Eight-stage pseudo-symplectic Runge–Kutta methods of order (4, 8)

Misha Stepanov stepanov@math.arizona.edu

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

Abstract

Using simplifying assumptions that are related to the time reversal symmetry, a 1-dimensional family of 8-stage pseudo-symplectic Runge–Kutta methods of order $(4, 8)$ is derived. An example of 7-stage method of order $(4, 9)$ is given.

Keywords: pseudo-symplectic Runge–Kutta methods

MSC Classification: 65L05 , 65L06

For the system $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{f}(t, \boldsymbol{x})$, in order to propagate by the step size h and update the position, $\boldsymbol{x}(t) \mapsto \tilde{\boldsymbol{x}}(t+h)$, where $\tilde{\boldsymbol{x}}(t+h)$ is a numerical approximation to the exact solution $\boldsymbol{x}(t+h)$, an s-stage Runge–Kutta method (which is determined by the coefficients a_{ij}, weights b_j, and nodes c_i) would form the following system of equations for $\boldsymbol{X}_1, \boldsymbol{X}_2, ..., \boldsymbol{X}_s$:

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

solve it, and then compute $\tilde{\boldsymbol{x}}(t+h) = \boldsymbol{x}(t) + h \sum_{j=1}^{s} b_j \boldsymbol{F}_j$. It is natural and will be assumed that $\sum_{j=1}^{s} a_{ij} = c_i$ for all i.

Unless a Hamiltonian is of a special type, *e.g.*, is separable: $\mathcal{H}(\boldsymbol{p}, \boldsymbol{x}) = T(\boldsymbol{p}) + U(\boldsymbol{x})$, where $\boldsymbol{x}$ and $\boldsymbol{p}$ are canonical coordinates, symplectic methods are implicit. In (Aubry & Chartier, 1998) the concept of so-called pseudo-symplectic methods was introduced. A method is said to be of pseudo-symplectic order (p, q) if it is of order p, and the symplectic structure is conserved up to the order q. It was shown that methods with $q \geq 2p$ have better Hamiltonian conservation properties (Aubry & Chartier, 1998, thm. 2.6), and an explicit 5-stage pseudo-symplectic Runge–Kutta method of order $(3, 6)$ was constructed (Aubry & Chartier, 1998, fig. 4.1).

There is no 6-stage explicit method of order $(4, 8)$ (Aubry & Chartier, 1998, prop. 4.2), but there are known 6-stage methods of order $(4, 7)$: (Calvo *et al.*, 2010, p. 262) and (Capuano *et al.*, 2017, p. 90).

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.

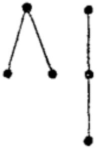
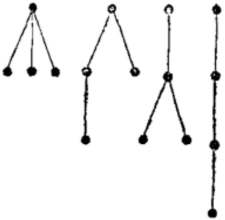
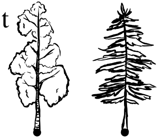
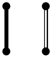


Fig. 3.



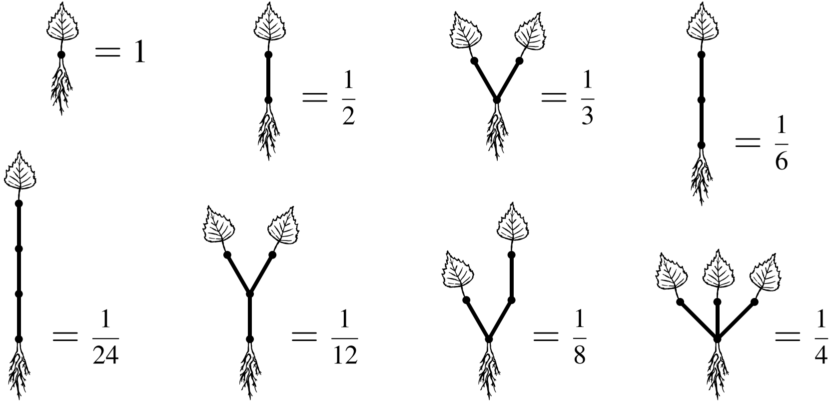
Similarly to (Penrose, 1971) graphical notation, an object that is a tensor of type (m, n) will be depicted by a symbol of the object connected by lines to m and n black dots below and above it, respectively:

	vector $\mathbf{1}$
t 	$\boldsymbol{\Phi}(\bullet) = \mathbf{1}$ and $\boldsymbol{\Phi}\big([\mathrm{t}_1\,\mathrm{t}_2\ldots\mathrm{t}_n]\big) = \prod_{m=1}^{n} \boldsymbol{A}\boldsymbol{\Phi}(\mathrm{t}_m)$ $\boldsymbol{\Phi}(\mathrm{t})$ or an arbitrary vector
	matrix $\boldsymbol{A}$ and identity matrix $\boldsymbol{I}$
	weights row vector $\boldsymbol{b}$
	element-wise product of vectors

Lines coming both from below and from above to a dot produce a tensor contraction, *i.e.*, the summation over the values of the corresponding tensor index. Outer products are obtained by simply drawing objects next to each other (Penrose, 1971, p. 224).

The drawings of a leaf, a root, of trees *Betula pendula* and *Larix sibirica* are by Olga Stepanova, used with permission.

A Runge–Kutta method of order 4 should satisfy the order conditions $\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t}) = 1/\mathrm{t}!$ for all rooted trees t with $|\mathrm{t}| \leq 4$:



or $\boldsymbol{b1} = 1, \boldsymbol{bc} = \frac{1}{2}, \boldsymbol{bc}^2 = \frac{1}{3}, \boldsymbol{bAc} = \frac{1}{6}, \boldsymbol{bc}^3 = \frac{1}{4}, \boldsymbol{b}\big(\boldsymbol{c}.(\boldsymbol{Ac})\big) = \frac{1}{8}, \boldsymbol{bAc}^2 = \frac{1}{12}, \boldsymbol{bA}^2\boldsymbol{c} = \frac{1}{24}$. Here $|\mathrm{t}|$ is the order of tree t, *i.e.*, the number of vertices in t. The factorial t! is recursively defined as $\bullet! = 1$ and if $\mathrm{t} = [\mathrm{t}_1\,\mathrm{t}_2 \dots \mathrm{t}_n]$, then $\mathrm{t}! = |\mathrm{t}| \prod_{m=1}^{n} \big(\mathrm{t}_m\big)!$.

