On Runge–Kutta methods of order 10

Misha Stepanov stepanov@arizona.edu

Department of Mathematics and Program in Applied Mathematics,
University of Arizona, Tucson, AZ 85721, USA

Abstract

A family of explicit 15-stage Runge–Kutta methods of order 10 is derived.

Keywords: minimal number of stages, explicit Runge–Kutta methods

MSC Classification: 65L05 , 65L06

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$$

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$$

$$\boldsymbol{x}(t+h) = \boldsymbol{x}(t) + \int_{t}^{t+h} \mathrm{d}t' \, \boldsymbol{f}\big(t', \boldsymbol{x}(t')\big)$$

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$$

$$\boldsymbol{x}(t+h) = \boldsymbol{x}(t) + \int_t^{t+h} \mathrm{d}t' \, \boldsymbol{f}\big(t', \boldsymbol{x}(t')\big) = \boldsymbol{x}(t) + h \int_0^1 \mathrm{d}\theta \, \boldsymbol{f}\big(t + \theta h, \boldsymbol{x}(t + \theta h)\big)$$

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$$

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s-stage Runge–Kutta method

$$i = 1, 2, \ldots, s, \qquad \boldsymbol{X}_i = \boldsymbol{x}(t) + h \sum_{j=1}^{s} a_{ij} \boldsymbol{f}\big(t + c_j h, \boldsymbol{X}_j\big)$$

$$\tilde{\boldsymbol{x}}(t+h) = \boldsymbol{x}(t) + h \sum_{j=1}^{s} b_j \boldsymbol{f}\big(t + c_j h, \boldsymbol{X}_j\big)$$

it is natural and will be assumed that $\sum_{j=1}^{s} a_{ij} = c_i$ for all i

Higher-order derivatives are connected with rooted trees (Cayley, 1857):

XXVIII. *On the Theory of the Analytical Forms called Trees.*
By A. Cayley, *Esq.**

A SYMBOL such as $A\partial_x + B\partial_y + \ldots$, where A, B, &c. contain the variables x, y, &c. in respect to which the differentiations are to be performed, partakes of the natures of

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this to the question in hand, PU consists of a single term repre-

Fig. 1.

Fig. 2.

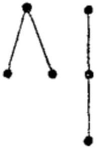
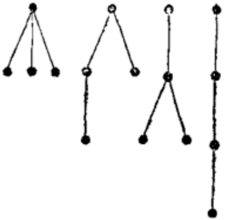


Fig. 3.



order conditions

$$\frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} = \boldsymbol{f}\big(t, \boldsymbol{x}(t)\big)$$

$$\boldsymbol{x}(t+h) = \boldsymbol{x}(t) + h\int_0^1 \mathrm{d}\theta\, \boldsymbol{f}\big(t+\theta h, \boldsymbol{x}(t+\theta h)\big)$$

$$\boldsymbol{X}_i = \boldsymbol{x}(t) + h\sum_{j=1}^{s} a_{ij}\,\boldsymbol{f}\big(t+c_j h, \boldsymbol{X}_j\big), \qquad i = 1, 2, ..., s$$

$$\tilde{\boldsymbol{x}}(t+h) = \boldsymbol{x}(t) + h\sum_{j=1}^{s} b_j\,\boldsymbol{f}\big(t+c_j h, \boldsymbol{X}_j\big)$$

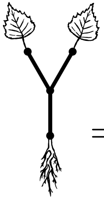
$\boldsymbol{\Phi}(\mathrm{t})$

	vector **1**
	matrix $\boldsymbol{A}$
	weights row vector $\boldsymbol{b}$
	element-wise product of vectors

