

DISCRETE VARIATIONAL METHODS AND SYMPLECTIC GENERALIZED ADDITIVE RUNGE–KUTTA METHODS

ANTONELLA ZANNA[†]

ABSTRACT. We consider a Lagrangian system $L(q, \dot{q}) = \sum_{l=1}^N L^{\{l\}}(q, \dot{q})$, where the q -variable is treated by a Generalized Additive Runge–Kutta (GARK) method. Applying the technique of discrete variations, we show how to construct symplectic schemes. Assuming the diagonal methods for the GARK given, we present some techniques for constructing the transition matrices. We address the problem of the order of the methods and discuss some semi-separable and separable problems, showing some interesting constructions of methods with non-square coefficient matrices.

1. INTRODUCTION

In this paper we are interested in studying a family of variational method that are obtained when considering a system with a Lagrangian

$$L(q, \dot{q}) = \sum_{l=1}^N L^{\{l\}}(q, \dot{q}), \quad q \in \mathbb{R}^d,$$

or a Hamiltonian system, split in elementary Hamiltonian systems,

$$H(q, p) = \sum_{l=1}^N H^{\{l\}}(q, p), \quad q, p \in \mathbb{R}^d,$$

where each term is treated by a different method of Runge–Kutta (RK) type. The idea of treating different terms with different methods is by no means new. Additive Runge–Kutta (ARK) methods were introduced already in the 80's [CS83] to deal with stiff ODEs, where the stiff term would be treated by a different Runge–Kutta method than the non-stiff term, typically using an explicit method for the non-stiff part and an implicit one for the stiff-part. In the mid-90's, these methods were studied in detail from the Hamiltonian viewpoint, and order conditions and conditions for symplecticity were established [AMSS97]. The use of additivity, especially in the context of DAEs was studied in [Jay98], and later in [Tan18], the latter especially in the context of the formalism of Generalized Additive Runge–Kutta (GARK) methods introduced in [SG15].

Parallel to the Hamiltonian approach, there is the Lagrangian approach, popular in the community of computational mechanics [MW01] and optimal control [OBJM11]. In the Lagrangian setting, the action integral is discretized by an appropriate quadrature, the variable is replaced by an appropriate polynomial interpolant and discrete variational equations are derived. As the discrete variational equations are essentially the same as generating functions, the resulting methods are automatically symplectic. Recently, a splitting of the Lagrangian, where each term was treated by a different method, was used in the context of higher order variational integrators for dynamical systems with holonomic constraints [WOBL17] and in order to devise mixed order integrators for systems with multiple scales [WOBL16]. The order analysis of these methods is not straightforward.

Date: January 20, 2020.

[†] Matematisk institutt, Universitetet i Bergen, Norway, email: Antonella.Zanna@uib.no.

It is known that there is an equivalence between symplectic Partitioned RK methods and some discrete variational methods, see [EH06, MW01], but it is not known whether more complicated variational methods can be written in a RK-type formalism. The advantage a RK formalism is that it would make order analysis of the methods considerably easier, as the order analysis of RK and PRK methods is well understood (see [EH06] chapter III and references therein).

In a recent paper [Zan], we introduced a family of Runge–Kutta methods of additive type for highly oscillatory problems. The methods were derived from a variational formulation, using different quadrature formulas for different parts of the Lagrangian. In this paper we identify those methods as a particular case of partitioned symplectic GARK methods, that are, in turn, GARK methods. The main idea is that the q -variables are treated by a GARK method, thus generating a discrete Lagrangian that uses a different RK for each part rather than the same RK for all terms. Performing discrete variations, we arrive to a partitioned GARK method that is automatically symplectic. The GARK framework allows us to significantly simplify the formulation of the methods, that can be written in a ready-to-use formalism, and the order analysis, as only known algebraic relations for the coefficients need to be verified.