For the system $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{f}(t,\boldsymbol{x})$ its integral form

$$\boldsymbol{x}(t+h) = \boldsymbol{x}(t) + \int_{t}^{t+h} \mathrm{d}t'\, \boldsymbol{f}\big(t', \boldsymbol{x}(t')\big) = \boldsymbol{x}(t) + h\int_{0}^{1} \mathrm{d}\theta\, \boldsymbol{f}\big(t+\theta h, \boldsymbol{x}(t+\theta h)\big)$$

can be interpreted as the application of an idealized Runge–Kutta method with stages being indexed by an interval $[0,1]$ (Plato's Form of a Runge–Kutta method).

In the upper half of the following table:

$\mathbf{1}$	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
$\boldsymbol{A}\boldsymbol{c}^n - \frac{1}{n+1}\boldsymbol{c}^{n+1}$	0
$\boldsymbol{\Phi}(\mathrm{t})$	$\lvert\mathrm{t}\rvert\, \theta^{\lvert\mathrm{t}\rvert-1}/\mathrm{t}!$
$\boldsymbol{b}\boldsymbol{\Phi}(\mathrm{t})$	$1/\mathrm{t}!$

the process/result of the substitution of entries in the left column with what is on the right will be called a *transfiguration*.

For the system $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{f}(t, \boldsymbol{x})$ its integral form

$$\boldsymbol{x}(t+h) = \boldsymbol{x}(t) + \int_{t}^{t+h} \mathrm{d}t' \, \boldsymbol{f}\big(t', \boldsymbol{x}(t')\big) = \boldsymbol{x}(t) + h \int_{0}^{1} \mathrm{d}\theta \, \boldsymbol{f}\big(t+\theta h, \boldsymbol{x}(t+\theta h)\big)$$

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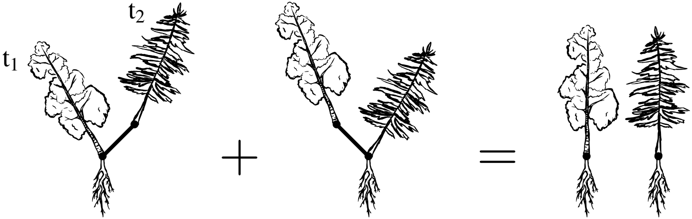
$\boldsymbol{u}.\boldsymbol{v}$	point-wise product $u(\theta)v(\theta)$

The transfiguration of, *e.g.*, the statement $\boldsymbol{bAc}^2 = \frac{1}{12}$ is

$$\begin{array}{ccccccccccc}
\int_0^1 \mathrm{d}\theta & \int_0^\theta \mathrm{d}\theta' & \Big(& \left(\int_0^{\theta'} \mathrm{d}\theta''\right) & . & \left(\int_0^{\theta'} \mathrm{d}\theta'''\right) & \Big) & = & \int_0^1 \mathrm{d}\theta & \int_0^\theta \mathrm{d}\theta' & \theta'^2 = \int_0^1 \mathrm{d}\theta \, \frac{\theta^3}{3} = \frac{1}{12} \\
\boldsymbol{b} & \boldsymbol{A} & (& (\boldsymbol{A}\mathbf{1}) & . & (\boldsymbol{A}\mathbf{1}) &) & = & \boldsymbol{b} & \boldsymbol{A} & \boldsymbol{c}^2
\end{array}$$

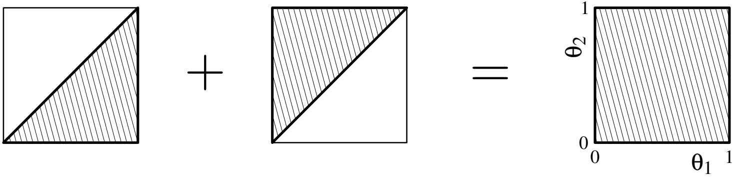
Let $D\big(\mathbf{\Phi}(\mathrm{t}_1), \mathbf{\Phi}(\mathrm{t}_2)\big)$ denote the following property (see (Aubry & Chartier, 1998, eq. (2.5))):



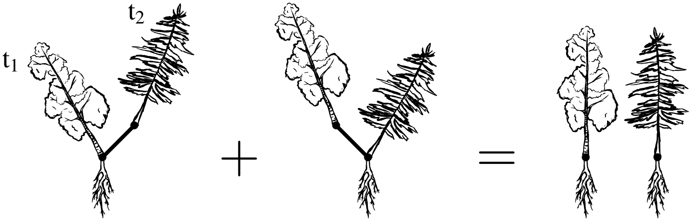
$$\boldsymbol{b}\big(\mathbf{\Phi}(\mathrm{t}_1).\big(\boldsymbol{A}\mathbf{\Phi}(\mathrm{t}_2)\big)\big) + \boldsymbol{b}\big(\big(\boldsymbol{A}\mathbf{\Phi}(\mathrm{t}_1)\big).\mathbf{\Phi}(\mathrm{t}_2)\big) = \big(\boldsymbol{b}\mathbf{\Phi}(\mathrm{t}_1)\big)\big(\boldsymbol{b}\mathbf{\Phi}(\mathrm{t}_2)\big)$$

whose transfiguration or continuous analog $D(u,v)$ would be

$$\int_0^1 \mathrm{d}\theta\, u(\theta) \int_0^\theta \mathrm{d}\theta'\, v(\theta') + \int_0^1 \mathrm{d}\theta \left(\int_0^\theta \mathrm{d}\theta'\, u(\theta')\right) v(\theta) = \left(\int_0^1 \mathrm{d}\theta\, u(\theta)\right)\left(\int_0^1 \mathrm{d}\theta\, v(\theta)\right)$$

