A GENERALIZED W-TRANSFORMATION FOR CONSTRUCTING SYMPLECTIC PARTITIONED RUNGE-KUTTA METHODS

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Abstract.

This paper deals with the construction of implicit symplectic partitioned Runge-Kutta methods (PRKM) of high order for separable and general partitioned Hamiltonian systems. The main tool is a generalized W-transformation for PRKM based on different quadrature formulas. Methods of high order and special properties can be determined using the transformed coefficient matrices. Examples are given.

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1 Introduction.

Consider the partitioned system of ordinary differential equations

$$\dot{p} = f(p, q), \qquad \dot{q} = g(p, q), \tag{1.1}$$

where $p = (p_1, ..., p_d)^T$, $q = (q_1, ..., q_d)^T$. Dots represent differentiation with respect to time. This includes the important class of Hamiltonian systems of differential equations, where f and g are given as

$$f = -\frac{\partial H(p, q)}{\partial q}, \qquad g = \frac{\partial H(p, q)}{\partial p} \tag{1.2}$$

with $H(p, q)$ a sufficiently smooth function. A system is called *separable*, if

$$\dot{p} = f(q), \qquad \dot{q} = g(p), \tag{1.3}$$

which means $H(p, q) = T(p) + V(q)$ in the Hamiltonian case.

The most important feature of Hamiltonian systems is their symplecticity property. Numerical integrators conserving this property for each step-size and all Hamiltonian systems are called *symplectic*. Recently there is much interest in the numerical integration of Hamiltonian systems by symplectic methods (c.f. Sanz-Serna [8]). These methods are especially suited for long-time integration. In many applications separable systems appear. In this paper mainly partioned Runge-Kutta methods which are symplectic for separable systems are investigated.

To prepare the following sections the usual simplifying assumptions for Runge-Kutta methods are extended to more general conditions in section 2. In an analogous way to the Runge-Kutta case the order of partitioned Runge-Kutta methods in association with the new simplifying assumptions is studied. By use of these simplifying assumptions a generalization of the W-transformation is stated in section 3. The W-transformation is very useful for characterization and construction of A-stable Runge-Kutta methods (cf. Hairer and Wanner [4]). The standard W-transformation is also practicable to construct symplectic Runge-Kutta type methods (cf. Sun [9], [10]). In a similar way as the matrix W for the W-transformation the two matrices $W^{(1)}$ and $W^{(2)}$ for the generalized W-transformation are constructed. In section 4 the W-transformed matrices $X^{(1)}$ and $X^{(2)}$ of the partitioned Runge-Kutta method are used to construct implicit symplectic partitioned Runge-Kutta methods for separable and partitioned systems. The statements are illustrated by several examples.

2 Simplifying assumptions

A partitioned Runge-Kutta method with s stages is specified by the tableau $(c^{(1)}, A^{(1)}, b^{(1)}; c^{(2)}, A^{(2)}, b^{(2)})$ and applied to system (1.1) reads

$$
\begin{aligned}
p_{n+1} &= p_n + h\sum_{i=1}^{s} b_i^{(1)} f(P_i, Q_i),\\
q_{n+1} &= q_n + h\sum_{i=1}^{s} b_i^{(2)} g(P_i, Q_i),
\end{aligned}
$$

with

$$
\begin{aligned}
P_i &= p_n + h\sum_{j=1}^{s} a_{ij}^{(1)} f(P_j, Q_j), \qquad i = 1, ..., s,\\
Q_i &= q_n + h\sum_{j=1}^{s} a_{ij}^{(2)} g(P_j, Q_j), \qquad i = 1, ..., s.
\end{aligned}
$$

The basic quadrature formulas having s nodes and s weights are given by $(c^{(1)}, b^{(1)})$ and $(c^{(2)}, b^{(2)})$. In the case of a separable system f depends only on Q_i and g depends only on P_i. Using the tableau $(c^{(1)}, A^{(1)}, b^{(1)}; c^{(2)}, A^{(2)}, b^{(2)})$ the following simplifying assumptions are checked easily (cf. Görtz and Scherer [2]).