The paper is organized as follows. We commence by reviewing the formalism of GARK methods and the equivalence with ARK methods, see § 2. In Section 3 we use GARK methods for the splitted Lagrangian to obtain variational equations and symplectic partitioned GARK methods. In Section 4 we present the general form of the methods for both Lagrangian and Hamiltonian problems, the latter split in Hamiltonian sub-problems. In Section 5 we review some results about the order conditions for GARK methods and reformulate them in a simple and elegant way. In section 6 we introduce two main techniques that can be used to construct the transfer matrices between the different methods. The transfer matrices constructed in this way can be used as generators for other transfer matrices. As the transfer matrices are not unique (in facts there are infinitely many of those), this gives the possibility of tuning the methods to obey qualitative properties which would be hard to obey in the classical setting. For instance, in [Zan] we constructed higher order symplectic methods that were P-stable using a diagonal method that was not P-stable. In Section 7 we relate the order of the partitioned symplectic method to the order of the underlying GARK method, thus simplifying the order analysis. In Section 8 we consider the special case when the number of splitting terms is $N = 2$. We consider a semi-separable case $L(q, \dot{q}) = L^{\{1\}}(q, \dot{q}) + L^{\{2\}}(q)$, and a fully separable case, $L(q, \dot{q}) = L^{\{1\}}(\dot{q}) + L^{\{2\}}(q)$, together with the corresponding Hamiltonian cases. For this latter case, we show, as an example of the new possibilities opened by this framework, a fourth order symplectic method with three stages for q and two stages for p , thus having rectangular coefficient matrices. The method is constructed from the Gauss–Legendre and Gauss–Lobatto of order four but is implicit only in the second stage Q_2 for q . Finally, Section 9 is devoted to some concluding remarks.

2. GARK METHODS

A GARK method for the problem

$$(1) \quad \dot{x} = f(t, x) = \sum_{l=1}^N f^{\{l\}}(t, x)$$

reads

$$\begin{aligned} X_i^{\{l\}} &= x_n + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} f^{\{m\}}(t_j^{\{m\}}, X_j^{\{m\}}), \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N, \\ x_{n+1} &= x_n + h \sum_{l=1}^N \sum_{j=1}^{s^{\{l\}}} b_j^{\{l\}} f^{\{l\}}(t_j^{\{l\}}, X_j^{\{j\}}), \end{aligned}$$

with $t_j^{\{l\}} = t_n + c_j^{\{l\}}h$, and the corresponding generalized Butcher tableau of coefficients

$$(2) \quad \begin{array}{c|ccc} c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} \end{array}$$

[SG15]. The diagonal blocks of the type $(A^{\{l,l\}}, b^{\{l\}}, c^{\{l\}})$, $l = 1, \dots, N$, are usually chosen as some standard RK methods, while the off-diagonal blocks $A^{\{l,m\}}$, $l \neq m$, are coupling (or transfer) coefficients.

2.1. The equivalence of ARK and GARK. The formalism of the GARK methods is equivalent to that of Additive RK methods, and RK method, providing a unified approach. For instance, when $N = 2$, the ARK method

$$\frac{c \mid A^{\{1\}} \quad A^{\{2\}}}{\mid b^{\{1\}} \quad b^{\{2\}}} \text{ is equivalent to the GARK method } \frac{c \mid A^{\{1\}} \quad A^{\{2\}}}{c \mid A^{\{1\}} \quad A^{\{2\}}}{\mid b^{\{1\}} \quad b^{\{2\}}}.$$

Vice versa, the GARK method

$$\frac{c^{\{1\}} \mid A^{\{1,1\}} \quad A^{\{1,2\}}}{c^{\{2\}} \mid A^{\{2,1\}} \quad A^{\{2,2\}}}{\mid b^{\{1\}} \quad b^{\{2\}}} \text{ is equivalent to the ARK method } \frac{\left[\begin{array}{c|c} c^{\{1\}} & \\ \hline c^{\{2\}} & \end{array} \right] \mid \left[\begin{array}{c|c} A^{\{1,1\}} & 0 \\ \hline A^{\{2,1\}} & 0 \end{array} \right]}{\left[\begin{array}{c|c} b^{\{1\}} & 0 \\ \hline 0 & b^{\{2\}} \end{array} \right]}$$

The advantage of the GARK fomulation is that it clarifies the coupling between the various methods, in addition to eliminating zero quadrature weights in the ARK formalism, hence the analysis of special cases.