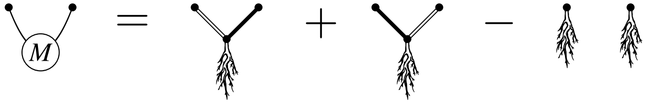


Let $D\big(\boldsymbol{\Phi}(\mathrm{t}_1), \boldsymbol{\Phi}(\mathrm{t}_2)\big)$ denote the following property (see (Aubry & Chartier, 1998, eq. (2.5))):



$$\boldsymbol{b}\big(\boldsymbol{\Phi}(\mathrm{t}_1).\big(\boldsymbol{A\Phi}(\mathrm{t}_2)\big)\big) + \boldsymbol{b}\big(\big(\boldsymbol{A\Phi}(\mathrm{t}_1)\big).\boldsymbol{\Phi}(\mathrm{t}_2)\big) = \big(\boldsymbol{b\Phi}(\mathrm{t}_1)\big)\big(\boldsymbol{b\Phi}(\mathrm{t}_2)\big)$$

Consider the following bilinear form M:

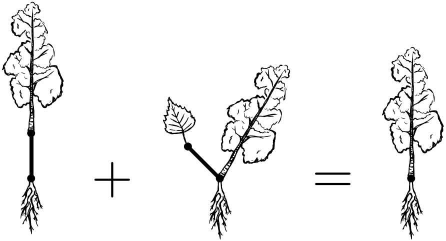


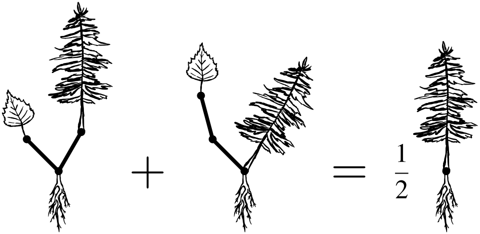
whose matrix $\boldsymbol{M} = \big[m_{ij}\big]$, with $m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$, is symmetric. The property $D(\boldsymbol{u}, \boldsymbol{v})$ can be written as $M(\boldsymbol{u}, \boldsymbol{v}) = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{v} = 0$.

An order p Runge–Kutta method is said to be pseudo-symplectic of order (p, q) if $D\big(\boldsymbol{\Phi}(\mathrm{t}_1), \boldsymbol{\Phi}(\mathrm{t}_2)\big)$ for all trees t_1 and t_2 such that $|\mathrm{t}_1| + |\mathrm{t}_2| \leq q$ (Aubry & Chartier, 1998, cor. 2.2 and eq. (2.7)).

The property $\left(D\left(\mathbf{\Phi}, \boldsymbol{u}\right) \text{ for all } \boldsymbol{u} \in \mathbf{R}^s\right)$ will be shortened as $\boldsymbol{D}\left(\mathbf{\Phi}\right)$ (see (Aubry & Chartier, 1998, def. 3.1)). It is equivalent to the linear form $\boldsymbol{u} \mapsto M\left(\mathbf{\Phi}, \boldsymbol{u}\right)$ being a zero function, or $\boldsymbol{M}\mathbf{\Phi} = \mathbf{0}$. Assuming that $\boldsymbol{b}\mathbf{1} = 1$ and $\boldsymbol{bc} = \frac{1}{2}$, here are the diagrams for $\boldsymbol{D}(\mathbf{1})$ and $\boldsymbol{D}(\boldsymbol{c})$:

$$\boldsymbol{bAu} + \boldsymbol{b}(\boldsymbol{c}.\boldsymbol{u}) = \boldsymbol{bu}$$





$$\boldsymbol{b}\left(\boldsymbol{c}.(\boldsymbol{Au})\right) + \boldsymbol{b}\left((\boldsymbol{Ac}).\boldsymbol{u}\right) = \tfrac{1}{2}\boldsymbol{bu}$$

Let a function $u(\theta)$ be called $[0,1]$-even or $[0,1]$-odd, if $u(1-\theta) = u(\theta)$ or $u(1-\theta) = -u(\theta)$, respectively. The following parity properties are true:

$$\begin{aligned} &\text{if } u(\theta) \text{ is } [0,1]\text{-odd, then } U(\theta) = \textstyle\int_0^\theta d\theta'\, u(\theta') \text{ is } [0,1]\text{-even} \\ &\text{if } u(\theta) \text{ is } [0,1]\text{-even and } \textstyle\int_0^1 d\theta\, u(\theta) = 0, \text{ then } U(\theta) = \textstyle\int_0^\theta d\theta'\, u(\theta') \text{ is } [0,1]\text{-odd} \end{aligned} \qquad (1)$$