$$
\begin{aligned}
\hat{B}(p) \quad &: \quad \sum_{i=1}^{s} b_i^{(1)} \left(c_i^{(2)}\right)^{\nu-1} = \sum_{i=1}^{s} b_i^{(2)} \left(c_i^{(1)}\right)^{\nu-1} = \frac{1}{\nu}, \qquad \nu = 1, ..., p, \\
\hat{C}(k) \quad &: \quad \sum_{j=1}^{s} a_{ij}^{(1)} \left(c_j^{(2)}\right)^{\nu-1} = \frac{1}{\nu} \left(c_i^{(1)}\right)^{\nu}, \qquad \nu = 1, ..., k, \quad i = 1, ..., s, \\
&\quad\;\; \sum_{j=1}^{s} a_{ij}^{(2)} \left(c_j^{(1)}\right)^{\nu-1} = \frac{1}{\nu} \left(c_i^{(2)}\right)^{\nu}, \qquad \nu = 1, ..., k, \quad i = 1, ..., s, \\
\hat{D}(l) \quad &: \quad \sum_{i=1}^{s} b_i^{(1)} \left(c_i^{(2)}\right)^{\nu-1} a_{ij}^{(2)} = \frac{1}{\nu} b_j^{(2)} \left(1 - \left(c_j^{(1)}\right)^{\nu}\right), \qquad \nu = 1, ..., l, \; j = 1, ..., s, \\
&\quad\;\; \sum_{i=1}^{s} b_i^{(2)} \left(c_i^{(1)}\right)^{\nu-1} a_{ij}^{(1)} = \frac{1}{\nu} b_j^{(1)} \left(1 - \left(c_j^{(2)}\right)^{\nu}\right), \qquad \nu = 1, ..., l, \; j = 1, ..., s, \\
P \quad &: \quad c_i^{(1)} = c_i^{(2)}, \quad b_i^{(1)} = b_i^{(2)}, \qquad i = 1, ..., s, \\
S \quad &: \quad b_i^{(1)} a_{ij}^{(2)} + b_j^{(2)} a_{ji}^{(1)} - b_i^{(1)} b_j^{(2)} = 0, \qquad i, j = 1, ..., s.
\end{aligned}
$$

These assumptions deliver simple criteria for the order of a partitioned Runge-Kutta method by application to partitioned and to separable systems. The known conditions concerning the coefficients of partitioned Runge-Kutta methods to be symplectic in the separable case (cf. Sanz-Serna [7], Suris [11]) and in the general partitioned case (cf. Sanz-Serna [1], Sanz-Serna [10]) are taken into consideration by the conditions P and S. The results are summarized in the following theorem, which is the starting point for the generalization of the W-Transformation.

THEOREM 2.1. *Assume that a partitioned Runge-Kutta method satisfies simplifying assumptions:*

1. *If $\hat{B}(p)$, $\hat{C}(k)$ and $\hat{D}(l)$ with $p \leq k+l+1$ and $p \leq 2k+2$, then the method has at least order p by application on separable systems.*
2. *If $\hat{B}(p)$, $\hat{C}(k)$, $\hat{D}(l)$and P with $p \leq k+l+1$ and $p \leq 2k+2$, then the method has at least order p by application on general partitioned systems.*
3. *If S, then the method is symplectic by application on separable systems.*
4. *If S and P, then the method is symplectic by application on general partitioned systems.*

To prove the first and second statement graph theory is used in the usual way. The effect of $\hat{C}(k)$ and $\hat{D}(l)$, respectively, on the order conditions represented by trees is checked. The statements follow in the same way as the statement for Runge-Kutta methods (cf. Butcher [5]). Under the given assumptions all trees of order $\leq p$ are equivalent to "bush"-trees of order $\leq p$. The order conditions to these trees are satisfied because of $\hat{B}(p)$.

3 Generalization of the W-transformation.

To construct symplectic partitioned Runge-Kutta methods the W-transformation is slightly generalized (cf. Hairer and Wanner [3], [4]). After some definitions and lemmata the W-transformations

$$X^{(1)} = {W^{(1)}}^T B^{(2)} A^{(1)} W^{(2)}, \qquad X^{(2)} = {W^{(2)}}^T B^{(1)} A^{(2)} W^{(1)}$$

are established. The standard W-transformation for Runge-Kutta methods is a special case of the W-transformation investigated here. The generalized W-transformation is useful to construct partitioned Runge-Kutta methods with special properties for separable and general partitioned systems. The construction of symplectic Runge-Kutta methods (cf. Sun [9]) and partitioned Runge-Kutta methods for general partitoned systems without proof of the order and the same quadrature formula (cf. Sun [10]) are special cases of the generalized W-transformation.