1	function $1(\theta) \equiv 1$
$\boldsymbol{A}$	operator $u(\theta) \mapsto \int_0^\theta \mathrm{d}\theta'\, u(\theta')$
$\boldsymbol{b}$	functional $u(\theta) \mapsto \int_0^1 \mathrm{d}\theta\, u(\theta)$
$\boldsymbol{u}.\boldsymbol{v}$	point-wise product $u(\theta)v(\theta)$
$\boldsymbol{c}$	θ
$\boldsymbol{\Phi}(\mathrm{t})$	$\lvert\mathrm{t}\rvert\theta^{\lvert\mathrm{t}\rvert-1}/\mathrm{t}!$
$\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t})$	$1/\mathrm{t}!$ (Butcher, 1963)

for all $\lvert\mathrm{t}\rvert \leq p$

order conditions

 $= \frac{1}{12}$

$$\int_0^1 d\theta \int_0^\theta d\theta' \left(\int_0^{\theta'} d\theta''\right)\left(\int_0^{\theta'} d\theta'''\right) = \int_0^1 d\theta \int_0^\theta d\theta'\, \theta'^2 = \int_0^1 d\theta\, \frac{\theta^3}{3} = \frac{1}{12}$$

$$\boldsymbol{b} \quad \boldsymbol{A} \quad \big(\; (\boldsymbol{A1}) \;\; . \;\; (\boldsymbol{A1}) \; \big) = \boldsymbol{b} \quad \boldsymbol{A} \quad \boldsymbol{c}^2$$

$\Phi(\mathrm{t})$

	vector **1**
	matrix $\boldsymbol{A}$
	weights row vector $\boldsymbol{b}$
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for all $\lvert\mathrm{t}\rvert \le p$

order conditions of Q-type

$$\boldsymbol{Q}\big([\bullet^n]\big) = \boldsymbol{q}_n = \boldsymbol{A}\boldsymbol{c}^n - \tfrac{1}{n+1}\boldsymbol{c}^{n+1}$$

$$\downarrow$$

$$\boldsymbol{Q}(\mathrm{t}) = \boldsymbol{A}\boldsymbol{\Phi}(\mathrm{t}) - \boldsymbol{c}^{|\mathrm{t}|}/\mathrm{t}!$$

$$\downarrow$$

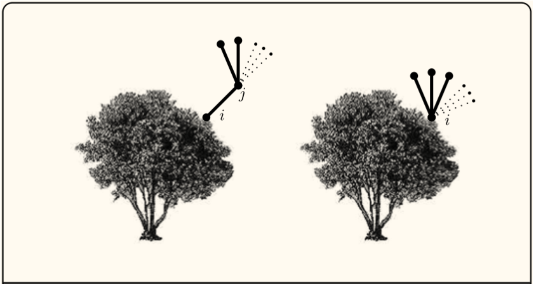


Figure 321(i) The $C(k)$ condition relating $\sum_j a_{ij} c_j^{k-1}$ (left-hand tree) to c_i^k (right-hand tree). The underlying tree is a pohutukawa (*Metrosideros excelsa*), also known as the ‘New Zealand Christmas tree’ because its bright red flowers bloom at Christmas-time.

J. C. Butcher, *Numerical methods for ordinary differential equations*, 3rd ed., John Wiley & Sons Ltd (2016).

$\left(\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t}) = \dfrac{1}{\mathrm{t}!} \text{ for all } |\mathrm{t}| \le p\right)$ — order conditions for a method of order p

$$\Updownarrow$$

quadrature order conditions $\boldsymbol{b}\boldsymbol{c}^n = \frac{1}{n+1}$ for $0 \le n < p$
and order conditions of *Q-type*

$$\boldsymbol{b}\big(\boldsymbol{Q}(\mathrm{t}_1).\boldsymbol{Q}(\mathrm{t}_2).\cdots.\boldsymbol{Q}(\mathrm{t}_k).\boldsymbol{c}^n\big) = 0 \text{ for } k \ge 1 \text{ and } |\mathrm{t}_1| + |\mathrm{t}_2| + \ldots + |\mathrm{t}_k| + n < p$$

order conditions of D-type

$$\boldsymbol{D}\big([\bullet^n]\big) = \boldsymbol{d}_n =$$
$$= (\boldsymbol{b}.\boldsymbol{c}^{n\mathrm{T}})\boldsymbol{A} - \tfrac{1}{n+1}\boldsymbol{b}.(\mathbf{1} - \boldsymbol{c}^{n+1})^{\mathrm{T}}$$