A pseudo-symplectic Runge–Kutta method of order $(4,8)$ will be searched for within 8-stage explicit methods with $c_4 = c_5 = \frac{1}{2}$, $c_6 = 1 - c_3$, $c_7 = 1 - c_2$, $c_8 = 1$, $b_6 = b_3$, $b_7 = b_2$, and $b_8 = b_1$. Vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ of 8 components are going to be called "even" and "odd" if $x_6 = x_3$, $x_7 = x_2$, $x_8 = x_1$, and $y_1 + y_8 = y_2 + y_7 = y_3 + y_6 = y_4 = y_5 = 0$, respectively. Let $\boldsymbol{p}_1 = 2\boldsymbol{c} - \mathbf{1}$, $\boldsymbol{p}_2 = 6\boldsymbol{c}^2 - 6\boldsymbol{c} + \mathbf{1}$, and $\boldsymbol{p}_3 = 20\boldsymbol{c}^3 - 30\boldsymbol{c}^2 + 12\boldsymbol{c} - \mathbf{1}$ be the analogs of shifted Legendre polynonials, orthogonal on $[0,1]$. The vectors $\mathbf{1}$, $\boldsymbol{b}^{\mathrm{T}}$, and $\boldsymbol{p}_2$ are "even"; while $\boldsymbol{p}_1$ and $\boldsymbol{p}_3$ are "odd". With such a definition of "even" and "odd" vectors, the eq. (1) could be viewed as the transfiguration of the statements

$$\begin{aligned} &\text{if } \boldsymbol{u} \text{ is "odd", then } \boldsymbol{A}\boldsymbol{u} \text{ is "even"} \\ &\text{if } \boldsymbol{u} \text{ is "even" and } \boldsymbol{b}\boldsymbol{u} = 0, \text{ then } \boldsymbol{A}\boldsymbol{u} \text{ is "odd"} \end{aligned}$$

To imitate these parity properties, it will be demanded that $\boldsymbol{A}\boldsymbol{p}_1$ is "even" (this implies that the vector $\boldsymbol{q}_1 = \boldsymbol{A}\boldsymbol{c} - \frac{1}{2}\boldsymbol{c}^2 = \frac{1}{2}\boldsymbol{A}\boldsymbol{p}_1 + \frac{1}{2}\boldsymbol{c}(\mathbf{1} - \boldsymbol{c})$ is "even" too), and that $\boldsymbol{A}\boldsymbol{p}_2$ and $\boldsymbol{A}\boldsymbol{q}_1$ are "odd". Also the properties $\boldsymbol{D}(\mathbf{1})$ and $\boldsymbol{D}(\boldsymbol{c})$ will be assumed.

Let a function $u(\theta)$ be called $[0,1]$-even or $[0,1]$-odd, if $u(1-\theta) = u(\theta)$ or $u(1-\theta) = -u(\theta)$, respectively. The following parity properties are true:

$$\begin{array}{l} \text{if } u(\theta) \text{ is } [0,1]\text{-odd, then } U(\theta) = \int_0^\theta \mathrm{d}\theta'\, u(\theta') \text{ is } [0,1]\text{-even} \\ \text{if } u(\theta) \text{ is } [0,1]\text{-even and } \int_0^1 \mathrm{d}\theta\, u(\theta) = 0, \text{ then } U(\theta) = \int_0^\theta \mathrm{d}\theta'\, u(\theta') \text{ is } [0,1]\text{-odd} \end{array} \tag{1}$$

0								
c_2	c_2							
c_3	a_{31}	a_{32}						
c_4	a_{41}	a_{42}	a_{43}					
c_5	a_{51}	a_{52}	a_{53}	a_{54}				
c_6	a_{61}	a_{62}	a_{63}	a_{64}	a_{65}			
c_7	a_{71}	a_{72}	a_{73}	a_{74}	a_{75}	a_{76}		
c_8	a_{81}	a_{82}	a_{83}	a_{84}	a_{85}	a_{86}	a_{87}	
	b_1	b_2	b_3	b_4	b_5	b_6	b_7	b_8

Let a function $u(\theta)$ be called $[0,1]$-even or $[0,1]$-odd, if $u(1-\theta)=u(\theta)$ or $u(1-\theta)=-u(\theta)$, respectively. The following parity properties are true:

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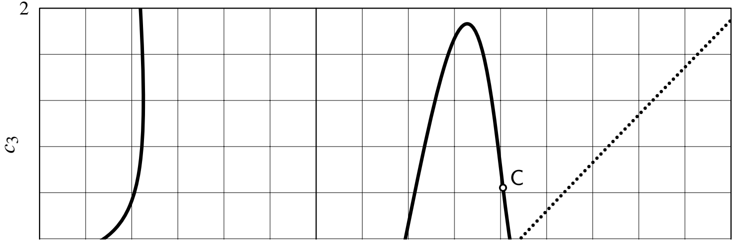
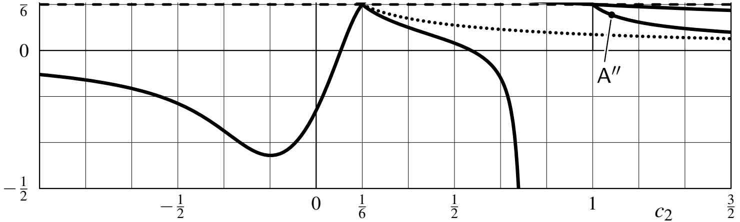
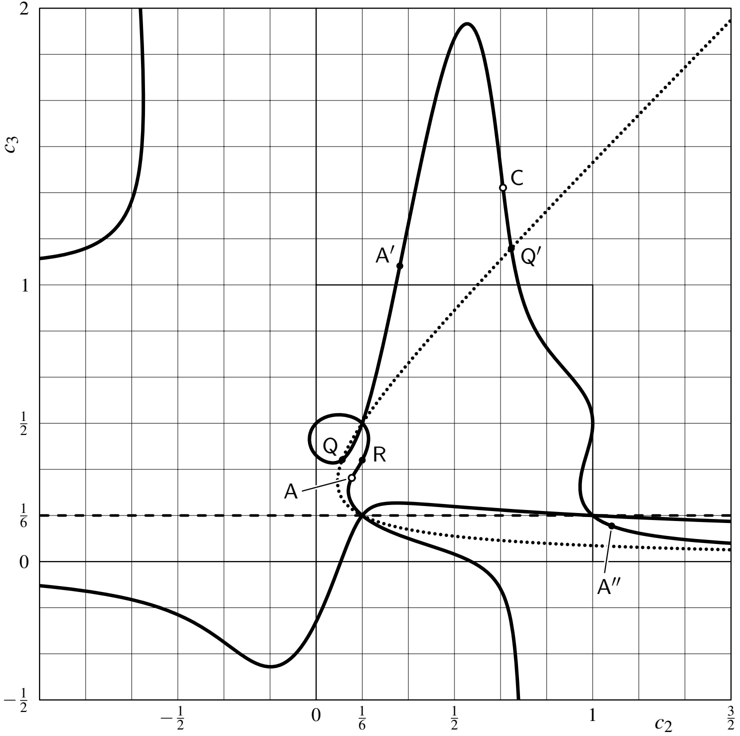
$$\begin{array}{c|cccccccc}
0 & & & & & & & & \\
c_2 & c_2 & & & & & & & \\
c_3 & a_{31} & a_{32} & & & & & & \\
\frac{1}{2} & a_{41} & a_{42} & a_{43} & & & & & \\
\frac{1}{2} & a_{51} & a_{52} & a_{53} & a_{54} & & & & \\
1-c_3 & a_{31} & a_{32} & 0 & a_{64} & a_{65} & & & \\
1-c_2 & c_2 & 0 & a_{32}\frac{b_3}{b_2} & a_{74} & a_{75} & a_{32}\frac{b_3}{b_2} & & \\
1 & 0 & c_2\frac{b_2}{b_1} & a_{31}\frac{b_3}{b_1} & a_{84} & a_{85} & a_{31}\frac{b_3}{b_1} & c_2\frac{b_2}{b_1} & \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_5 & b_3 & b_2 & b_1
\end{array}$$



