# Multistage and Multistep Methods

- Euler's method is only first-order accurate
- Multistage method is a one-step method achieving high-order accuracy.
- Another way to achieve high accuracy is the Multistep method using several steps of previous values.

## General R-stage Runge-Kutta family

$$U^{n+1} = U^n + \Delta t\, \Phi(U^n, t_n; \Delta t)$$
$$\Phi = \sum_{r=1}^{R} b_r k_r$$

$$k_r = f(Y_r,\ t_n + c_r \Delta t)$$
$$Y_r = U^n + \Delta t \sum_{j=1}^{R} a_{rj} f(Y_j, t_n + c_j \Delta t)$$

with

$$k_1 = f(U^n, t_n)$$
$$\sum_{j=1}^{R} a_{ij} = c_i, \quad i = 1, \dots, R$$
$$\sum_{j=1}^{R} b_j = 1.$$

Butcher table

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1R} \\ \vdots & \vdots & & \vdots \\ c_R & a_{R1} & \cdots & a_{RR} \\ \hline & b_1 & \cdots & b_R \end{array}$$

Examples. 1. one-stage Runge-Kutta method $R=1$

$$U^{n+1} = U^n + \Delta t\, f(U^n, t) \qquad \begin{array}{c|c} 0 & \\ \hline & 1 \end{array}$$

2. A two-stage explicit Runge-Kutta method

$$U^* = U^n + \tfrac{1}{2}\Delta t\, f(U^n, t_n)$$
$$U^{n+1} = U^n + \Delta t\, f(U^*, t_n + \tfrac{1}{2}\Delta t) \qquad \begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{2} & \\ \hline & 0 & 1 \end{array}$$

$\left( U^* \simeq \dfrac{U^{n+1}+U^n}{2} \quad \text{with } u(t_{n+1}) = u(t_n) + \int_{t_n}^{t_{n+1}} f(u,t)\,dt \right)$

Combine the two steps

$$U^{n+1} = U^n + \Delta t\, f(U^n + \tfrac{1}{2}\Delta t\, f(U^n), \ t_n + \tfrac{1}{2}\Delta t)$$

$$\tau^n = \frac{u(t_{n+1}) - u(t_n)}{\Delta t} - f(u(t_n) + \tfrac{1}{2}\Delta t\, f(u(t_n), t_n),\ t_n + \tfrac{1}{2}\Delta t)$$

$$= u'(t_n) + \tfrac{1}{2}u''(t_n)\Delta t + \tfrac{1}{6}u'''(t_n)\Delta t$$

$$- \left[ f + \tfrac{1}{2}\Delta t\,(f_u f + f_t) + \tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2 (f_{uu} f^2 + 2 f_{tu} f + f_{tt}) \right]$$
$$+ h.o.t.$$

$$= O(\Delta t^2)$$

Notice that

$$u' = f, \quad u'' = \frac{df}{dt} = f_u u' + f_t$$
$$f(u(t_n) + \tfrac{1}{2}\Delta t\, f(u(t_n), t_n)) = f(u(t_n) + \tfrac{1}{2}\Delta t\, u'(t_n))$$

Remark. We may also use the special test func. $u' = \lambda u$

with $u(t_{n+1}) = e^{\lambda \Delta t} u(t_n)$

$$U^{n+1} = U^n + \Delta t \lambda \, (U^n + \tfrac{1}{2} \Delta t \, \lambda U^n)$$

$$= U^n + (\Delta t \lambda) U^n + \tfrac{1}{2} (\Delta t \lambda)^2 U^n$$

$$= e^{\Delta t \lambda} U^n + O(\Delta t^2)$$

This is also a fundamental tool in stability analysis.

3. Trapezoidal rule for integral

$$U^{n+1} = U^n + \frac{1}{2} \Delta t \, f(U^n, t_n) + \frac{1}{2} \Delta t \, f(U^{n+1}, t_{n+1})$$

Another explicit two-stage RK

$$U^* = U^n + \Delta t \, f(U^n, t_n)$$

$$U^{n+1} = U^n + \frac{1}{2} \Delta t \, f(U^n, t_n) + \frac{1}{2} \Delta t \, f(U^*, t_{n+1})$$

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

4. A very popular 4th-order RK method

$$U^{(1)} = U^n$$

$$U^{(2)} = U^n + \frac{1}{2} \Delta t \, f(U^{(1)}, t_n)$$

$$U^{(3)} = U^n + \frac{1}{2} \Delta t \, f(U^{(2)}, t_n + \tfrac{1}{2} \Delta t)$$

$$U^{(4)} = U^n + \Delta t \, f(U^{(3)}, t_n + \tfrac{1}{2} \Delta t)$$

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

$$U^{n+1} = U^n + \frac{1}{6} \Delta t \Big[ f(U^{(1)}, t_n) + 2 f(U^{(2)}, t_n + \tfrac{1}{2} \Delta t) + 2 f(U^{(3)}, t_n + \tfrac{1}{2} \Delta t) + f(U^{(4)}, t_n + \Delta t) \Big]$$

