partial f_i}{\partial x_i} - f_i\frac{\partial f_i}{\partial u_i}\right)}_{C} + O(h^2) \qquad (12)$$

$\Longrightarrow$ 1st order accurate ? - Not quite!

C $\quad \frac{d}{dx}(u_i') = u_i''$; $df_i = x_i\frac{\partial f_i}{\partial x_i} + u_i\frac{\partial f_i}{\partial u_i}$

$$\frac{df_i}{dx_i} = \frac{\partial f_i}{\partial x_i} + f_i\frac{\partial f_i}{\partial u_i}$$

$$\Longrightarrow u_i'' - \frac{\partial f_i}{\partial x_i} - f_i\frac{\partial f_i}{\partial u_i} = \frac{d}{dx}(\cancel{u_i' - f_i})$$

Exact Solution

$\Longrightarrow$ Improved Euler Method is 2^{nd} order accurate.

3.) Runge-Kutta Method

- The 4^{th} order Runge-Kutta method is very popular because of its high accuracy.
- Given a fixed step size h, the 4 steps of the Runge-Kutta method read:

$$\boxed{\begin{aligned} a_i &= h \cdot f(x_i, u_i) \\ b_i &= h \cdot f\left(x_i + \frac{h}{2}, u_i + \frac{a_i}{2}\right) \\ c_i &= h \cdot f\left(x_i + \frac{h}{2}, u_i + \frac{b_i}{2}\right) \\ d_i &= h \cdot f(x_i + h, u_i + c_i) \end{aligned}} \qquad (13a)$$

- Thus, the update form for the 4^{th} order Runge-Kutta method becomes

$$\boxed{u_{i+1} = u_i + \frac{1}{6}(a_i + 2b_i + 2c_i + d_i)} \qquad (13b)$$

- It can be shown w/ some algebra that the truncation error (TE) is indeed of the form $\mathcal{O}(h^4)$.

Example: Let us demonstrate that the 4th order Runge-Kutta method does indeed integrate a 4th order polynomial exactly.

- Consider the following initial value problem:

$$\begin{cases} u'(x) = 4x^3 \\ u_0 = x_0{}^4 \end{cases} \qquad (14)$$

- From (13a) we find that

$$\begin{cases} a_0 = 4h\,x_0{}^3 \\ b_0 = 4h\left(x_0 + \frac{h}{2}\right)^3 \\ c_0 = 4h\left(x_0 + \frac{h}{2}\right)^3 \\ d_0 = 4h\,(x_0 + h)^3 \end{cases} \qquad (15a)$$

- From (13b) we can now expand u_1 as:

$$u_1 = x_0^4 + \frac{2}{3}h\,x_0^3 + \frac{2}{3}h\left(x_0+\frac{h}{2}\right)^3 \cdot 4 + \frac{2}{3}h\,(x_0+h)^3$$

$$= x_0^4 + \frac{2}{3}h\,x_0^3 + \frac{8}{3}h\left(x_0^3 + \frac{3}{2}x_0^2 h + \frac{3}{4}x_0 h^2 + \frac{1}{8}h^3\right) + \frac{2}{3}h\left(x_0^3 + 3x_0^2 h + 3x_0 h^2 + h^3\right)$$

$$= x_0^4 + 4x_0^3 h + 6x_0^2 h^2 + 4x_0 h^3 + h^4$$

$$= (x_0+h)^4 = x_1^4 \qquad \textbf{EXACT!} \qquad (16)$$

4.) Polynomials as Test Functions

- Polynomials are very useful in testing/ensuring the accuracy of a numerical scheme.
- Why? – Because the Taylor expansion of a polynomial is finite:

Example: $f(x) = 2x^3 + 4x^2 - x + 7$

$f'(x) = 6x^2 + 8x - 1 \quad ; \quad f''(x) = 12x + 8 \quad ; \quad f'''(x) = 12$

$f^{(IV)}(x) = 0 \quad ; \quad \dots \quad f^{(\dots)}(x) = 0$

Discrete:
$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + \underbrace{\frac{\Delta x^4}{4!} f^{(IV)}(x_i) + \dots}_{\doteq 0}$$

- Therefore, a 4th order accurate numerical method such as the Runge-Kutta method can solve exactly polynomials up to order 4. (even if the governing PDE is nonlinear!)

Example: "Self-similar incompressible viscous flow over a flat plate" [Blasius, 1908]

$$\boxed{f''' + \frac{1}{2} f f'' = 0} \quad ; \quad f = f(y) \qquad (17)$$

- This is a 3rd order nonlinear ODE. A non-trivial test for the integration scheme can be done by introducing a source term on the r.h.s. as:

$$\boxed{f''' + \frac{1}{2} f f'' = g(y)} \qquad (17a)$$

- Say (as a hypothetical test) that

$$\underline{f(y) = \frac{1}{6} y^3} \; ; \; f'(y) = \frac{1}{2} y^2 \; ; \; f''(y) = y \; ; \; f'''(y) = 1$$

then (17a) is satisfied if

$$\boxed{g(y) = 1 + \frac{1}{2}\frac{1}{6} y^3 \cdot y = 1 + \frac{1}{12} y^4} \qquad (17b)$$

- Solving (17a) using the 4th order Runge-Kutta method, the exact solution $f(y) = \frac{1}{6} y^3$ has to be recovered. – <u>How To Do?</u>

- Remember that <u>any</u> ODE of order n can be transformed into a system of 1st order ODEs.

5.) Numerical solution of ODEs of order n

- Consider the following 3rd order ODE in $y(x)$

$$\boxed{y''' + 3y' - 2y = 0} \qquad (18)$$

- Define $n-1$ new unknowns ...

$$u_1 = y \quad ; \quad u_2 = y' \quad ; \quad u_3 = y'' \qquad (19)$$

- Note that we can replace (18) by

$$\boxed{y''' = -3y' + 2y} \qquad (18a)$$

or

$$\boxed{u_3' = -3u_2 + 2u_1} \qquad (18b)$$

- Now we can write a system of 1st order ODEs as:

$$\left.\begin{aligned} u_1' &= y' = u_2 \\ u_2' &= y'' = u_3 \\ u_3' &= y''' = -3u_2 + 2u_1 \end{aligned}\right\} \qquad (20)$$

- Equation (20) can be written in matrix form

$$u_1' = 0\,u_1 + 1\,u_2 + 0\,u_3$$
$$u_2' = 0\,u_1 + 0\,u_2 + 1\,u_3 \qquad (21)$$
$$u_3' = 2\,u_1 - 3\,u_2 + 0\,u_3$$

or $\underline{u}' = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}' \Rightarrow \boxed{\underline{u}' = A\,\underline{u}}$ (22)

where $A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 2 & -3 & 0 \end{pmatrix}$

- As an example, we chose the initial conditions for (18) to be

$$y(0) = 0 \; ; \; y'(0) = 1 \; ; \; y''(0) = 0 \qquad (23)$$

Now you need to translate the initial conditions to

$$u_1(0) = 0 \; ; \; u_2(0) = 1 \; ; \; u_3(0) = 0 \qquad (23a)$$

- How do you solve (22) & (23a) using the 4th order Runge-Kutta method?

1.) The initial conditions in (23a) allow us to advance each 1st order ODE in (22) from $i=0$ to $i=i+1=1$.

2.) This is done by performing (13a) & (13b) for each 1st order ODE in (22).

3.) The solution @ $i+1$ for the system of 1st order ODEs serves as an initial condition to advancing the system (22) to the next spatial step $i+2$.