Validated Explicit and Implicit Runge-Kutta Methods

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Initial Value Problem of Ordinary Differential Equations

Consider an IVP for ODE, over the time interval $[0, T]$

$$\dot{\mathbf{y}} = f(\mathbf{y}) \quad \text{with} \quad \mathbf{y}(0) = \mathbf{y}_0$$

IVP has a unique solution $\mathbf{y}(t; \mathbf{y}_0)$ if $f : \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz in $\mathbf{y}$
but for our purpose we suppose f smooth enough i.e., of class C^k

Goal of numerical integration

- Compute a sequence of time instants: $t_0 = 0 < t_1 < \cdots < t_n = T$
- Compute a sequence of values: $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_n$ such that

$$\forall i \in [0, n], \quad \mathbf{y}_i \approx \mathbf{y}(t_i; \mathbf{y}_0) \ .$$

- s.t. $\mathbf{y}_{n+1} \approx \mathbf{y}(t_n + h; \mathbf{y}_n)$ with an error $\mathcal{O}(h^{p+1})$ where
  - h is the integration **step-size**
  - p is the **order** of the method
  - true with *localization assumption* i.e., $\mathbf{y}_n = \mathbf{y}(t_n; y_0)$.

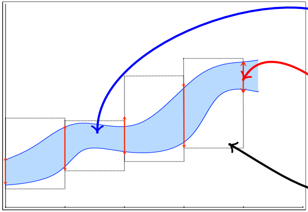
Validated solution of IVP for ODE

Goal of validated numerical integration

- Compute a sequence of time instants: $t_0 = 0 < t_1 < \cdots < t_n = T$
- Compute a sequence of values: $[\mathbf{y}_0], [\mathbf{y}_1], \ldots, [\mathbf{y}_n]$ such that

$$\forall i \in [0, n], \quad [\mathbf{y}_i] \ni \mathbf{y}(t_i; \mathbf{y}_0) \enspace .$$

A two-step approach



- Exact solution of $\dot{\mathbf{y}} = f(\mathbf{y}(t))$ with $\mathbf{y}(0) \in \mathcal{Y}_0$
- Safe approximation at discrete time instants
- Safe approximation between time instants

State of the art

Taylor methods

They have been developed since 60's (Moore, Lohner, Makino and Berz, Rhim, Jackson and Nedialkov, etc.)

- prove the existence and uniqueness: **high order interval Picard-Lindelöf**
- works very well on various kinds of problems:
  - **non stiff** and **moderately stiff** linear and non-linear systems,
  - with **thin uncertainties on initial conditions**
  - with (a writing process) **thin uncertainties on parameters**
- **very efficient** with automatic differentiation techniques
- **wrapping effect fighting**: interval centered form and QR decomposition
- **many software**: AWA, COSY infinity, VNODE-LP, CAPD, etc.

Some extensions

- Taylor polynomial with Hermite-Obreskov (Jackson and Nedialkov)
- Taylor polynomial in Chebyshev basis (T. Dzetkulic)

One question

Why bother to define new methods?

Answer 1: it may fail

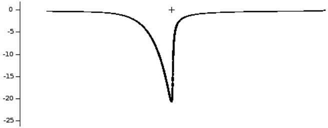
A chemical reaction simulated with VNODE-LP

$$\begin{cases} \dot{y} = z \\ \dot{z} = z^2 - \dfrac{3}{0.001 + y^2} \end{cases} \quad \text{with} \quad \begin{cases} y(0) = 10 \\ z(0) = 0 \end{cases} \quad \text{and} \quad t \in [0, 50]$$

Result: it is stuck around $t = 1$ with various order between 5 and 40.

With validated Lobatto-3C (order 4) method with tolerance 10^{-10}, we get in about 7.6s (Intel i7 3.4Ghz)

- $\text{width}(y_1(50.0)) = 7.67807 \cdot 10^{-5}$
- $\text{width}(y_2(50.0)) = 2.338 \cdot 10^{-6}$



Note: CAPD can solve this problem

Answer 2: there is no silver bullet

Numerical solutions of IVP for ODEs are produced by

- Adams-Bashworth/Moulton methods
- BDF methods
- Runge-Kutta methods
- etc.

each of these methods is adapted to a particular class of ODEs

Runge-Kutta methods

- have **strong stability** properties for various kinds of problems (A-stable, L-stable, algebraic stability, etc.)
- may preserve quadratic algebraic invariant (symplectic methods)
- can produce continuous output (polynomial approximation of $y(t)$)

Can we benefit these properties in validated computations?