Simpson's quadrature rule

$$u(t_{n+1}) - u(t_n) \simeq \Delta t \Big[ \frac{1}{6} f(u(t_n), t_n) + \frac{4}{6} f(u(t_n + \tfrac{1}{2} \Delta t), t_n + \tfrac{1}{2} \Delta t)$$

$$+\frac{1}{6}f(u(t_{n+1}), t_{n+1})\Big]$$

- Explicit RK methods: $a_{ij}=0,\ j\geq i$
- Diagonally implicit RK methods: $a_{ij}=0,\ j>i$

## Order of accuracy

An $R$-stage explicit RK method can have order at most $R$.

| # of stages $R$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| attainable order (explicit RK) | 1 | 2 | 3 | 4 | 4 | 5 | 6 | 6 | 7 | 7 |

Among implicit RK methods, $R$-stage methods of order $2R$ exist.

Example. Explicit three-stage Runge-Kutta method $R=3$

$$U^{n+1}=U^n+\Delta t(b_1k_1+b_2k_2+b_3k_3)$$

$$k_1=f(U^n, t_n)$$

$$k_2=f(U^n+a_{21}\Delta t\, k_1,\ t_n+c_2\Delta t)$$

$$k_3=f(U^n+a_{31}\Delta t\, k_1+a_{32}\Delta t\, k_2,\ t_n+c_3\Delta t)$$

$$\begin{array}{c|ccc} 0 & & & \\ c_2 & a_{21} & & \\ c_3 & a_{31} & a_{32} & \\ \hline & b_1 & b_2 & b_3 \end{array}$$

$$c_2=a_{21},\quad c_3=a_{31}+a_{32}$$

Taylor series about $(U^n, t_n)$ yields

$$k_2 = f + \Delta t\, c_2 (f_t + k_1 f_u) + \frac{1}{2}\Delta t^2 c_2^2 (f_{tt} + 2k_1 f_{tu} + k_1^2 f_{uu})$$

$f^{2''}$ $+ O(\Delta t^3)$

$$= f + \Delta t\, c_2 F_1 + \frac{1}{2}\Delta t^2 c_2^2 + O(\Delta t^3)$$

with

$$F_1 = f_t + f f_u, \quad F_2 = f_{tt} + 2 f f_{tu} + f^2 f_{uu}$$

$$k_3 = f + \Delta t \{ c_3 f_t + [(c_3 - a_{32}) k_1 + a_{32} k_2] f_u \}$$
$$+ \frac{1}{2}\Delta t^2 \{ c_3^2 f_{tt} + 2 c_3 [(c_3 - a_{32}) k_1 + a_{32} k_2] f_{tu}$$
$$+ [(c_3 - a_{32}) k_1 + a_{32} k_2^2] f_{uu} \} + O(\Delta t^3)$$

$$= f + \Delta t\, c_3 F_1 + \Delta t^2 (c_2 a_{32} F_1 f_u + \frac{1}{2} c_3^2 F_2) + O(\Delta t^3)$$

$$\Phi(U^n, t_n; \Delta t) = (b_1 + b_2 + b_3) f + \Delta t (b_2 c_2 + b_3 c_3) F_1$$
$$+ \frac{1}{2}\Delta t^2 [2 b_3 c_2 a_{32} F_1 f_u + (b_2 c_2^2 + b_3 c_3^2) F_2] + O(\Delta t^3)$$

match with with the Taylor series

$$\frac{u(t_{n+1}) - u(t_n)}{\Delta t} = u'(t_n) + \frac{1}{2}\Delta t\, u''(t_n) + \frac{1}{6}\Delta t^2 u'''(t_n) + O(\Delta t^3)$$
$$= f + \frac{1}{2}\Delta t\, F_1 + \frac{1}{6}\Delta t^2 (F_1 f_u + F_2) + O(\Delta t^3)$$

$$\Rightarrow \quad b_1 + b_2 + b_3 = 1$$
$$b_2 c_2 + b_3 c_3 = \frac{1}{2}$$
$$b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3}$$
$$b_3 c_2 a_{32} = \frac{1}{6}.$$

(i) Heun's method

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

(ii) Standard 3rd-order RK

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

## Absolute stability of RK methods

Consider $\quad u' = \lambda u, \quad u(0) = u_0 \neq 0, \qquad (*)$

and $\lambda < 0$ real.