$$\downarrow$$

$$\boldsymbol{D}(\mathrm{t}) = \big(\boldsymbol{b}.\boldsymbol{\Phi}^{\mathrm{T}}(\mathrm{t})\big)\boldsymbol{A} - \big(\boldsymbol{b}.(\mathbf{1} - \boldsymbol{c}^{|\mathrm{t}|})^{\mathrm{T}}\big)/\mathrm{t}!$$

$$\downarrow$$

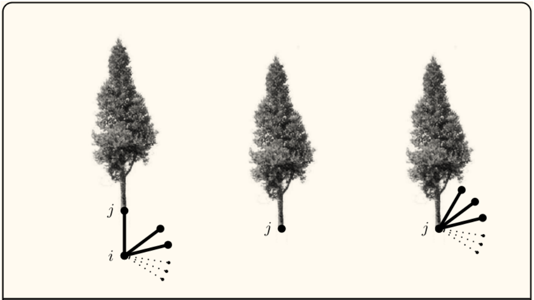


Figure 321(ii) The $D(k)$ condition relating $\sum_i b_i c_i^{k-1} a_{ij}$ (left-hand tree) to b_j (middle tree) and $b_j c_j^k$ (right-hand tree). The underlying tree is a kauri (*Agathis australis*). Although the immature tree shown is only a few metres tall, the most famous kauri tree, Tane Mahuta (Lord of the Forest), has a height of 40 m and a diameter, 1.5 m above ground level, of 5.21 m.

J. C. Butcher, *Numerical methods for ordinary differential equations*, 3rd ed., John Wiley & Sons Ltd (2016).

$\left(\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t}) = \dfrac{1}{\mathrm{t}!} \text{ for all } |\mathrm{t}| \le p\right)$ — order conditions for a method of order p

$$\Updownarrow$$

quadrature order conditions $\boldsymbol{b}\boldsymbol{c}^n = \frac{1}{n+1}$ for $0 \le n < p$
and order conditions of *D-type*

$$\boldsymbol{D}(\mathrm{t})\boldsymbol{\Phi}(\mathrm{t}') = 0 \text{ for all rooted trees t and t}' \text{ such that } |\mathrm{t}| + |\mathrm{t}'| \le p$$

$$\boldsymbol{d}_0 = \boldsymbol{b}\boldsymbol{A} - \boldsymbol{b}.(\boldsymbol{1} - \boldsymbol{c}) = \boldsymbol{0} \qquad \big(d_{0,s} = b_s(c_s - 1) = 0\big) \Longrightarrow (c_s = 1)$$

6-points Lobatto quadrature:

$$\int_0^1 \mathrm{d}\theta\, f(\theta) \approx \sum_{k=1}^{6} w_k f(\theta_k), \qquad \alpha, \beta = \sqrt{\tfrac{1}{21}(7 \pm 2\sqrt{7})}$$

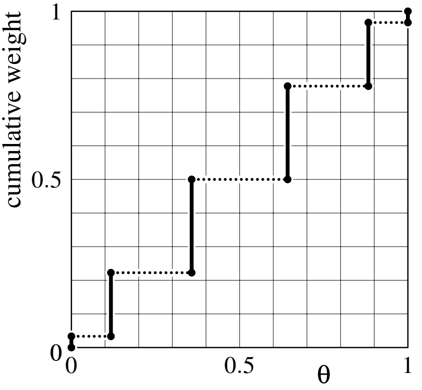
$$\theta_1 = 0, \qquad \theta_{2,5} = \tfrac{1}{2}(1 \mp \alpha), \qquad \theta_{3,4} = \tfrac{1}{2}(1 \mp \beta), \qquad \theta_6 = 1$$

$$w_1 = w_6 = \tfrac{1}{30}, \quad w_2 = w_5 = \tfrac{1}{60}(14 - \sqrt{7}), \quad w_3 = w_4 = \tfrac{1}{60}(14 + \sqrt{7})$$