$$\zeta(c_2, c_3) = \sum_{m,n} \zeta_{mn}\, c_2^m (2c_3)^n = 0$$

ζ_{mn}	$m=0$	$m=1$	2	3	4
5	9	−9			
4	−21	−15	−108	216	
3	15	75	294	−576	
2	−1	−93	−198	396	72
$n=1$	−3	53	18	−132	
$n=0$	1	−13	20		




2
1
$\frac{1}{2}$
$\frac{1}{6}$
0
$-\frac{1}{2}$
c_3
$-\frac{1}{2}$
0
$\frac{1}{6}$
$\frac{1}{2}$
1
$\frac{3}{2}$
c_2
C
A′
Q′
Q
R
A
A″

At the point $(c_2, c_3) = \mathsf{C} = (2\gamma, 4\gamma)$, where $\gamma = \left(2 + 2^{1/3} + 2^{-1/3}\right)/12 = 1/4(2 - 2^{1/3}) = 0.33780...$ the method becomes equivalent to

$$\begin{array}{c|ccccccc}
0 & & & & & & & \\
2\gamma & 2\gamma & & & & & & \\
4\gamma & 0 & 4\gamma & & & & & \\
\frac{1}{2} & 2\gamma & 0 & \frac{1}{2}-2\gamma & & & & \\
1-4\gamma & 0 & 4\gamma & 0 & 1-8\gamma & & & \\
1-2\gamma & 2\gamma & 0 & \frac{1}{2}-2\gamma & 0 & \frac{1}{2}-2\gamma & & \\
1 & 0 & 4\gamma & 0 & 1-8\gamma & 0 & 4\gamma & \\
\hline
 & \gamma & 2\gamma & \frac{1}{4}-\gamma & \frac{1}{2}-4\gamma & \frac{1}{4}-\gamma & 2\gamma & \gamma
\end{array} \tag{2}$$

This 7-stage pseudo-symplectic Runge–Kutta method of order $(4, 9)$ is strongly connected to a well-known explicit symplectic method for separated Hamiltonians (Forest & Ruth, 1990, eqs. (4.9) and (4.12)), (Yoshida, 1990, eq. (2.11)).

1-dimensional family of 8-stage pseudo-symplectic Runge–Kutta methods of order (4, 8) indexed by a parameter ψ:

$$
\begin{array}{c|cccccccc}
0 & & & & & & & & \\
c_2 & c_2 & & & & & & & \\
c_3 & 0 & c_3 & & & & & & \\
\frac{1}{2} & \frac{1}{2}-c_2 & c_2+c_3-1 & 1-c_3 & & & & & \\
\frac{1}{2} & a_{51} & a_{52} & a_{53} & a_{54} & & & & \\
1-c_3 & 0 & c_3 & 0 & a_{64} & a_{65} & & & \\
1-c_2 & c_2 & 0 & \frac{1}{2}-2c_2 & a_{74} & a_{75} & \frac{1}{2}-2c_2 & & \\
1 & 0 & c_3 & 0 & a_{64} & a_{65} & 0 & c_3 & \\
\hline
 & \frac{1}{2}c_2 & \frac{1}{2}c_3 & \frac{1}{4}-c_2 & b_4 & b_5 & \frac{1}{4}-c_2 & \frac{1}{2}c_3 & \frac{1}{2}c_2
\end{array}
$$

$$
\begin{bmatrix} \boldsymbol{a}_{4*} \\ \boldsymbol{a}_{5*} \end{bmatrix} = \begin{bmatrix} \varphi c_2 & (1-\varphi)c_3 & \varphi(\frac{1}{2}-2c_2) & \varphi c_2+(1-\varphi)(\frac{1}{2}-c_3) & 0 & 0 & 0 & 0 \\ \psi c_2 & (1-\psi)c_3 & \psi(\frac{1}{2}-2c_2) & \psi c_2+(1-\psi)(\frac{1}{2}-c_3) & 0 & 0 & 0 & 0 \end{bmatrix}
$$

$$
\begin{bmatrix} a_{64} & a_{65} \\ a_{74} & a_{75} \\ b_4 & b_5 \end{bmatrix} = \begin{bmatrix} 2(\frac{1}{2}-c_3)(1-\chi) & 2(\frac{1}{2}-c_3)\chi \\ 2c_2(1+\chi) & -2c_2\chi \\ \frac{1}{2}(a_{64}+a_{74}) & \frac{1}{2}(a_{65}+a_{75}) \end{bmatrix}, \qquad \chi = \frac{4(1-3c_2)}{(1-6c_2)(\varphi-\psi)}
$$

$$
c_2(c_2-\tfrac{1}{2})(c_2-1) = \tfrac{1}{24},\ c_3 = c_2(1-c_2)/(\tfrac{1}{2}-c_2) = 1/6(1-2c_2)^2,\ \varphi = 1/2c_2-1
$$