We discuss R-stage RK method with order of accuracy R

that is, $1 \le R \le 4$.

1) $R = 1$, forward Euler's method

$$U^{n+1} = (1 + h)U^n, \quad n \ge 0 \quad \text{with } h = \lambda \Delta t$$

$\Rightarrow U^n = (1+h)^n U^0$

$\Rightarrow$ sequence $\{U^n\}_{n=0}^{\infty}$ will converge iff $|1+h| < 1$

$\Rightarrow \lambda\Delta t = h \in (-2, 0)$.

Euler's method is absolutely stable in $(-2, 0)$

The interval $(-2, 0)$ is referred to as interval of absolute stability

2) $R=2$

$$U^{n+1} = U^n + \Delta t(b_1 k_1 + b_2 k_2)$$

where $k_1 = f(U^n, t_n)$, $k_2 = f(U^n + a_{21}\Delta t k_1, t_n + c_2 \Delta t)$

and $b_1 + b_2 = 1$, $c_2 b_2 = a_{21} b_2 = \frac{1}{2}$

Applying this to (*) yields

$$U^{n+1} = (1 + h + \tfrac{1}{2}h^2) U^n \qquad h = \lambda \Delta t$$

$$\Rightarrow \quad U^n = (1 + h + \tfrac{1}{2}h^2)^n U^0$$

$\Rightarrow$ absolutely stable iff

$$|1 + h + \tfrac{1}{2}h^2| < 1 \iff h \in (-2, 0).$$

3) $R=3$ analogous argument shows

$$U^{n+1} = (1 + \tilde{h} + \tfrac{1}{2}\tilde{h}^2 + \tfrac{1}{6}\tilde{h}^3) U^n$$

$$|1 + \tilde{h} + \tfrac{1}{2}\tilde{h}^2 + \tfrac{1}{6}\tilde{h}^3| < 1$$

$$\iff \tilde{h} \in (-2.51, 0).$$

4) $R=4$

$$U^{n+1} = (1 + \tilde{h} + \tfrac{1}{2}\tilde{h}^2 + \tfrac{1}{6}\tilde{h}^3 + \tfrac{1}{24}\tilde{h}^4)^n U^0$$

$$\iff \tilde{h} \in (-2.87, 0).$$

In general, we will have

$$U^{n+1} = A_R(h)\, U^n$$

however, for $R \geq 5$ in addition to $h$, the expression for $A_R(h)$ also depends on the coefficients of the RK method.

## Taylor series methods

$$u(t_{n+1}) \approx u(t_n) + \Delta t\, u'(t_n) + \frac{1}{2}\Delta t^2 u''(t_n) + \cdots$$
$$+ \frac{1}{p!}\Delta t^p u^{(p)}(t_n)$$

with
$$u'(t) = f(u(t), t)$$
$$u''(t) = f_u(u(t), t)\, u'(t) + f_t(u(t), t)$$
$$= f_u(u(t), t)\, f(u(t), t) + f_t(u(t), t)$$

Example. Solving $u'(t) = t^2 \sin(u(t))$

$$u''(t) = 2t \sin(u(t)) + t^2 \cos(u(t))\, u'(t)$$

$$= 2t \sin(u(t)) + t^4 \cos(u(t)) \sin(u(t))$$

A Second-order method

$$U^{n+1} = U^n + \Delta t\, t_n^2 \sin(U^n) + \frac{\Delta t^2}{2}\left[2t_n \sin(U^n) + t_n^4 \cos(U^n)\sin(U^n)\right].$$

## One-step v.s. Multistep Methods

* RK methods are one-step methods:
  $U^{n+1}$ depends on $U^n$ but not on previous $U^{n-1}, U^{n-2}, \ldots$

Advantages of one-step method:

- self-starting from $U^0$ the initial data;
- time step $k$ can be changed at any point;
- Solution $u(t)$ can be non-smooth at some point $t^*$.

Disadvantages:

- Cumbersome and expensive to implement
  (especially high-order RK methods)
- function values expensive to compute
- difficulty in implicit (nonlinear) systems.