2.2. Partitioned Runge–Kutta methods are GARK methods. Consider a generic problem with a partitioning of the variables of the type

$$\begin{aligned} \dot{q} &= v(q, p) \\ \dot{p} &= f(q, p), \end{aligned}$$

and a Partitioned Runge–Kutta method $(A^{\{1\}}, b^{\{1\}}, c^{\{1\}})$, $(A^{\{2\}}, b^{\{2\}}, c^{\{2\}})$. It is usual to choose $b^{\{2\}} = b^{\{1\}} = b$ and $c^{\{2\}} = c^{\{1\}} = c$. Let variable $y = [q, p]^T$ and the splitting

$$\dot{y} = \mathcal{F}(y) = \mathcal{F}^{\{1\}}(y) + \mathcal{F}^{\{2\}}(y) = \begin{bmatrix} v(q, p) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ f(q, p) \end{bmatrix}.$$

It is easy to see that the PRK method corresponds to the GARK method

$$\frac{c \mid A^{\{1\}} \quad A^{\{2\}}}{c \mid A^{\{1\}} \quad A^{\{2\}}}{\mid b \quad b}.$$

In facts, by virtue of the fact that the q -part of $\mathcal{F}^{\{2\}}$ is zero, one has $Q_i^{\{1\}} = Q_i^{\{2\}}$ for all the stages of the methods. By a similar argument, $P_i^{\{1\}} = P_i^{\{2\}}$ and the statement follows. In particular, if the problem is Hamiltonian, that is

$$v(q, p) = \frac{\partial H(q, p)}{\partial p}, \quad f(q, p) = -\frac{\partial H(q, p)}{\partial q}$$

and if the PRK is symplectic, then the above GARK becomes $(A^{\{1\}} = A)$

$$\frac{c \mid A \quad \widehat{A}}{c \mid A \quad \widehat{A}}{\mid b \quad b},$$

with the symplectic condition $b_i b_j = b_i \widehat{a}_{i,j} + b_j a_{j,i}$.

3. VARIATIONAL DERIVATION OF PARTITIONED SYMPLECTIC GARK METHODS

Assume a Lagrangian $L(q, \dot{q}) = \sum_{l=1}^N L^{\{l\}}(q, \dot{q})$ given. We consider a discrete action approximation

$$(3) \quad \int_0^h L(q, \dot{q}) \approx h \sum_{l=1}^N \sum_{k=1}^{s^{\{l\}}} b_k^{\{l\}} L^{\{l\}}(Q_k^{\{l\}}, \dot{Q}_k^{\{l\}}),$$

where we assume that the q -variables are resolved by a GARK method

$$(4) \quad Q_i^{\{l\}} = q_0 + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} \dot{Q}_j^{\{m\}}, \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N$$

$$(5) \quad q_1 = q_0 + h \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} \dot{Q}_i^{\{l\}},$$

corresponding to the GARK tableau for the q variables,

$$Q : \begin{array}{c|ccc} c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} \end{array}$$

with $b_i^{\{l\}} \neq 0$ for $i = 1, \dots, s^{\{l\}}$, $l = 1, \dots, N$. We construct the *augmented discrete Lagrangian* by taking

$$L_\lambda(q_0, q_1) = h \sum_{l=1}^N \sum_{k=1}^{s^{\{l\}}} b_k^{\{l\}} L^{\{l\}}(Q_k^{\{l\}}, \dot{Q}_k^{\{l\}}) - \lambda(q_1 - q_0 - h \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} \dot{Q}_i^{\{l\}}).$$