$$\int_0^1 \mathrm{d}\theta\, \theta^n = \sum_{k=1}^{6} w_k \theta_k^n = \frac{1}{n+1} \text{ for } 0 \le n \le 9$$

$$\sum_{k=1}^{6} w_k \theta_k^{10} = \frac{4811}{52920} = \frac{1}{11} + \frac{1}{582120}$$

order of accuracy is 10



node clusters

Definition 1. Let $\mathscr{S} = \{1, 2, ..., s\}$ be the set of all stages. A *node cluster* is a triple $\mathscr{C} = (S, Q, D)$, where S is a non-empty subset of $\mathscr{S}$ such that the nodes corresponding to any two stages i, j in S are identical: $c_i = c_j$; and $Q \subseteq \mathbf{R}^{|S|}$ and $D \subseteq (\mathbf{R}^{|S|})^*$ are subspaces that satisfy the following orthogonality conditions:

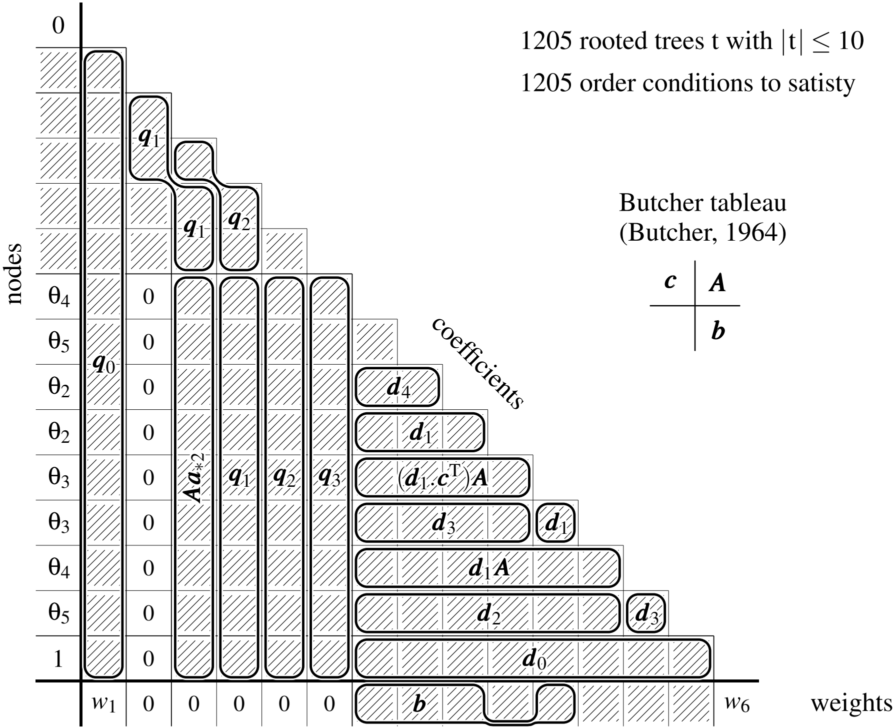
$$Q = \left\{ \boldsymbol{q} \in \mathbf{R}^{|S|} \,\middle|\, \sum_{i \in S} b_i q_i = \sum_{i \in S} d_i q_i = 0 \text{ for all } \boldsymbol{d} \in D \right\}$$
$$D = \left\{ \boldsymbol{d} \in (\mathbf{R}^{|S|})^* \,\middle|\, \sum_{i \in S} d_i = \sum_{i \in S} d_i q_i = 0 \text{ for all } \boldsymbol{q} \in Q \right\}$$

i.e., Q and D are the orthogonal complements of $D + \mathrm{span}(\boldsymbol{b}|_S)$ and $Q + \mathrm{span}(\mathbf{1}|_S)$, respectively. If $\sum_{i \in S} b_i \neq 0$, then $\mathscr{C}$ is said to be a *quadrature cluster*.