# Linear Multistep Methods (LMMs)

In general, an $r$-step LMM has the form

$$\sum_{j=0}^{r} \alpha_j U^{n+j} = \Delta t \sum_{j=0}^{r} \beta_j f(U^{n+j}, t_{n+j})$$

- $\beta_r = 0$, explicit ; $\beta_r \neq 0$, implicit.
- normalization $\alpha_r = 1$

Example. 1. Apply Simpson's rule

$$u(t_{n+1}) = u(t_{n-1}) + \int_{t_{n-1}}^{t_{n+1}} f(u(t), t)\, dt$$

$$\approx u(t_{n-1}) + \frac{1}{3}\Delta t \left[ f(u(t_{n-1}), t_{n-1}) + 4 f(u(t_n), t_n) + f(u(t_{n+1}), t_{n+1}) \right]$$

$$U^{n+1} = U^{n-1} + \frac{\Delta t}{3}\left[ f(U^{n-1}, t_{n-1}) + 4 f(U^n, t_n) + f(U^{n+1}, t_{n+1}) \right]$$

2. <u>Adams Methods</u>

$$U^{n+r} = U^{n+r-1} + \Delta t \sum_{j=0}^{r} \beta_j f(U^{n+j})$$

$\beta_j$ coefficients are chosen to maximize the order of accuracy.

$$u(t_{n+r}) = u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} u'(t)\, dt$$

$$= u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} f(u(t))\, dt$$

$$\approx u(t_{n+r-1}) + \Delta t \sum_{j=1}^{r-1} \beta_j f(u(t_{n+j}))$$

Explicit Adams-Bashforth

1-step: $U^{n+1} = U^n + \Delta t\, f(U^n)$ (FE)

2-step: $U^{n+2} = U^{n+1} + \frac{\Delta t}{2}[-f(U^n) + 3f(U^{n+1})]$

3-step: $U^{n+3} = U^{n+2} + \frac{\Delta t}{12}[5f(U^n) - 16f(U^{n+1}) + 23f(U^{n+2})]$.

Implicit Adams-Moulton

1-step: $U^{n+1} = U^n + \frac{\Delta t}{2}[f(U^n) + f(U^{n+1})]$ (trapezoidal rule)

2-step: $U^{n+2} = U^{n+1} + \frac{\Delta t}{12}[-f(U^n) + 8f(U^{n+1}) + 5f(U^{n+2})]$

3-step: $U^{n+3} = U^{n+2} + \frac{\Delta t}{24}[f(U^n) - 5f(U^{n+1}) + 19f(U^{n+2}) + 9f(U^{n+3})]$.

3. Nyström methods

$$U^{n+r} = U^{n+r-2} + \Delta t \sum_{j=0}^{r-1} \beta_j f(U^{n+j})$$

( $r=2$ Simpson's rule )

## Local truncation error (LTE)

$$\tau(t_{n+r}) = \frac{1}{\Delta t}\left(\sum_{j=0}^{r} \alpha_j u(t_{n+j}) - \Delta t \sum_{j=0}^{r} \beta_j u'(t_{n+j})\right)$$

with

$$u(t_{n+j}) = u(t_n) + j\Delta t\, u'(t_n) + \frac{1}{2}(j\Delta t)^2 u''(t_n) + \dots$$

$$u'(t_{n+j}) = u'(t_n) + j\Delta t\, u''(t_n) + \frac{1}{2}(j\Delta t)^2 u'''(t_n) + \dots$$

therefore,

$$\tau(t_{n+r}) = \frac{1}{\Delta t}\left(\sum_{j=0}^{r} \alpha_j\right) u(t_n) + \left(\sum_{j=0}^{r} (j\alpha_j - \beta_j)\right) u'(t_n) + O(\Delta t).$$

The method is <u>consistent</u> if $\tau \to 0$ as $\Delta t \to 0$,

which requires

$$\sum_{j=0}^{r} \alpha_j = 0, \quad \sum_{j=0}^{r} j\alpha_j = \sum_{j=0}^{r} \beta_j .$$

## Characteristic Polynomials of LMM

$$\rho(x) = \sum_{j=0}^{r} \alpha_j x^j$$

$$\sigma(x) = \sum_{j=0}^{r} \beta_j x^j .$$

note that

$$\rho(1) = \sum_{j=0}^{r} a_j \qquad \rho'(x) = \sum_{j=0}^{r} j a_j x^{j-1}$$

the consistent condition gives

$$\rho(1) = 0, \qquad \rho'(1) = \sigma(1).$$

Example. 2-step Adams-Moulton

$$\rho(x) = x^2 - x$$

$$\sigma(x) = \frac{1}{12}(-1 + 8x + 5x^2)$$

Comments.

- Starting values

  Using $r$-stage LMMs, $U^0, U^1, \dots, U^{r-1}$ are needed.

- Predictor - corrector methods

$$\hat{U}^{n+1} = U^n + \Delta t\, f(U^n)$$

$$U^{n+1} = U^n + \frac{\Delta t}{2}\left[ f(U^n) + f(\hat{U}^{n+1}) \right]$$

( ode113 in MATLAB uses this approach,

with Adams-Bashforth-Moulton of orders 1-12 )