The augmentation of the Lagrangian takes care of the linear dependence in the variables. Proceeding in a manner similar to the derivation of symplectic PRK, we use the $\dot{Q}_j^{\{m\}}$, $j = 1, \dots, s^{\{m\}}$, $m = 1, \dots, N$ as the principal variables. Taking derivative with respect to $\dot{Q}_j^{\{m\}}$, we obtain the following $s^{\{1\}} + \dots + s^{\{N\}}$ conditions

$$(6) \quad h \sum_{l=1}^N \sum_{k=1}^{s^{\{l\}}} b_k^{\{l\}} (\dot{P}_k^{\{l\}} \frac{\partial Q_k^{\{l\}}}{\partial \dot{Q}_j^{\{m\}}} + P_k^{\{l\}} \frac{\partial \dot{Q}_k^{\{l\}}}{\partial \dot{Q}_j^{\{m\}}}) + \lambda h b_j^{\{m\}} = 0, \quad j = 1, \dots, s^{\{m\}}, \quad m = 1, \dots, N,$$

where we have denoted

$$\dot{P}_k^{\{l\}} = \frac{\partial}{\partial q} L^{\{l\}}(Q_k^{\{l\}}, \dot{Q}_k^{\{l\}}), \quad P_k^{\{l\}} = \frac{\partial}{\partial \dot{q}} L^{\{l\}}(Q_k^{\{l\}}, \dot{Q}_k^{\{l\}}).$$

Using the fact that $\frac{\partial Q_k^{\{l\}}}{\partial \dot{Q}_j^{\{m\}}} = h a_{k,j}^{\{l,m\}} I$ and substituting into (6), we obtain

$$(7) \quad h \sum_{l=1}^N \sum_{k=1}^{s^{\{l\}}} b_k^{\{l\}} (\dot{P}_k^{\{l\}} h a_{k,j}^{\{l,m\}}) + h^2 b_j^{\{m\}} P_j^{\{m\}} + \lambda h b_j^{\{m\}} = 0, \quad j = 1, \dots, s^{\{m\}}, \quad m = 1, \dots, N.$$

The symplectic numerical method is obtained by considering the discrete Euler equations for $L_\lambda(q_0, q_1)$

$$\frac{\partial}{\partial q_0} L_\lambda(q_0, q_1) + \frac{\partial}{\partial q_1} L_\lambda(q_{-1}, q_0) = 0,$$

(variations are zero at the endpoint of integration) and eliminating the Lagrange multiplier λ , giving a two-step type method in q_{-1}, q_0, q_1 . The method can be reduced to a one-step method by using the the Legendre transform

$$p_0 = -\frac{\partial}{\partial q_0} L_\lambda(q_0, q_1), \quad p_1 = \frac{\partial}{\partial q_1} L_\lambda(q_0, q_1),$$

and we shall consider the latter approach. We have

$$\frac{\partial L_\lambda}{\partial q_0} = h \sum_{l=1}^N \sum_{k=1}^{s^{(l)}} b_k^{\{l\}} (\dot{P}_k^{\{l\}} \frac{\partial Q_k^{\{l\}}}{\partial q_0} + P_k^{\{l\}} \frac{\partial \dot{Q}_k^{\{l\}}}{\partial q_0}) + \lambda (I + h \sum_{l=1}^N \sum_{k=1}^{s^{(l)}} b_k^{\{l\}} \frac{\partial \dot{Q}_k^{\{l\}}}{\partial q_0}),$$

and, taking into account that

$$\frac{\partial Q_k^{\{l\}}}{\partial q_0} = I + h \sum_{m=1}^N \sum_{j=1}^{s^{(m)}} a_{k,j}^{\{l,m\}} \frac{\partial \dot{Q}_j^{\{m\}}}{\partial q_0},$$

together with (7), we obtain

$$(8) \quad p_0 = -h \sum_{l=1}^N \sum_{k=1}^{s^{(l)}} b_k^{\{l\}} \dot{P}_k^{\{l\}} - \lambda.$$