The definitions and the lemmata in the following refer to the usual notations (cf. Hairer and Wanner [3],p. 82 ff.). The $P_j(x)$ denote the Legendre polynomials shifted to the interval $[0, 1]$.

Definition 3.1. *Let $k, l \in \{0, ..., s-1\}$. The matrix W satisfies $T(k, l)$ for the quadrature formula (c,b) if and only if*

$$i) \quad W = (w_{ij})_{i,j=1,\dots,s} \quad \textit{is nonsingular},$$

$$ii) \quad w_{ij} = P_{j-1}(c_i), \qquad i = 1, ..., s, \quad j = 1, ..., \max\{k, l\} + 1,$$

$$iii) \quad W^T B W = \begin{bmatrix} I & 0 \\ 0 & R \end{bmatrix},$$

where I is the $(l+1) \times (l+1)$ identity matrix and R is an arbitrary $(s-l-1) \times (s-l-1)$ matrix, are satisfied.

There are theorems about the existence of such a matrix W (cf. Hairer and Wanner [3]). We repeat the most important for theoretical and practical use.

Lemma 3.1. *Let the quadrature formula (c, b) be of order p. Then there exists a matrix W satisfying $T(k, l)$ if and only if*

$$p \geq k + l + 1, \qquad p \geq 2l + 1, \tag{3.1}$$

and at least max$\{k, l\} + 1$ nodes c_i are distinct.

Lemma 3.2. *If the quadrature formula (c, b) has s distinct nodes c_i and is of order $p \geq s + l$, then*

$$W \quad = \quad (P_{j-1}(c_i))_{i,j=1,\dots,s} \tag{3.2}$$

satisfies $T(k, l)$ with arbitrary $k \in \{0, ..., s-1\}$.

Now the generalized W-transformation for partitioned Runge-Kutta methods is stated.

THEOREM 3.3. *Assume that $W^{(1)}$ and $W^{(2)}$ satisfy $T(k,l)$, $k \le l$, for the quadrature formula $(c^{(1)}, b^{(2)})$ and $(c^{(2)}, b^{(1)})$, respectively, with nonvanishing weights $b_i^{(1)}$ and $b_i^{(2)}$. Then for the s-stage partitioned Runge-Kutta methods $(c^{(1)}, A^{(1)}, b^{(1)}; c^{(2)}, A^{(2)}, b^{(2)})$ with*

$$X^{(1)} = {W^{(1)}}^T B^{(2)} A^{(1)} W^{(2)} \quad \text{and} \quad X^{(2)} = {W^{(2)}}^T B^{(1)} A^{(2)} W^{(1)}$$

it holds

$$\text{a)} \quad \hat{C}(k) \quad \text{equivalent to} \quad \left\{ \begin{array}{lcl} X^{(1)} I_k & = & X_G I_k \\ X^{(2)} I_k & = & X_G I_k \end{array} \right. , \tag{3.3}$$

$$\text{b)} \quad \hat{D}(l) \quad \text{equivalent to} \quad \left\{ \begin{array}{lcl} I_l X^{(1)} & = & I_l X_G \\ I_l X^{(2)} & = & I_l X_G \end{array} \right. , \tag{3.4}$$

$$\text{c)} \quad S \quad \text{equivalent to} \quad X^{(1)} + X^{(2)T} - e_1 e_1^T = 0, \tag{3.5}$$

where

$$I_k = diag(\underbrace{1, ..., 1}_{k}, 0, .., 0), \quad \xi_k = \frac{1}{2\sqrt{4k^2 - 1}}, \quad k = 1, ..., s-1, \quad \text{and}$$

$$X_G = \begin{bmatrix} \frac{1}{2} & -\xi_1 & & & 0 \\ \xi_1 & 0 & -\xi_2 & & \\ & \xi_2 & 0 & \ddots & \\ & & \ddots & \ddots & -\xi_{s-1} \\ 0 & & & \xi_{s-1} & 0 \end{bmatrix}.$$

The conditions $X^{(1)} I_l = X_G I_l$ and $I_l X^{(2)} = I_l X_G$, respectively, state that the first k columns or rows of $X^{(i)}$ are those from X_G.