Subspaces of $(\mathbf{R}^s)^*$: $D_0 = \{\mathbf{0}\}$, $D_1 = \mathrm{span}(\boldsymbol{d}_0)$, and D_p is generated by D_{p-1}, $D_{p-1}.\boldsymbol{c}$, $D_{p-1}\boldsymbol{A}$, and $\boldsymbol{D}(\mathrm{t})$ for all rooted trees t with $|\mathrm{t}| = p$. For example, if $\boldsymbol{d}_0 = \mathbf{0}$, then $D_2 = \mathrm{span}(\boldsymbol{d}_1)$ and $D_3 = \mathrm{span}\big(\boldsymbol{d}_1, \boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}}, \boldsymbol{d}_1\boldsymbol{A}, \boldsymbol{d}_2, (\boldsymbol{b}.(\boldsymbol{Ac})^{\mathrm{T}})\boldsymbol{A} - \boldsymbol{b}.(\mathbf{1} - \boldsymbol{c}^3)^{\mathrm{T}}/6\big)$. For a method of order p the D-type order conditions could be written as $D_{p-1}\mathbf{1} = \{0\}$.

Definition 2. A node cluster $\mathscr{C} = (S, Q, D)$ is said to be of *cluster order* at least p if $\boldsymbol{Q}(\mathrm{t})$ restricted to S is in the subspace Q for all rooted trees t with $|\mathrm{t}| \leq p$.

Definition 3. A node cluster $\mathscr{C} = (S, Q, D)$ is said to be of *cluster co-order* at least p if for any row vector $\boldsymbol{d}$ in the subspace D_p its restriction to S lies in D.


1205 rooted trees t with |t| ≤ 10
1205 order conditions to satisty
Butcher tableau
(Butcher, 1964)
c
A
b
nodes
0
θ4
θ5
θ2
θ2
θ3
θ3
θ4
θ5
1
coefficients
q0
q1
q1
q2
Aa*2
q1
q2
q3
d4
d1
(d1.cT)A
d3
d1
d1A
d2
d3
d0
b
w1
0
0
0
0
0
w6
weights

To absorb non-zero values of, *e.g.*, $d_{1,14} = w_6 a_{15,14} - b_{14}(1-\theta_5^2)/2 = b_{14}(1-\theta_5)^2/2$, the stages are lumped into node clusters $S_4 = \{7, 13\}$, $S_5 = \{8, 14\}$, $S_2 = \{9, 10\}$, and $S_3 = \{11, 12\}$ of both cluster order and co-order 4.

$$\boldsymbol{d}_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -d_{1,13} & -d_{1,14} & -d_{1,10} & d_{1,10} & -d_{1,12} & d_{1,12} & d_{1,13} & d_{1,14} & 0 \end{bmatrix}$$

$$\boldsymbol{d}_2 = \gamma_{20}\boldsymbol{d}_1 + \gamma_{21}(\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}}), \qquad \boldsymbol{d}_1\boldsymbol{A} = \gamma_{a0}\boldsymbol{d}_1 + \gamma_{a1}(\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}})$$

$$\begin{aligned} \boldsymbol{d}_3 &= \gamma_{30}\boldsymbol{d}_1 + \gamma_{31}(\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}}) + \gamma_{32}(\boldsymbol{d}_1.\boldsymbol{c}^{2\mathrm{T}}) \\ (\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}})\boldsymbol{A} &= \gamma_{c0}\boldsymbol{d}_1 + \gamma_{c1}(\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}}) + \gamma_{c2}(\boldsymbol{d}_1.\boldsymbol{c}^{2\mathrm{T}}) \end{aligned}$$

this requires $c_{11} = c_{12}$

$$\boldsymbol{d}_4 = \gamma_{40}\boldsymbol{d}_1 + \gamma_{41}(\boldsymbol{d}_1.\boldsymbol{c}^{\mathrm{T}}) + \gamma_{42}(\boldsymbol{d}_1.\boldsymbol{c}^{2\mathrm{T}}) + \gamma_{43}(\boldsymbol{d}_1.\boldsymbol{c}^{3\mathrm{T}}) + \gamma_{4c}(\boldsymbol{d}_1.\boldsymbol{c}^{2\mathrm{T}})\boldsymbol{A}$$

this requires $c_9 = c_{10}$

From `jcbutcher.com/p8`:

The first eighth order Runge–Kutta methods

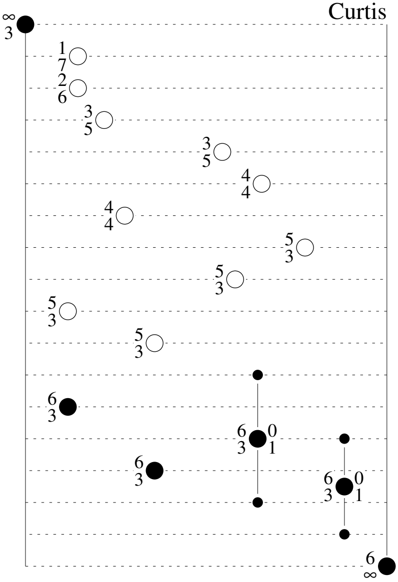
Jim Verner, 2021-10-01

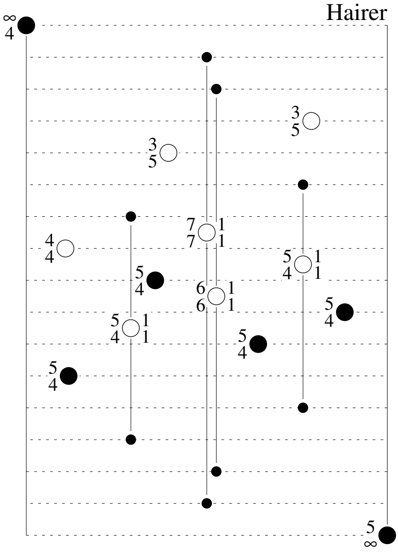
... Accordingly, I wrote an Algol program to solve for the 40 nonzero coefficients, and selected a few sequences of the nodes to determine values of the remaining constraint. Unfortunately, no sequence of the nodes that I chose led to the hoped-for result. (Because each test required overnight computing, there was insufficient time to test all possible sequencings of the nodes before Graeme was to return.)

I explained to Graeme in detail what I had discovered. He was pleased with the fact that there had been some progress, and suggested that I return the next day after he had reviewed my results in detail. I had told him all of the possible distributions of the nodes, and of the few selections I had made and tested although none of the particular sequences of nodes I had selected for testing satisfied all 200 order conditions.

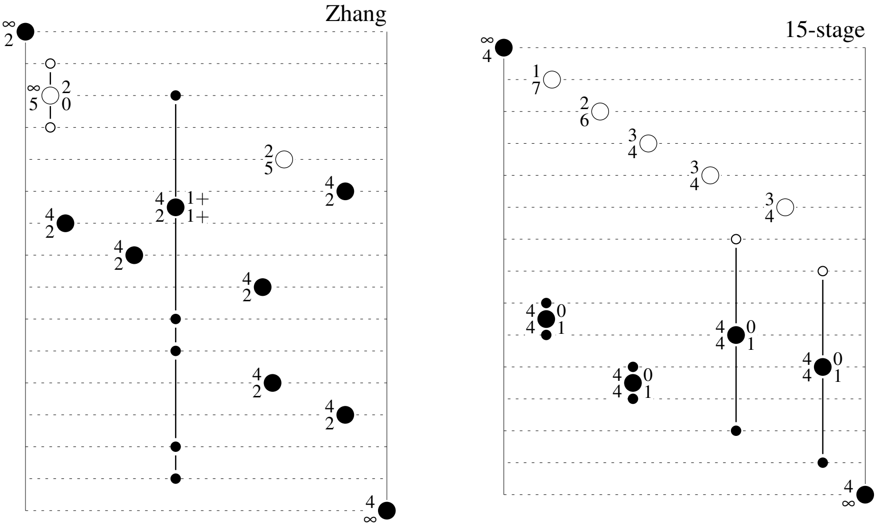
The next day, he observed to me that of the trial choices I had made, each pair of adjacent nodes was distinct, and suggested I resequence the nodes so that up to three adjacent pairs were equal. He suggested that, should some such choice lead to the anticipated result, he would invite me to the Club to share a pint. It is very likely you can guess what happened next! Indeed — that pint showed me that the completion of my program was in sight. Graeme's suggestion did lead to a method of order 8. ...