Similarly,

$$\frac{\partial L_\lambda}{\partial q_1} = h \sum_{l=1}^N \sum_{k=1}^{s^{(l)}} (\dot{P}_k^{\{l\}} \frac{\partial Q_k^{\{l\}}}{\partial q_1} + P_k^{\{l\}} \frac{\partial \dot{Q}_k^{\{l\}}}{\partial q_1}) - \lambda I,$$

and, again, expanding in terms of $\frac{\partial \dot{Q}_k^{\{l\}}}{\partial q_1}$ and using (7), we obtain

$$p_1 = -\lambda I,$$

from which,

$$p_1 = p_0 + h \sum_{l=1}^N \sum_{k=1}^{s^{(l)}} b_k^{\{l\}} \dot{P}_k^{\{l\}}.$$

The internal stages for the $P_i^{\{l\}}$ s can now be retrieved combining (7) and (8):

$$(9) \quad P_j^{\{l\}} = p_0 + h \sum_{m=1}^N \sum_{k=1}^{s^{(m)}} (b_k^{\{m\}} - \frac{b_k^{\{m\}}}{b_j^{\{l\}}} a_{k,j}^{\{m,l\}}) \dot{P}_k^{\{m\}} \quad j = 1, \dots, s^{(l)}$$

thus obtaining a Partitioned Symplectic GARK method

$$(10) \quad Q : \begin{array}{c|ccc} c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} \end{array}, \quad P : \begin{array}{c|ccc} c^{\{1\}} & \widehat{A}^{\{1,1\}} & \dots & \widehat{A}^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & \widehat{A}^{\{N,1\}} & \dots & \widehat{A}^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} \end{array},$$

where¹

$$(11) \quad \widehat{A}^{\{l,m\}} = (\mathbb{1}^{\{l,m\}} - (B^{\{l\}})^{-1} (A^{\{m,l\}})^T) B^{\{m\}}, \quad l, m = 1, \dots, N,$$

$B^{\{k\}} = \text{diag}(b^{\{k\}})$ are required to be invertible, and $\mathbb{1}^{\{l,m\}} = \mathbb{1}_{s^{\{l\}} \times s^{\{m\}}}$ is the matrix of ones of dimension $s^{\{l\}} \times s^{\{m\}}$. It is easy to see that

$$A^{\{m,l\}} = (\mathbb{1}^{\{l,m\}} - (B^{\{m\}})^{-1} (\widehat{A}^{\{l,m\}})^T) B^{\{l\}}, \quad l, m = 1, \dots, N,$$

¹For consistency, we will require $c^{\{l\}} = A^{\{l,m\}} \mathbb{1}^{\{m\}}$.

From the relation (11) above, it is clear that, once the GARK method for the q -variables is chosen, the matrices $\hat{A}^{\{l,m\}}$, $l, m = 1, \dots, N$, exist and are uniquely defined, as long as the weights in $b^{\{l\}}, b^{\{m\}}$ are all nonzero. Moreover the correspondence is one to one. As the p -variables are conjugate to the q variables, the one-to-one relation (11) justifies the following definition.

Definition 3.1 (Symplectic conjugate GARK methods). *The couple of GARK methods $(A^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$, $(\hat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$, $l, m = 1, \dots, N$, with $\hat{A}^{\{l,m\}}$ defined as in (11) and $b_i^{\{l\}} \neq 0$, $i = 1, \dots, s^{\{l\}}$, $l = 1, \dots, N$, will be called a symplectic conjugate GARK method and denoted by $(A^{\{l,m\}}, \hat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$, $l, m = 1, \dots, N$.*

The relation (11) can be written as a generalization of the well known symplectic condition

$$b_i^{\{l\}} b_j^{\{m\}} = b_i^{\{l\}} \hat{a}_{i,j}^{\{l,m\}} + b_j^{\{m\}} a_{j,i}^{\{m,l\}} \quad \forall i = 1, \dots, s^{\{l\}}, \quad j = 1, \dots, s^{\{m\}}, \quad \forall l, m = 1, \dots, N.$$

Note that the diagonal blocks of the Q and P variables are precisely symplectic conjugate PRK pairs $(A^{\{l,l\}}, \hat{A}^{\{l,l\}}, b^{\{l\}}, c^{\{l\}})$.