Proof of Theorem 3.3. $\hat{C}(k)$ can be written in terms of quadrature formulas

$$\sum_{j=1}^{s} a_{ij}^{(q)} p(c_j^{(3-q)}) = \int_0^{c_i^{(q)}} p(x)dx, \quad i = 1, ..., s, \quad q = 1, 2, \quad p \in \mathcal{P}_{k-1}, \tag{3.6}$$

where $\mathcal{P}_{k-1}$ denotes the space of all polynomials with degree $\le k-1$. Inserting the Legendre polynomials P_ν for $\nu = 0, 1, ..., k-1$ instead of $p \in \mathcal{P}_{k-1}$ and using the known integral relations (cf. Hairer and Wanner [3], p.78), it follows

$$\begin{aligned} \sum_{j=1}^{s} a_{ij}^{(q)} P_0(c_j^{(3-q)}) &= \xi_1 P_1(c_i^{(q)}) + \frac{1}{2} P_0(c_i^{(q)}), \qquad i = 1, ..., s, \quad q = 1, 2, \\ \sum_{j=1}^{s} a_{ij}^{(q)} P_\nu(c_j^{(3-q)}) &= \xi_{\nu+1} P_{\nu+1}(c_i^{(q)}) - \xi_\nu P_{\nu-1}(c_i^{(q)}), \qquad \nu = 1, ..., k-1. \end{aligned}$$

Using $T(k,l)$ the previous conditions are given in matrix notation

$$A^{(q)} W^{(3-q)} I_k = W^{(q)} X_G I_k, \quad q = 1, 2.$$

Multiplication with ${W^{(1)}}^T B^{(2)}$ or ${W^{(2)}}^T B^{(1)}$, respectively, yields

$$ {W^{(q)}}^T B^{(3-q)} W^{(q)} {W^{(q)}}^{-1} A^{(q)} W^{(3-q)} I_k \quad = \quad {W^{(q)}}^T B^{(3-q)} W^{(q)} X_G I_k, \quad q = 1, 2. $$

Because of

$$ {W^{(q)}}^T B^{(3-q)} W^{(q)} X_G I_k = X_G I_k, \quad q = 1, 2, $$

statement a) follows.

$\hat{D}(l)$ can be written as $(q = 1, 2)$

$$ \sum_{i=1}^{s} b_i^{(q)} a_{ij}^{(3-q)} P_\nu(c_i^{(3-q)}) \quad = \quad b_j^{(3-q)} \int_{c_j^{(q)}}^{1} P_\nu(x) dx, \quad \nu = 1, ..., l-1, \quad j = 1, ..., s. $$

Using the integral relations it follows $(q = 1, 2)$

$$ \begin{aligned} \sum_{i=1}^{s} b_i^{(q)} a_{ij}^{(3-q)} P_0(c_i^{(3-q)}) \quad &= \quad b_j^{(3-q)} (\frac{1}{2} P_0(c_j^{(q)}) - \xi_1 P_1(c_j^{(q)})), \quad \nu = 1, ..., l-1, \\ \sum_{i=1}^{s} b_i^{(q)} a_{ij}^{(3-q)} P_\nu(c_i^{(3-q)}) \quad &= \quad b_j^{(3-q)} (\xi_\nu P_{\nu-1}(c_j^{(q)}) - \xi_{\nu+1} P_{\nu+1}(c_j^{(q)})), \quad j = 1, ..., s, \end{aligned} $$

or in matrix notation using $T(k, l)$

$$ I_l {W^{(3-q)}}^T B^{(q)} A^{(3-q)} \quad = \quad I_l X_G {W^{(q)}}^T B^{(3-q)}, \quad q = 1, 2. $$

Statement b) follows from multiplication from the right with $W^{(1)}$ or $W^{(2)}$, respectively.