Maximizing b_5 but keeping $b_4 \geq 0$ leads to $b_4 = 0$, $\psi = 2c_3$:

$$
\begin{array}{c|cccccccc}
0 & & & & & & & & \\
c_2 & c_2 & & & & & & & \\
c_3 & 0 & c_3 & & & & & & \\
\frac{1}{2} & \frac{1}{2}-c_2 & c_2+c_3-1 & 1-c_3 & & & & & \\
\frac{1}{2} & 2c_2c_3 & (1-2c_3)c_3 & (1-4c_2)c_3 & 4c_2c_3 & & & & \\
1-c_3 & 0 & c_3 & 0 & 4c_2-2 & \frac{1}{2c_2}-2 & & & \\
1-c_2 & c_2 & 0 & \frac{1}{2}-2c_2 & 2-4c_2 & 6c_2-2 & \frac{1}{2}-2c_2 & & \\
1 & 0 & c_3 & 0 & 4c_2-2 & \frac{1}{2c_2}-2 & 0 & c_3 & \\
\hline
 & \frac{1}{2}c_2 & \frac{1}{2}c_3 & \frac{1}{4}-c_2 & 0 & \frac{1}{2}+c_2-c_3 & \frac{1}{4}-c_2 & \frac{1}{2}c_3 & \frac{1}{2}c_2
\end{array}
\qquad
\begin{array}{l}
c_2 = \frac{1}{2} - \frac{1}{\sqrt{3}}\sin\left(\frac{2\pi}{9}\right) \\
c_3 = \frac{1}{2} - \frac{1}{\sqrt{3}}\sin\left(\frac{\pi}{9}\right)
\end{array}
\tag{3}
$$

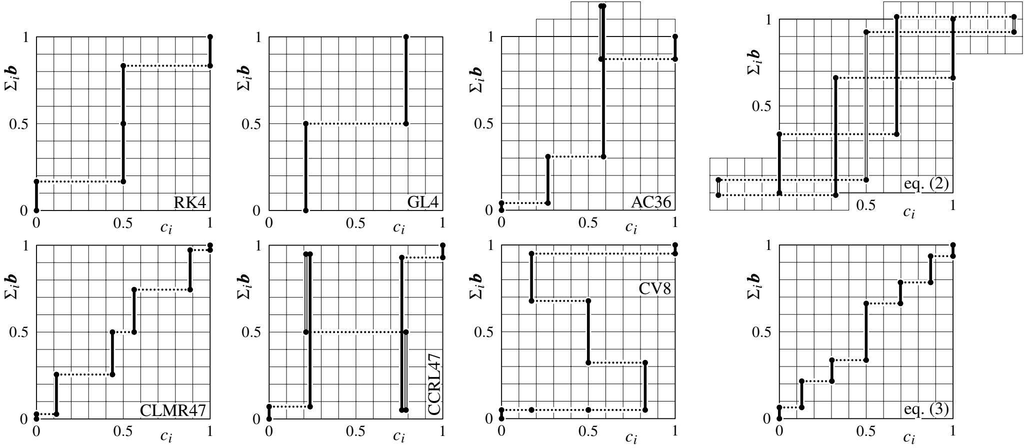
$c_2^2 = -\frac{1}{12} + \frac{7}{6}c_2 - \frac{1}{6}c_3$, $c_2c_3 = -\frac{1}{12} + \frac{1}{6}c_2 + \frac{1}{3}c_3$, $c_3^2 = -\frac{1}{3} + \frac{1}{6}c_2 + \frac{4}{3}c_3$

$a_{65} = a_{85} = 1/2c_2 - 2 = \varphi - 1 = 3 - 4c_2 - 2c_3$

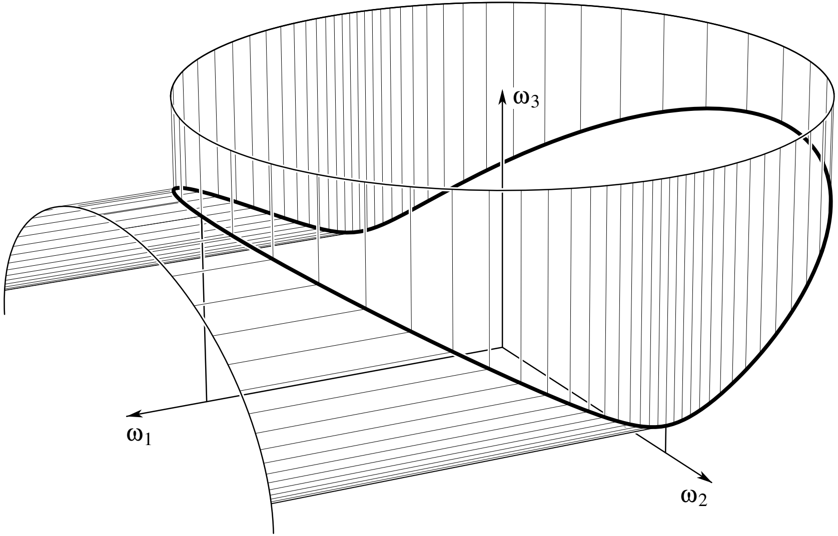
	s	p	q	$10^4 \times T_4$	$10^3 \times T_5$	$10^3 \times T_6$	$R(z)R(-z) - 1$
RK4	4	4	4	0	14.504...	16.035...	0.01388888... z^6
AC36	5	3	6	7.5690...	2.3451...	3.9611...	−0.00057870... z^8
CLMR47	6	4	7	0	0.29185...	0.39787...	0.00024760... z^8
CCRL47	6	4	7	0	1.4813...	1.6278...	−0.00030365... z^8
eq. (2)	7	4	9	0	112.99...	132.54...	−0.00144678... z^{10}
eq. (3)	8	4	8	0	0.64048...	0.91796...	0.00000950... z^{10}
CV8	11	8	8	0	0	0	0.00000627... z^{10}
GL4	2	4	∞	0	4.3306...	5.6178...	0