node cluster structures





node cluster structures



	s	$10^6 \times T_{11}$	$10^6 \times T_{12}$	$10^6 \times T_{13}$	$\max_{ij}\lvert a_{ij}\rvert$	$\min_j b_j$
Curtis	18	3.50...	8.14...	13.06...	5.4724...	0.03333...
Hairer	17	5.27...	17.22...	36.01...	1.0549...	−0.18
Ōno	17	1.25...	3.01...	4.71...	1.3763...	−0.17892...
Feagin	17	21.89...	64.01...	113.71...	5.7842...	−0.05
Zhang	16	1.42...	21.70...	37.89...	4.9406...	−1.19177...
15-stage	15	3.49...	8.48...	14.07...	2.2415...	0.03333...

	z_R	$\tilde{x}(\pi/2)$	$\tilde{y}(\pi/2)$	$\tilde{x}(\pi/2)$	$\tilde{y}(\pi/2)$
Curtis	−3.8269...	−0.00001559...	1.0000226...	0.000093...	1.000561...
Hairer	−2.7046...	−0.00071183...	1.0004307...	0.011791...	1.007904...
Ōno	−3.3815...	−0.00006422...	1.0000264...	0.000151...	1.000116...
Feagin	−2.5279...	−0.00091244...	1.0007372...	−0.004805...	0.996073...
Zhang	−4.7240...	−0.00000464...	1.0000090...	−0.004199...	0.997594...
15-stage	−4.4293...	−0.00000074...	1.0000335...	0.000203...	1.000054...

error coefficients $T_p^2 = \sum_{\mathrm{t},\, |\mathrm{t}|=p} \frac{1}{\sigma^2(\mathrm{t})} \left(\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t}) - \frac{1}{\mathrm{t}!} \right)^2$

$\sigma(\mathrm{t})$ is the order of the symmetry group of the tree t

interval of absolute stability $[z_R, 0] \subseteq \left\{ z \,\middle|\, z \in \mathbf{R} \text{ and } |R(z)| \le 1 \right\}$

$R(z) = 1 + \sum_{n=0}^{s-1} z^{n+1} \boldsymbol{b}\boldsymbol{A}^n \mathbf{1}$ is the stability function

	s	$10^6 \times T_{11}$	$10^6 \times T_{12}$	$10^6 \times T_{13}$	$\max_{ij} \lvert a_{ij} \rvert$	$\min_j b_j$
Curtis	18	3.50...	8.14...	13.06...	5.4724...	0.03333...
Hairer	17	5.27...	17.22...	36.01...	1.0549...	−0.18
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Feagin	17	21.89...	64.01...	113.71...	5.7842...	−0.05
Zhang	16	1.42...	21.70...	37.89...	4.9406...	−1.19177...
15-stage	15	3.49...	8.48...	14.07...	2.2415...	0.03333...

	z_R	$\tilde{x}(\pi/2)$	$\tilde{y}(\pi/2)$	$\tilde{x}(\pi/2)$	$\tilde{y}(\pi/2)$
Curtis	−3.8269...	−0.00001559...	1.0000226...	0.000093...	1.000561...
Hairer	−2.7046...	−0.00071183...	1.0004307...	0.011791...	1.007904...
Ōno	−3.3815...	−0.00006422...	1.0000264...	0.000151...	1.000116...
Feagin	−2.5279...	−0.00091244...	1.0007372...	−0.004805...	0.996073...
Zhang	−4.7240...	−0.00000464...	1.0000090...	−0.004199...	0.997594...
15-stage	−4.4293...	−0.00000074...	1.0000335...	0.000203...	1.000054...