Condition S reads in matrix notation

$$ B^{(1)} A^{(2)} + {A^{(1)}}^T B^{(2)} - b^{(1)} {b^{(2)}}^T = 0. $$

Because of $T(k, l)$ it holds

$$ {W^{(q)}}^T B^{(3-q)} W^{(q)} e_1 = e_1 = {W^{(q)}}^T B^{(3-q)} e, \quad q = 1, 2 $$

with $e_1 = (1, 0, ..., 0)^T$ and $e = (1, ..., 1)^T$. Then using

$$ {W^{(2)}}^T B^{(1)} A^{(2)} W^{(1)} + {W^{(2)}}^T {A^{(1)}}^T B^{(2)} W^{(1)} - {W^{(2)}}^T B^{(1)} e ({W^{(1)}}^T B^{(2)} e)^T = 0, $$

statement c) follows. □

4 Partitioned Runge-Kutta methods

The following theorem immediately offers the tool for constructing symplectic partitioned Runge-Kutta methods of high order for separable and general partitioned systems.

THEOREM 4.1. *Assume that $W^{(1)}$ and $W^{(2)}$ satisfy $T(k,k)$ for the quadrature formula $(c^{(1)}, b^{(2)})$ and $(c^{(2)}, b^{(1)})$ of order p_1 and p_2, respectively, with nonvanishing weights $b_i^{(1)}$ and $b_i^{(2)}$. Choose*

$$X^{(i)} = \begin{bmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & & \ddots & & \\ & \ddots & & -\xi_k & \\ & & \xi_k & \boxed{Q^{(i)}} \end{bmatrix}, \quad i = 1, 2,$$

with ${Q^{(1)}} + {Q^{(2)}}^T = 0$. Then the partitioned Runge-Kutta method specified by the tableau

$$(c^{(1)}, {B^{(2)}}^{-1} {W^{(1)}}^{-T} X^{(1)} {W^{(2)}}^{-1}, b^{(1)}; c^{(2)}, {B^{(1)}}^{-1} {W^{(2)}}^{-T} X^{(2)} {W^{(1)}}^{-1}, b^{(2)})$$

is of order $p = min\{2k+1, p_1, p_2\}$ and is symplectic for separable systems. Further, if $b^{(1)} = b^{(2)}$ and $c^{(1)} = c^{(2)}$, then the method is of order p and is symplectic for general partitioned systems.

In the following examples the construction of methods using Theorem 4.1 is demonstrated.

EXAMPLE 4.1. *With the polynomial M (cf. Hairer and Wanner [3])*

$$M(x) = P_2(x) + \sqrt{\frac{5}{3}} \alpha_i P_1(x), \quad i = 1, 2.$$

Consider the quadrature formulas

$$(c^{(1)}, b^{(2)}) = \left(\begin{array}{c|c} \frac{3-a_1-\alpha_1}{6} & \frac{a_1-\alpha_1}{2a_1} \\ \frac{3+a_1-\alpha_1}{6} & \frac{a_1+\alpha_1}{2a_1} \end{array} \right), \qquad (c^{(2)}, b^{(1)}) = \left(\begin{array}{c|c} \frac{3-a_2-\alpha_2}{6} & \frac{a_2-\alpha_2}{2a_2} \\ \frac{3+a_2-\alpha_2}{6} & \frac{a_2+\alpha_2}{2a_2} \end{array} \right),$$

where $\alpha_1, \alpha_2 \in I\!R$ and $a_i = \sqrt{3 + \alpha_i^2}$, $i = 1, 2$. The W-matrices are

$$W^{(1)} = \begin{bmatrix} 1 & -\frac{a_1+\alpha_1}{\sqrt{3}} \\ 1 & \frac{a_1-\alpha_1}{\sqrt{3}} \end{bmatrix}, \qquad W^{(2)} = \begin{bmatrix} 1 & -\frac{a_2+\alpha_2}{\sqrt{3}} \\ 1 & \frac{a_2-\alpha_2}{\sqrt{3}} \end{bmatrix}.$$