Examples of Runge-Kutta methods

Single-step fixed step-size explicit Runge-Kutta method

e.g. explicit Trapzoidal method (or Heun's method)[1] is defined by:

$$\mathbf{k}_1 = f(t_n, \mathbf{y}_n) \;, \qquad \mathbf{k}_2 = f(t_n + 1h_n, \mathbf{y}_n + h1\mathbf{k}_1)$$

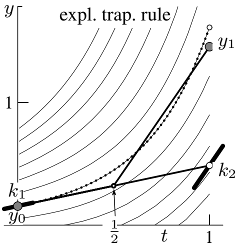
$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right)$$

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

Intuition

- $\dot{y} = t^2 + y^2$
- $y_0 = 0.46$
- $h = 1.0$

dotted line is the exact solution.



[1] example coming from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

Single-step fixed step-size implicit Runge-Kutta method

e.g. Runge-Kutta Gauss method (order 4) is defined by:

$$\mathbf{k}_1 = f\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h_n, \quad \mathbf{y}_n + h\left(\frac{1}{4}\mathbf{k}_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)\mathbf{k}_2\right)\right) \tag{1a}$$

$$\mathbf{k}_2 = f\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h_n, \quad \mathbf{y}_n + h\left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)\mathbf{k}_1 + \frac{1}{4}\mathbf{k}_2\right)\right) \tag{1b}$$

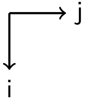
$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right) \tag{1c}$$

Remark: A non-linear system of equations must be solved at each step.

Runge-Kutta methods

s-stage Runge-Kutta methods are described by a Butcher tableau

$$
\begin{array}{c|ccccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s} & \\
\vdots & \vdots & \vdots & & \vdots & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} & \\
\hline
 & b_1 & b_2 & \cdots & b_s & \\
 & b'_1 & b'_2 & \cdots & b'_s & \text{(optional)}
\end{array}
$$



Which induces the following recurrence:

$$
\mathbf{k}_i = f\left(t_n + c_i h_n, \quad \mathbf{y}_n + h\sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right) \qquad \mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{i=1}^{s} b_i\mathbf{k}_i \tag{2}
$$

- **Explicit** method (ERK) if $a_{ij} = 0$ is $i \leqslant j$
- **Diagonal Implicit** method (DIRK) if $a_{ij} = 0$ is $i \leqslant j$ and at least one $a_{ii} \neq 0$
- **Implicit** method (IRK) otherwise

Validated Runge-Kutta methods

Challenges

1. Computing with sets of values taking into account dependency problem and wrapping effect;
2. Bounding the approximation error of Runge-Kutta formula.

Our approach

- **Problem 1** is solved using **affine arithmetic** avoiding centered form and QR decomposition
- **Problem 2** is solved by bounding the **Local truncation error** of Runge-Kutta method based on **B-series**

We focus on Problem 2 in this talk

Order condition for Runge-Kutta methods

Method order of Runge-Kutta methods and Local Truncation Error (LTE)

$$\mathbf{y}(t_n; \mathbf{y}_{n-1}) - \mathbf{y}_n = C \cdot \mathcal{O}\left(h^{p+1}\right) \quad \text{with} \quad C \in \mathbb{R}.$$

we want to bound this!

Order condition

This condition states that a method of Runge-Kutta family is of order p **iff**

- the Taylor expansion of the exact solution
- and the Taylor expansion of the numerical methods

have the same $p+1$ first coefficients.

Consequence

The LTE is the **difference of Lagrange remainders of two Taylor expansions**

. . . but how to compute it?