In what follows, we will use consistently the wide hat notation $\hat{}$ to denote a matrix that is constructed using (11).

4. GENERAL FORMAT OF THE METHODS: THE LAGRANGIAN AND HAMILTONIAN SETTING

The Symplectic Partitioned GARK methods read as follows:

$$(12) \quad \begin{aligned} Q_i^{\{l\}} &= q_0 + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} \dot{Q}_j^{\{m\}}, \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N \\ q_1 &= q_0 + h \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} \dot{Q}_i^{\{l\}}, \\ P_i^{\{l\}} &= p_0 + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} \hat{a}_{i,j}^{\{l,m\}} \dot{P}_j^{\{m\}} \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N \\ p_1 &= p_0 + h \sum_{l=1}^N \sum_{k=1}^{s^{\{l\}}} b_k^{\{l\}} \dot{P}_k^{\{l\}}. \end{aligned}$$

where $P^{\{l\}} = \frac{\partial}{\partial \dot{q}} L^{\{l\}}(Q^{\{l\}}, \dot{Q}^{\{l\}})$ (Legendre transform) and $\hat{A}^{\{l,m\}}$ defined as in (11). Assuming the latter to be invertible, we can solve for $\dot{Q}^{\{l\}}$ to obtain

$$\dot{Q}^{\{l\}} = V^{\{l\}}(Q^{\{l\}}, P^{\{l\}}),$$

so that

$$\dot{P}^{\{l\}} = \frac{\partial}{\partial q} L^{\{l\}}(Q^{\{l\}}, \dot{Q}^{\{l\}}) = F^{\{l\}}(Q^{\{l\}}, P^{\{l\}}).$$

Thus, the method can be written as a one step method $(q_0, p_0) \rightarrow (q_1, p_1)$ in the form

$$(13) \quad \begin{aligned} Q_i^{\{l\}} &= q_0 + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} V^{\{m\}}(Q_j^{\{m\}}, P_j^{\{m\}}) \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N \\ q_1 &= q_0 + h \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} V^{\{l\}}(Q_i^{\{l\}}, P_i^{\{l\}}) \\ P_i^{\{l\}} &= p_0 + h \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} \hat{a}_{i,j}^{\{l,m\}} F^{\{m\}}(Q_j^{\{m\}}, P_j^{\{m\}}) \quad i = 1, \dots, s^{\{l\}}, \quad l = 1, \dots, N \\ p_1 &= p_0 + h \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} F^{\{l\}}(Q_i^{\{l\}}, P_i^{\{l\}}). \end{aligned}$$

Note that the above formulation yields a symplectic method in the Hamiltonian setting, when

$$H(q, p) = \sum_{l=1}^N H^{\{l\}}(q, p), \quad V^{\{l\}}(q, p) = \frac{\partial H^{\{l\}}}{\partial p}(q, p), \quad F^{\{l\}}(q, p) = -\frac{\partial H^{\{l\}}}{\partial q}(q, p).$$

Next, consider a partitioning of the system

$$\dot{y} = \mathcal{F}(y) = \mathcal{F}^{\{1\}}(y) + \dots + \mathcal{F}^{\{2N\}}(y) = \sum_{l=1}^N \begin{bmatrix} V^{\{l\}}(q, p) \\ 0 \end{bmatrix} + \sum_{l=1}^N \begin{bmatrix} 0 \\ F^{\{l\}}(q, p) \end{bmatrix}.$$