Setting

$$A^{(q)} = {B^{(3-q)}}^{-1} {W^{(q)}}^{-T} X^{(q)} {W^{(3-q)}}^{-1} = W^{(q)} X^{(q)} {W^{(3-q)}}^T B^{(q)}, \quad q = 1, 2$$

with

$$X^{(1)} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} \\ \frac{1}{2\sqrt{3}} & w \end{bmatrix}, \qquad X^{(2)} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} \\ \frac{1}{2\sqrt{3}} & -w \end{bmatrix}, \quad \omega \in \mathbb{R}$$

and using Theorem 4.1 we get symplectic partitioned Runge-Kutta methods at least of order 3. The coefficients are computed to

$$A^{(1)} = \frac{1}{2a_2} \begin{bmatrix} \frac{(3-d_4)d_1}{6} + \frac{1}{2} + wd_4 & \frac{(3-d_4)d_2}{6} - \frac{1}{2} - wd_4 \\ \frac{(3+d_3)d_1}{6} + \frac{1}{2} - wd_3 & \frac{(3+d_3)d_2}{6} - \frac{1}{2} + wd_3 \end{bmatrix},$$

$$A^{(2)} = \frac{1}{2a_1} \begin{bmatrix} \frac{(3-d_2)d_3}{6} + \frac{1}{2} - wd_2 & \frac{(3-d_2)d_4}{6} - \frac{1}{2} + wd_2 \\ \frac{(3+d_1)d_3}{6} + \frac{1}{2} + wd_1 & \frac{(3+d_1)d_4}{6} - \frac{1}{2} - wd_1 \end{bmatrix},$$

where $d_1 = a_2 - \alpha_2$, $d_2 = a_2 + \alpha_2$, $d_3 = a_1 - \alpha_1$ *and* $d_4 = a_1 + \alpha_1$.

Sometimes the order of dispersion is more important than the classical order (cf. van der Houwen and Sommeijer [6]). The dispersion order is the largest p satisfying

$$\Phi(z) = z - \arccos\left(\frac{1}{2}\frac{\Psi_1(z^2) + \Psi_2(z^2)}{\Psi(z^2)}\right) = \mathcal{O}(z^{p+1}) \qquad (z \to 0^+)$$

with

$$\begin{aligned} \Psi_q(z) &= \det(I + zA^{(3-q)}A^{(q)} - zc^{(3-q)}b^{(q)^T}), \\ \Psi(z) &= \det(I + zA^{(3-q)}A^{(q)}), \qquad q = 1, 2. \end{aligned}$$

Using the generalized W-transformation this transforms into:

$$\begin{aligned} \Psi_q(z) &= \det(I + zX^{(3-q)}X^{(q)} - z \begin{bmatrix} \frac{1}{2} \\ \xi_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} e_1^T), \\ \Psi(z) &= \det(I + zX^{(3-q)}X^{(q)}), \qquad q = 1, 2. \end{aligned}$$

Now the symplectic methods of highest order of dispersion can easily be derived. This will be done in more detail in a forthcoming paper. The family above is a two parameter family of methods of the highest dispersion order 6 by choosing $w = \pm\frac{1}{30}\sqrt{15}$. The two-stage Gauss-Runge-Kutta method does not reach order of dispersion 6.

Example 4.2. *Using the Radau quadrature formulas*

$$(c^{(1)}, b^{(2)}) = \left(\begin{array}{c|c} 0 & \frac{1}{9} \\ \frac{6-\sqrt{6}}{10} & \frac{16+\sqrt{6}}{36} \\ \frac{6+\sqrt{6}}{10} & \frac{16-\sqrt{6}}{36} \end{array}\right), \qquad (c^{(2)}, b^{(1)}) = \left(\begin{array}{c|c} \frac{4-\sqrt{6}}{10} & \frac{16-\sqrt{6}}{36} \\ \frac{4+\sqrt{6}}{10} & \frac{16+\sqrt{6}}{36} \\ 1 & \frac{1}{9} \end{array}\right),$$

we get the W-matrices

$$W^{(1)} = \begin{bmatrix} 1 & -\sqrt{3} & \sqrt{5} \\ 1 & a_1 & a_3 \\ 1 & a_2 & a_4 \end{bmatrix}, \qquad W^{(2)} = \begin{bmatrix} 1 & -a_2 & a_4 \\ 1 & -a_1 & a_3 \\ 1 & \sqrt{3} & \sqrt{5} \end{bmatrix},$$

where $a_1 = \frac{\sqrt{3}(1-\sqrt{6})}{5}$, $a_2 = \frac{\sqrt{3}(1+\sqrt{6})}{5}$, $a_3 = \frac{-\sqrt{5}(2+3\sqrt{6})}{25}$ *and* $a_4 = \frac{-\sqrt{5}(2-3\sqrt{6})}{25}$.