	$C(2)$	$\boldsymbol{D}(\mathbf{1})$	$\boldsymbol{D}(\boldsymbol{c})$	$\boldsymbol{D}(\boldsymbol{c}^2)$	$\boldsymbol{D}(\boldsymbol{Ac})$	$\max_{ij}\lvert a_{ij}\rvert$	$\min_j b_j$
RK4	F	T	F	F	F	1	0.1666...
AC36	F	T	T	F	F	2.1621...	−0.3054...
CLMR47	F	T	T	T	T	4.4309...	0.0277...
CCRL47	F	T	T	T	T	2.9265...	−0.4488...
eq. (2)	F	T	T	T	T	1.7024...	−0.8512...
eq. (3)	F	T	T	T	T	1.8793...	0.0644...
CV8	T	T	F	F	F	14.728...	0.05
GL4	T	T	T	T	T	0.5386...	0.5

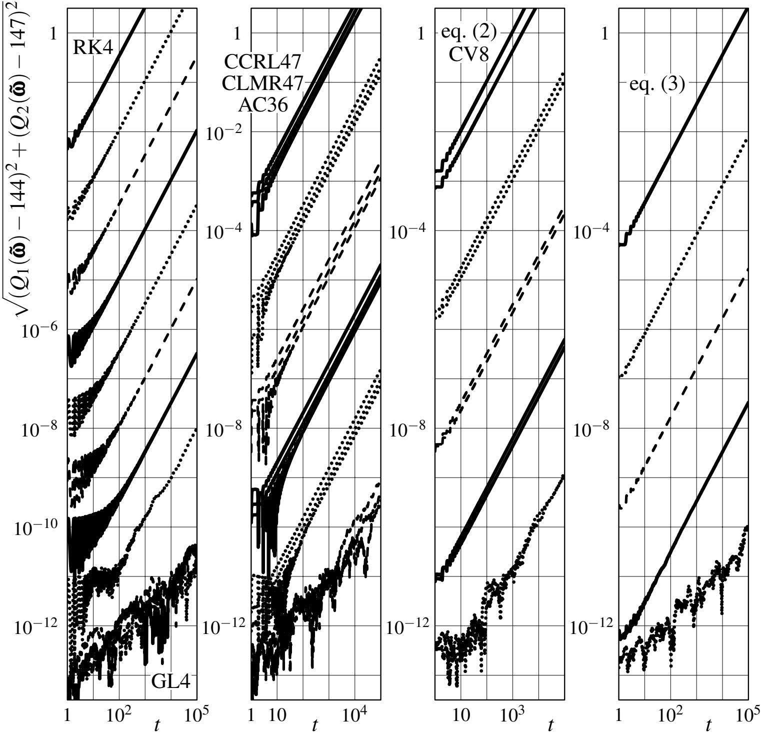
Table 1 A comparison of eight s-stage Runge–Kutta methods of order (p, q). Error coefficients are defined as $T_p^2 = \sum_{\mathrm{t},\,|\mathrm{t}|=p} \big(\boldsymbol{b\Phi}(\mathrm{t}) - 1/\mathrm{t}!\big)^2/\sigma^2(\mathrm{t}) = (1/p!)^2 \sum_{\mathrm{t},\,|\mathrm{t}|=p} \alpha^2(t)\big(\mathrm{t}!\,\boldsymbol{b\Phi}(\mathrm{t}) - 1\big)^2$, where $\sigma(\mathrm{t})$ is the order of the symmetry group of the tree t, and $\alpha(\mathrm{t})$ is the number of monotonic labelings of t.
The $R(z)R(-z) - 1$ column shows the first non-zero term in its Taylor expansion about $z = 0$.
The $\min_j b_j$ column shows the minimal value of a non-zero weight.



Quadrature scheme graphical depiction for the eight methods listed in Table 1. Here $\Sigma_i \boldsymbol{b} = \sum_{j=1}^{i} b_j$, where $1 \le i \le s$, are the cumulative weights, with $\Sigma_0 \boldsymbol{b} = 0$. Due to the order condition $\boldsymbol{b}\mathbf{1} = 1$ for an s-stage method one has $\Sigma_s \boldsymbol{b} = 1$. On the diagram the points $\left(c_i, \Sigma_{i-1} \boldsymbol{b}\right)$ and $\left(c_i, \Sigma_i \boldsymbol{b}\right)$, where $1 \le i \le s$, are connected by a thick line (with white filling if $\Sigma_i \boldsymbol{b} < \Sigma_{i-1} \boldsymbol{b}$). To easier follow the progression of the stages, the points $\left(c_i, \Sigma_i \boldsymbol{b}\right)$ and $\left(c_{i+1}, \Sigma_i \boldsymbol{b}\right)$, where $1 \le i < s$, are connected by dotted lines.