We consider first the case when $N = 2$. We have a splitting in four additive vector fields,

$$\begin{bmatrix} V^{\{1\}}(q, p) \\ 0 \end{bmatrix} + \begin{bmatrix} V^{\{2\}}(q, p) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ F^{\{1\}}(q, p) \end{bmatrix} + \begin{bmatrix} 0 \\ F^{\{2\}}(q, p) \end{bmatrix},$$

where, under the assumption that $F = \nabla H$ is Hamiltonian, we take $H(q, p) = H^{\{1\}}(q, p) + H^{\{2\}}(q, p)$, and

$$V^{\{l\}}(q, p) = \frac{\partial H^{\{l\}}}{\partial p}(q, p), \quad F^{\{l\}}(q, p) = -\frac{\partial H^{\{l\}}}{\partial q}(q, p), \quad l = 1, 2.$$

The method (10) coefficients $\widehat{A}^{\{l,m\}}$ satisfying (11) is then equivalent to a (symplectic) GARK method

$$(14) \quad \begin{array}{c|cccc} c^{\{1\}} & A^{\{1,1\}} & A^{\{1,2\}} & \widehat{A}^{\{1,1\}} & \widehat{A}^{\{1,2\}} \\ c^{\{2\}} & A^{\{2,1\}} & A^{\{2,2\}} & \widehat{A}^{\{2,1\}} & \widehat{A}^{\{2,2\}} \\ c^{\{1\}} & A^{\{1,1\}} & A^{\{1,2\}} & \widehat{A}^{\{1,1\}} & \widehat{A}^{\{1,2\}} \\ c^{\{2\}} & A^{\{2,1\}} & A^{\{2,2\}} & \widehat{A}^{\{2,1\}} & \widehat{A}^{\{2,2\}} \\ \hline & b^{\{1\}} & b^{\{2\}} & b^{\{1\}} & b^{\{2\}} \end{array}.$$

Also in this scheme we have redundancy, as $Q_i^{\{3\}} = Q_i^{\{1\}}$ for $i = 1, \dots, s^{\{1\}}$ and $Q_i^{\{4\}} = Q_i^{\{2\}}$ for $i = 1, \dots, s^{\{2\}}$, being the 3rd, 4th additive terms of the q -vector fields zero; similarly, one has $P_i^{\{1\}} = P_i^{\{3\}}$, $i = 1, \dots, s^{\{1\}}$ and $P_i^{\{2\}} = P_i^{\{4\}}$, $i = 1, \dots, s^{\{2\}}$, being the 1st, 2nd part of the p -vector field zero.

A generic N -terms symplectic partitioned GARK method (10) can, in turn, be written as a GARK method (with lots of redundancy) in a similar manner, by taking 2 copies of each set of q and p variables, so that $Q_i^{\{l+N\}} = Q_i^{\{l\}}$ and $P_i^{\{l\}} = P_i^{\{l+N\}}$, $i = 1, \dots, s^{\{l\}}$, $l = 1, \dots, N$, resulting in a $2N$ symplectic GARK method

$$(15) \quad \begin{array}{c|cccccc} c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} & \widehat{A}^{\{1,1\}} & \dots & \widehat{A}^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} & \widehat{A}^{\{N,1\}} & \dots & \widehat{A}^{\{N,N\}} \\ c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} & \widehat{A}^{\{1,1\}} & \dots & \widehat{A}^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} & \widehat{A}^{\{N,1\}} & \dots & \widehat{A}^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} & b^{\{1\}} & \dots & b^{\{N\}} \end{array}.$$

where $\widehat{A}^{\{l,m\}}$ is defined as in (11). The benefit of the above formulation is that we can take advantage of the existing order analysis already developed for GARK methods.