A quick view of Runge-Kutta order condition theory[2]

Starting from $\mathbf{y}^{(q)} = (f(\mathbf{y}))^{(q-1)}$ and with the Chain rule, we have

High order derivatives of exact solution y

$$
\begin{aligned}
\dot{\mathbf{y}} &= f(\mathbf{y}) \\
\ddot{\mathbf{y}} &= f'(\mathbf{y})\dot{\mathbf{y}} && f'(\mathbf{y}) \text{ is a linear map} \\
\mathbf{y}^{(3)} &= f''(\mathbf{y})(\dot{\mathbf{y}}, \dot{\mathbf{y}}) + f'(\mathbf{y})\ddot{\mathbf{y}} && f''(\mathbf{y}) \text{ is a bi-linear map} \\
\mathbf{y}^{(4)} &= f'''(\mathbf{y})(\dot{\mathbf{y}}, \dot{\mathbf{y}}, \dot{\mathbf{y}}) + 3f''(\mathbf{y})(\ddot{\mathbf{y}}, \dot{\mathbf{y}}) + f'(\mathbf{y})\mathbf{y}^{(3)} && f'''(\mathbf{y}) \text{ is a tri-linear map} \\
\mathbf{y}^{(5)} &= f^{(4)}(\mathbf{y})(\dot{\mathbf{y}}, \dot{\mathbf{y}}, \dot{\mathbf{y}}, \dot{\mathbf{y}}) + 6f'''(\mathbf{y})(\ddot{\mathbf{y}}, \dot{\mathbf{y}}, \dot{\mathbf{y}}) && \vdots \\
&\quad + 4f''(\mathbf{y})(\mathbf{y}^{(3)}, \dot{\mathbf{y}}) + 3f''(\mathbf{y})(\ddot{\mathbf{y}}, \ddot{\mathbf{y}}) + f'(\mathbf{y})\mathbf{y}^{(4)} \\
&\vdots
\end{aligned}
$$

[2] strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

A quick view of Runge-Kutta order condition theory[2]

Inserting the value of $\dot{\mathbf{y}}$, $\ddot{\mathbf{y}}$, ..., we have:

High order derivatives of exact solution y

$$
\begin{aligned}
\dot{\mathbf{y}} &= f \\
\ddot{\mathbf{y}} &= f'(f) \\
\mathbf{y}^{(3)} &= f''(f,f) + f'(f'(f)) \\
\mathbf{y}^{(4)} &= \ f'''(f,f,f) \ + \ {\color{red}3}f''(f'f,f) \ + \ f'(f''(f,f)) \ + \ f'(f'(f'(f))) \\
&\ \vdots
\end{aligned}
$$

- `Elementary differentials`, are denoted by $F(\tau)$

Remark a tree structure is made apparent in these computations

[2]strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

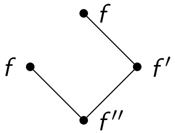
A quick view of Runge-Kutta order condition theory[2]

Rooted trees

- f is a leaf
- f' is a tree with one branch, ..., $f^{(k)}$ is a tree with k branches

Example

$f''(f'f, f)$ is associated to



Remark: this tree is not unique e.g., symmetry

[2] strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

A quick view of Runge-Kutta order condition theory[2]

Theorem 1 (Butcher, 1963)

The qth derivative of the **exact solution** is given by

$$\mathbf{y}^{(q)} = \sum_{r(\tau)=q} \alpha(\tau) F(\tau)(\mathbf{y}_0) \quad \text{with} \quad \begin{array}{l} r(\tau) \text{ the order of } \tau \text{ i.e., number of nodes} \\ \alpha(\tau) \text{ a positive integer} \end{array}$$

We can do the same for the numerical solution

Theorem 2 (Butcher, 1963)

The qth derivative of the **numerical solution** is given by

$$\mathbf{y}_1^{(q)} = \sum_{r(\tau)=q} \gamma(\tau)\phi(\tau)\alpha(\tau) F(\tau)(\mathbf{y}_0) \quad \text{with} \quad \begin{array}{l} \gamma(\tau) \text{ a positive integer} \\ \phi(\tau) \text{ depending on a Butcher tableau} \end{array}$$

Theorem 3, order condition (Butcher, 1963)

A Runge-Kutta method has order p iff $\phi(\tau) = \frac{1}{\gamma(\tau)} \quad \forall \tau, r(\tau) \leqslant p$

[2] strongly inspired from "Geometric Numerical Integration", Hairer, Lubich and Wanner.