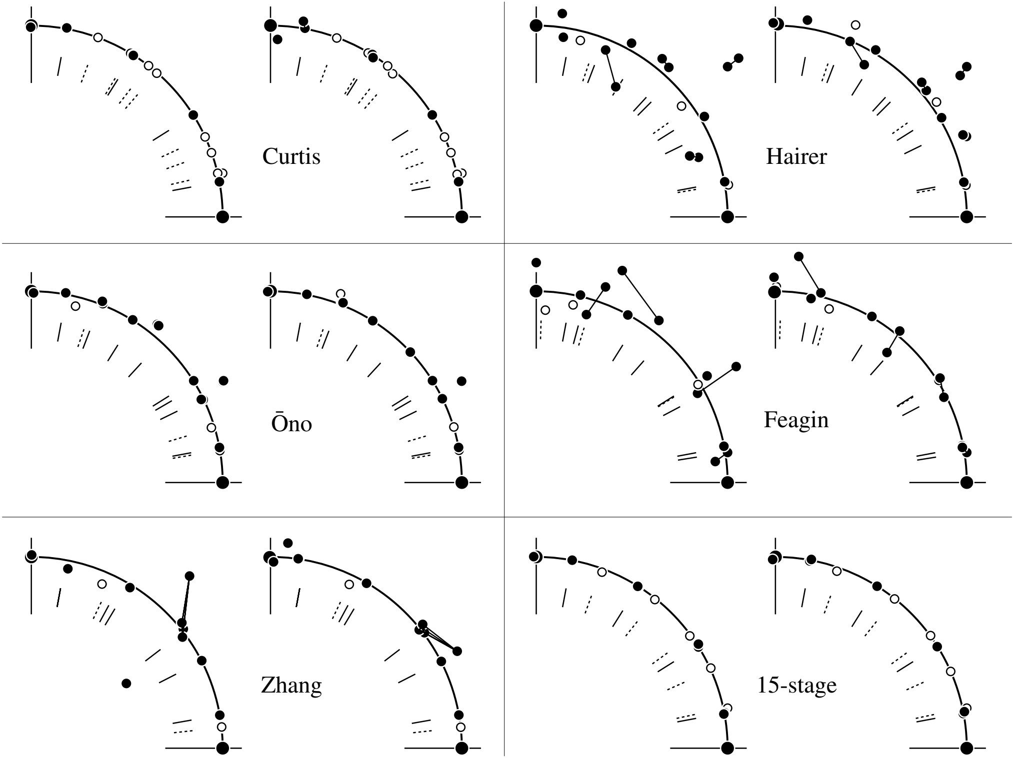
initial condition:
$x(0) = 1,\ y(0) = 0$

$$\begin{cases} \mathrm{d}x/\mathrm{d}t = -y \\ \mathrm{d}y/\mathrm{d}t = x \end{cases}$$

$$\begin{cases} \mathrm{d}x/\mathrm{d}t = -y/(x^2+y^2) \\ \mathrm{d}y/\mathrm{d}t = x/(x^2+y^2) \end{cases}$$

exact solution: $x(t) = \cos t,\ y(t) = \sin t$

one step $h = \pi/2$


Curtis
Hairer
Ōno
Feagin
Zhang
15-stage

Conclusions

- It is possible to construct an explicit Runge–Kutta method of order 10 with just 15 stages — an improvement upon 18 (Curtis, 1975), 17 (Hairer, 1978), and 16 (Zhang, 2024) stages.

- The notions of order conditions of D-type, dual method, node clusters, and cluster order and co-order, could simplify the future construction of [high order] explicit Runge–Kutta methods.

- I still do not completely understand why $c_9 = c_{10}$ and $c_{11} = c_{12}$ help to satisfy order conditions, but it was very convenient as it allowed for the so much needed repetition of nodes to form node clusters.

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