Setting

$$A^{(q)} = B^{(3-q)^{-1}} W^{(q)^{-T}} X^{(q)} W^{(3-q)^{-1}} = W^{(q)} X^{(q)} W^{(3-q)^{T}} B^{(q)}, \quad q = 1, 2$$

with

$$X^{(1)} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} & \\ \frac{1}{2\sqrt{3}} & & \frac{-1}{2\sqrt{15}} \\ & \frac{1}{2\sqrt{15}} & w \end{bmatrix}, \qquad X^{(2)} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} & \\ \frac{1}{2\sqrt{3}} & & \frac{-1}{2\sqrt{15}} \\ & \frac{1}{2\sqrt{15}} & -w \end{bmatrix}.$$

Using Theorem 4.1 a symplectic partitioned Runge-Kutta method of order at least 5 for separable systems is deduced. The coefficients are computed to $A^{(1)} = (a_{ij}^{(1)})_{i,j=1,\dots,s}$ *and* $A^{(2)} = (a_{ij}^{(2)})_{i,j=1,\dots,s}$ *with*

$a_{11}^{(1)} = \frac{1}{36}(1+10w)(-1+\sqrt{6})$, $a_{12}^{(1)} = -\frac{1}{36}(1+10w)(1+\sqrt{6})$, $a_{13}^{(1)} = \frac{1+10w}{18}$, $a_{21}^{(1)} = \frac{1}{1800}(-16+\sqrt{6})(-43+20w)$, $a_{22}^{(1)} = \frac{1}{360}(4+\sqrt{6})(47-18\sqrt{6}+20w)$, $a_{23}^{(1)} = -\frac{1}{450}(2+3\sqrt{6})(1+10w)$, $a_{31}^{(1)} = -\frac{1}{360}(\sqrt{6}-4)(47+18\sqrt{6}+20w)$, $a_{32}^{(1)} = -\frac{1}{1800}(16+\sqrt{6})(-43+20w)$, $a_{33}^{(1)} = \frac{1}{450}(-2+3\sqrt{6})(1+10w)$.

and

$a_{11}^{(2)} = -\frac{1}{450}(-2+3\sqrt{6})(-3\sqrt{6}-1+10w)$, $a_{12}^{(2)} = \frac{1}{1800}(16+\sqrt{6})(7+20w)$, $a_{13}^{(2)} = \frac{1}{360}(-4+\sqrt{6})(6\sqrt{6}-11+20w)$, $a_{21}^{(2)} = \frac{1}{450}(2+3\sqrt{6})(3\sqrt{6}-1+10w)$, $a_{22}^{(2)} = -\frac{1}{360}(4+\sqrt{6})(-6\sqrt{6}-11+20w)$, $a_{23}^{(2)} = -\frac{1}{1800}(-16+\sqrt{6})(7+20w)$, $a_{31}^{(2)} = \frac{1}{18}(1-10w)$, $a_{32}^{(2)} = \frac{1}{36}(1+\sqrt{6})(-1+3\sqrt{6}+10w)$, $a_{33}^{(2)} = -\frac{1}{36}(-1+\sqrt{6})(-1-3\sqrt{6}+10w)$.

Conclusion. The generalized W-transformation is especially suitable to construct partitioned Runge-Kutta methods for separable Hamiltonian systems. It will be a useful tool for improving methods like we show in the small example for the order of dispersion. The same can be done to identify the methods that are P-stable or the methods that are not symplectic but are of an higher order of dispersion. Further theorems can be given to construct methods that are not symplectic but are of higher order based on the same transformation for separable systems. The known results for Runge-Kutta methods and partitioned Runge-Kutta methods for general systems with the same quadrature formula are included.

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