LTE formula for **explicit and implicit** Runge-Kutta

From Theorem 1 and Theorem 2, if a Runge-Kutta has order p then

$$\mathbf{y}(t_n; \mathbf{y}_{n-1}) - \mathbf{y}_n = \frac{h^{p+1}}{(p+1)!} \sum_{r(\tau)=p+1} \alpha(\tau) \left[1 - \gamma(\tau)\phi(\tau)\right] F(\tau)(\mathbf{y}(\xi))$$

$$\xi \in [t_{n-1}, t_n]$$

- $\alpha(\tau)$ and $\gamma(\tau)$ are positive integer (with some combinatorial meaning)
- $\phi(\tau)$ function of the coefficients of the RK method,

Example

$\phi\Big($  $\Big)$ is associated to $\displaystyle\sum_{i,j=1}^{s} b_i a_{ij} c_j$ with $\displaystyle c_j = \sum_{k=1}^{s} a_{jk}$

Note: $y(\xi)$ may be over-approximated using Interval Picard-Lindelöf operator.

Implementation of LTE formula

Elementary differentials

$$F(\tau)(y) = f^{(m)}(y)\,(F(\tau_1)(y), \ldots, F(\tau_m)(y)) \quad \text{for} \quad \tau = [\tau_1, \ldots, \tau_m]$$

translate as a sum of partial derivatives of f associated to sub-trees

Notations

- n the state-space dimension
- p the order of a Rung-Kutta method

Two ways of computing $F(\tau)$

1. **Direct form** (current): complexity $\mathcal{O}(n^{p+1})$
2. **Factorized form** (under test): complexity $\mathcal{O}(n(p+1)^{\frac{5}{2}})$
   based on the work of Ferenc Bartha and Hans Munthe-Kaas
   "Computing of B-series by automatic differentiation", 2014

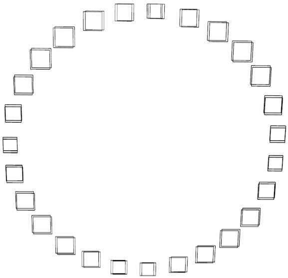
Experimentation

Toy example

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} -y_2 \\ y_1 \end{pmatrix} \quad \text{with} \quad \begin{pmatrix} y_1(0) = [0, 0.1] \\ y_2(0) = [0.95, 1.05] \end{pmatrix}$$

Validated RK4 method with tolerance 10^{-8} we get in about 3s (Intel i7 3.4Ghz)

- $\mathrm{width}(y_1(100.0)) = 0.146808$
- $\mathrm{width}(y_2(100.0)) = 0.146902$



Experimentation

Usefulness of affine arithmetic

$$\begin{cases} \dot{y}_1 = 1, & y_1(0) = 0 \\ \dot{y}_2 = y_3, & y_2(0) = 0 \\ \dot{y}_3 = \dfrac{1}{6}y_2^3 - y_2 + 2\sin(p \cdot y_1) \quad \text{with} \quad p \in [2.78, 2.79], & y_3(0) = 0 \end{cases} .$$

Validated RK4 method with tolerance 10^{-6} we get in about 2.3s (Intel i7 3.4Ghz)

- $\text{width}(y_1(10.0)) = 7.10543 \cdot 10^{-15}$
- $\text{width}(y_2(10.0)) = 6.11703$
- $\text{width}(y_3(10.0)) = 7.47225$

Note: none of the method in the Vericomp benchmark can reach 10s
Note 2: CAPD can solve it

Experimentation

Based on Vericomp benchmark [3] (around 70 problems)

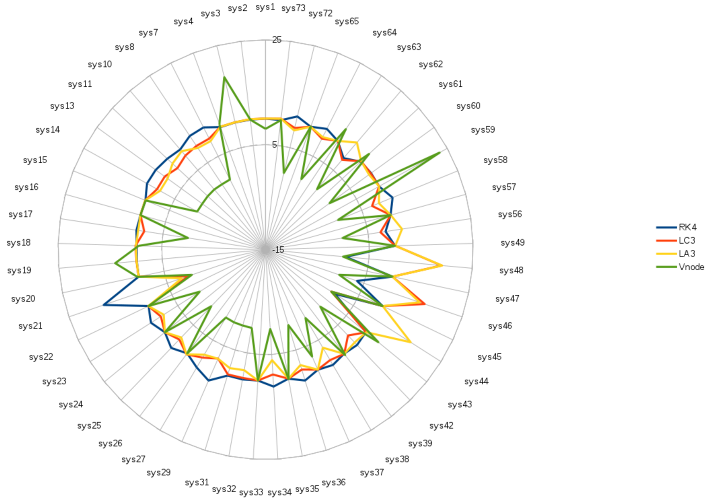
$$
\begin{tikzcd}
 & & & \text{simple (A)} \arrow[r] & \text{Uncertain (U) or not} \\
 & & \textcolor{blue}{\text{linear (L)}} \arrow[ur] \arrow[r] \arrow[dr] & \text{moderate (B)} \arrow[ur, dotted] & \\
\text{IVP} \arrow[r] & \text{non-stiff (P.I)} \arrow[ur] \arrow[dr] & & \text{complicate (C)} \arrow[uur, dotted] & \\
 & & \textcolor{orange}{\text{nonlinear } (\overline{L})} \arrow[r, dotted] & \text{idem} &
\end{tikzcd}
$$