Euler's equations describing free rotation of a rigid body with principal moments of inertia $I_1 = 1$, $I_2 = 2$, and $I_3 = 3$ are $\mathrm{d}\omega_1/\mathrm{d}t = -\omega_2\omega_3$, $\mathrm{d}\omega_2/\mathrm{d}t = \omega_1\omega_3$, and $\mathrm{d}\omega_3/\mathrm{d}t = -\frac{1}{3}\omega_1\omega_2$. Depicted is the solution $(\omega_1, \omega_2, \omega_3)(t) = (12\,\mathrm{cn}, 12\,\mathrm{sn}, 7\,\mathrm{dn})\big(7t, \frac{48}{49}\big)$, where cn, sn, and dn are the Jacobi elliptic functions. The circular and elliptic cylinders correspond to the quadratic invariants $Q_1(\boldsymbol{\omega}) = \omega_1^2 + \omega_2^2 = 144$ and $Q_2(\boldsymbol{\omega}) = \omega_2^2 + 3\omega_3^2 = 147$, respectively.



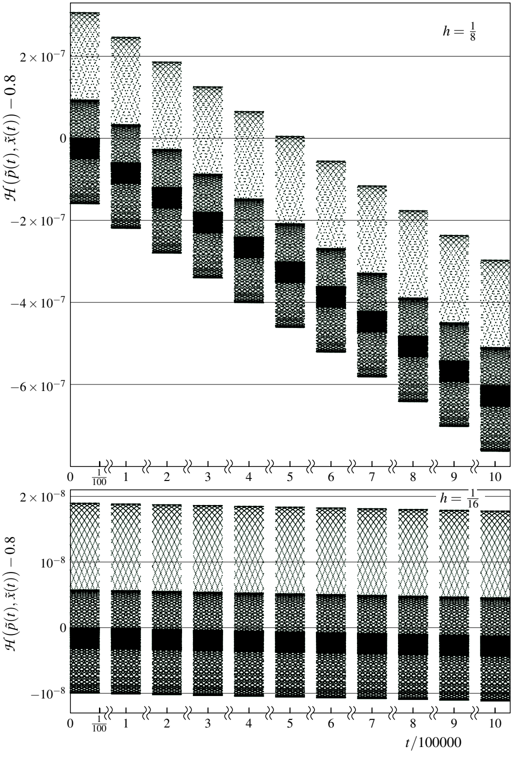
$\sqrt{(Q_1(\tilde{\boldsymbol{\omega}}) - 144)^2 + (Q_2(\tilde{\boldsymbol{\omega}}) - 147)^2}$
RK4
GL4
CCRL47
CLMR47
AC36
eq. (2)
CV8
eq. (3)
1
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
1
10
10^2
10^3
10^4
10^5
t

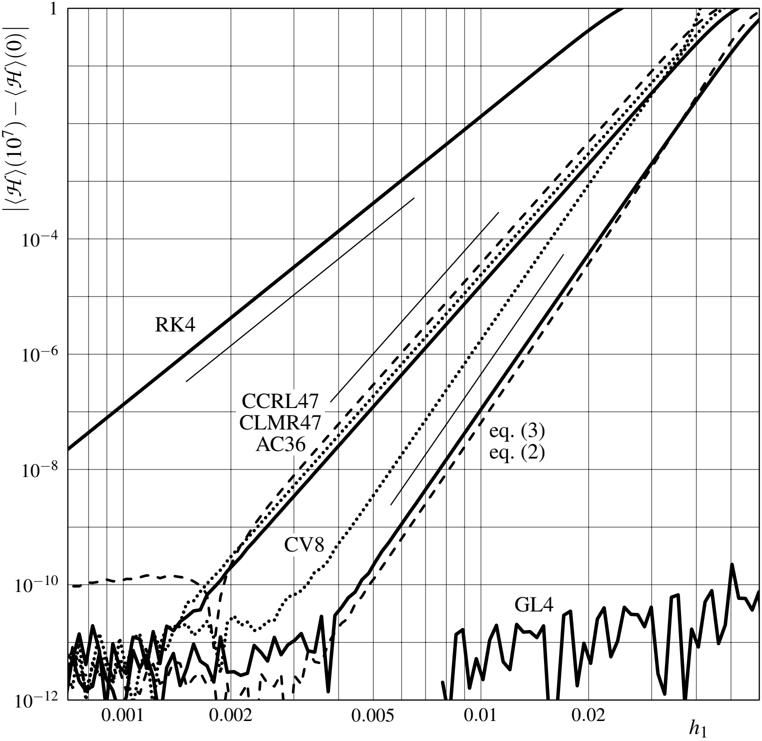
$$\mathrm{d}x/\mathrm{d}t = \partial\mathcal{H}/\partial p$$

$$\mathrm{d}p/\mathrm{d}t = -\partial\mathcal{H}/\partial x$$

$$\mathcal{H}(p,x) = \tfrac{1}{2}p^2 - \left(1 - \tfrac{1}{6}p\right)\cos(x)$$

The solution with initial condition $(x,p)\big|_{t=0} = \big(\arccos(-0.8), 0\big)$ forms a periodic trajectory along the closed level curve $\mathcal{H}(p,x) = 0.8$ around the origin.





$|\langle\mathcal{H}\rangle(10^7) - \langle\mathcal{H}\rangle(0)|$
1
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
0.001
0.002
0.005
0.01
0.02
h_1
RK4
CCRL47
CLMR47
AC36
CV8
eq. (3)
eq. (2)
GL4

Conclusions

- There are known 5- and 6-stage pseudo-symplectic Runge–Kutta methods of order $(3, 6)$ and $(4, 7)$, respectively.
- With 7 stages it is possible to come up with a method of order $(4, 9)$.
- Utilising 8 stages, one can construct robust, with non-negative weights and monotonically increasing nodes, methods of order $(4, 8)$.
- The newly derived methods, largely due to their higher order, have better quadratic invariants and energy preservation properties than previously known pseudo-symplectic methods.

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