with the following metrics:

- c5t: user time taken to simulate the problem for 1 second.
- c5w: the final diameter of the solution (infinity norm is used).
- c6t: the time to breakdown the method with a maximal limit of 10 seconds.
- c6w: the diameter of the solution a the breakdown time.

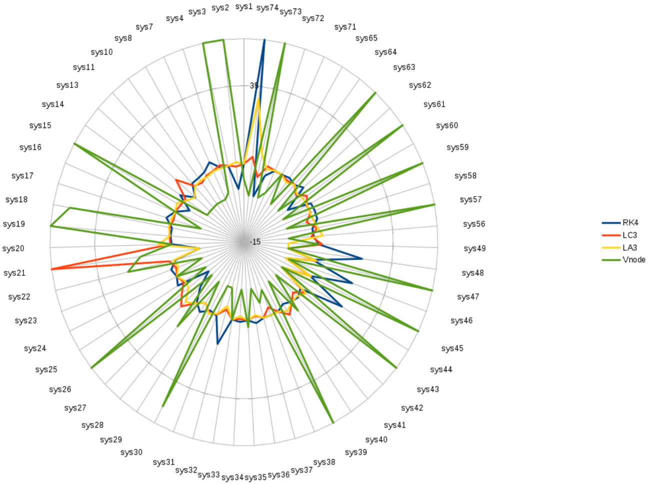
[3] `http://vericomp.inf.uni-due.de/`

Summary – RK vs Vnode-LP – c5w



- Vnode-LP: order 15, 20, 25 (tolerances 10^{-14})
- RK4, LC3, LA3: tolerances 10^{-8} to 10^{-14} (order 4)

Summary – RK vs Vnode-LP – c6w



- Vnode-LP: order 15, 20, 25 (tolerances 10^{-14})
- RK4, LC3, LA3: tolerances 10^{-8} to 10^{-14} (order 4)

Conclusion

We presented a new approach to validate Runge-Kutta methods

- a new formula to compute LTE based on B-series
- fully parametrized by a Butcher tableau
- affine arithmetic avoiding QR decomposition

implementation as a plugin of IBEX, code name DynIbex, available at
`http://perso.ensta-paristech.fr/~chapoutot/dynibex/`

Future work

- finish testing the implementation of LTE with automatic differentiation
- implement new *a priori* enclosure methods based on Runge-Kutta
- define new methods mixing different Runge-Kutta in one simulation
- solve new IVP problems such as for DAE (next talk) or DDE

BACKUP

Note on the number of trees (up to order 11 (left)):

```
Number of Rooted Trees
1842 719 286 115 48 20 9 4 2 1 1  (total 3047)
```

Quick remainder: Taylor series method

Taylor series development of $\mathbf{y}(t)$ (assume $\mathbf{y}(t_n) \in [\boldsymbol{y}_n]$)

$$\begin{aligned}
\mathbf{y}(t_{n+1}) &= \mathbf{y}(t_n) + \sum_{i=1}^{N-1} \frac{h^i}{i!} \frac{d^i \mathbf{y}}{dt^i}(t_n) + \frac{h_{n+1}^N}{N!} \frac{d^{\mathbf{Nx}}}{dt^N}(t') \\
&\in [\boldsymbol{y}_n] + \sum_{i=1}^{N-1} h^i f^{[i-1]}(\mathbf{y}(t_n)) + h^N f^{[N-1]}(\mathbf{y}(t')) \\
&\in [\boldsymbol{y}_n] + \sum_{i=1}^{N-1} h^i f^{[i-1]}([\boldsymbol{y}_n]) + h^N f^{[N-1]}([\tilde{\boldsymbol{y}}_n]) \triangleq [\boldsymbol{y}_{n+1}]
\end{aligned}$$

Challenges

- Computation of $[\tilde{\boldsymbol{y}}_n]$ such that $\forall t \in [t_n, t_{n+1}],\ \mathbf{y}(t) \in [\tilde{\boldsymbol{y}}_n]$
  Solution: interval Picard-Lindelöf operator
- With that formula: $\text{width}([\boldsymbol{y}_{n+1}]) \geqslant \text{width}([\boldsymbol{y}_n])$
  Solutions: interval centered form + QR decomposition

Single-step variable step-size explicit Runge-Kutta method

e.g. Bogacki-Shampine (ode23) is defined by:

$$
\begin{aligned}
\mathbf{k}_1 &= f(t_n, \mathbf{y}_n) \\
\mathbf{k}_2 &= f(t_n + \tfrac{1}{2}h_n, \mathbf{y}_n + \tfrac{1}{2}h\mathbf{k}_1) \\
\mathbf{k}_3 &= f(t_n + \tfrac{3}{4}h_n, \mathbf{y}_n + \tfrac{3}{4}h\mathbf{k}_2) \\
\mathbf{y}_{n+1} &= \mathbf{y}_n + h\left(\frac{2}{9}\mathbf{k}_1 + \frac{1}{3}\mathbf{k}_2 + \frac{4}{9}\mathbf{k}_3\right) \\
\mathbf{k}_4 &= f(t_n + 1h_n, \mathbf{y}_{n+1}) \\
\mathbf{z}_{n+1} &= \mathbf{y}_n + h\left(\frac{7}{24}\mathbf{k}_1 + \frac{1}{4}\mathbf{k}_2 + \frac{1}{3}\mathbf{k}_3 + \frac{1}{8}\mathbf{k}_4\right)
\end{aligned}
$$

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{3}{4} & 0 & \frac{3}{4} & & \\
1 & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} & \\
\hline
 & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} & \\
 & \frac{7}{24} & \frac{1}{4} & \frac{1}{3} & \frac{1}{8}
\end{array}
$$

Remark: the step-size h is adapted following $\| \mathbf{y}_{n+1} - \mathbf{z}_{n+1} \| \leqslant \text{tol}$

Gauss-Legendre methods

Single-step fixed step-size implicit Runge-Kutta method

e.g. Runge-Kutta Gauss method (order 4) is defined by:

$$\mathbf{k}_1 = f\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h_n, \quad \mathbf{y}_n + h\left(\frac{1}{4}\mathbf{k}_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)\mathbf{k}_2\right)\right) \tag{3a}$$

$$\mathbf{k}_2 = f\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h_n, \quad \mathbf{y}_n + h\left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)\mathbf{k}_1 + \frac{1}{4}\mathbf{k}_2\right)\right) \tag{3b}$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right) \tag{3c}$$

Remark: A non-linear system of equations must be solved at each step.

Note on building IRK Gauss' method

$$\dot{\mathbf{y}} = f(\mathbf{y}) \quad \text{with} \quad \mathbf{y}(0) = \mathbf{y}_0 \Leftrightarrow \mathbf{y}(t) = \mathbf{y}_0 + \int_{t_n}^{t_{n+1}} f(\mathbf{y}(s))ds$$

We solve this equation using quadrature formula.

IRK Gauss method is associated to a **collocation method** (polynomial approximation of the integral) such that for $i, j = 1, \ldots, s$:

$$a_{ij} = \int_0^{c_i} \ell_j(t)dt \qquad \text{and} \qquad b_j = \int_0^1 \ell_j(t)dt$$

with $\ell_j(t) = \prod_{k \neq j} \frac{t - c_k}{c_j - c_k}$ the **Lagrange polynomial**.
And the c_i are chosen as the solution of the **Shifted Legendre polynomial** of degree s:

$$P_s(x) = (-1)^s \sum_{k=0}^{s} \binom{s}{k} \binom{s+k}{s} (-x)^k$$

Example: 1, $2x - 1$, $6x^2 - 6x + 1$, $20x^3 - 30x^2 + 12x - 1$, etc.