5. ORDER CONDITIONS FOR GARK METHODS

In this section we consider a generic GARK method,

$$(16) \quad \begin{array}{c|ccc} c^{\{1\}} & A^{\{1,1\}} & \dots & A^{\{1,N\}} \\ \vdots & \vdots & \ddots & \vdots \\ c^{\{N\}} & A^{\{N,1\}} & \dots & A^{\{N,N\}} \\ \hline & b^{\{1\}} & \dots & b^{\{N\}} \end{array}$$

for the differential equation

$$\dot{y} = \mathcal{F}(y) = \sum_{l=1}^N \mathcal{F}^{\{l\}}(y), \quad \mathcal{F} : \mathbb{R}^d \rightarrow \mathbb{R}^d.$$

A study of the order conditions of ARK (which are equivalent to GARK) was carried out in [AMSS97]. The generalization to the GARK formalism was treated in [SG15] mostly with focus on implicit-explicit methods. A further treatment, especially with focus on DAEs and stiff systems, can be found in [Tan18]. All these methods use expansion in elementary differentials and colored trees (N-trees). For completeness, we summarize the order analysis in this section.

The order conditions for GARK methods can be derived in a similar manner to those of standard RK methods. The trees that define the order conditions are exactly those of RK methods, except for the fact that one has to consider all the possible combinations of colors $1, \dots, N$ associated to each of the vector field. The set NT of N-trees consists of all Butcher trees with colored vertices. The order of a N-tree $u \in \text{NT}$, denoted as $\rho(u)$, is the number vertices in u . The empty tree is denoted as \emptyset and to emphasize that a N-tree u has root of color ν , we will write $u^{[\nu]}$. Note that $u^{[\nu]} = [u_1, \dots, u_m]^{[\nu]}$, where u_1, \dots, u_m are the non-empty N-subtrees obtained removing the root of u . The set of N-trees with root ν is denoted by NT_ν . As in the setting of Butcher trees, we will denote by $\sigma(u)$ the number of symmetries of $u \in \text{NT}$ and by $\gamma(u)$ its density, which is defined in a recursive manner as

$$\begin{aligned} \gamma(\emptyset) &= 1 \\ \gamma(\tau^{[\nu]}) &= 1, \quad \nu = 1, \dots, N, \\ \gamma(u) &= \rho(u)\gamma(u_1) \cdots \gamma(u_m), \quad u = u^{[\nu]} = [u_1, \dots, u_m]^{[\nu]}, \end{aligned}$$

where $\tau^{[\nu]}$ denotes the single vertex of color ν .

For each tree $u \in \text{NT}$ there is an elementary differential $F(u) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ associated to it. Elementary differentials are multilinear maps and are recursively defined for each component $i = 1, \dots, d$ of the vector field \mathcal{F} as

$$\begin{aligned} F^i(\emptyset)(y) &= y^i \\ F^i(\tau^{[\nu]})(y) &= \mathcal{F}^{\{\nu\},i}(y), \quad \nu = 1, \dots, N \\ F^i(u)(y) &= \sum_{i_1, \dots, i_m=1}^d \frac{\partial^m \mathcal{F}^{\{\nu\},i}}{\partial y^{i_1} \cdots \partial y^{i_m}}(y) F^{i_1}(u_1)(y) \cdots F^{i_m}(u_m)(y), \quad u = u^{[\nu]} = [u_1, \dots, u_m]^{[\nu]}. \end{aligned}$$

Thus, defining $\mathbf{c} : \text{NT} \rightarrow \mathbb{R}$, a mapping assigning to each N-tree a real number, the exact solution $y(t+h)$ can be written as a formal power expansion,

$$y(t+h) = \text{NB}(\mathbf{c}, y(t)) = \sum_{u \in \text{NT}} \frac{h^{\rho(u)}}{\sigma(u)} \mathbf{c}(u) F(u)(y(t)),$$

with

$$\mathbf{c}(u) = \frac{1}{\gamma(u)}.$$

A similar expansion holds for the numerical method,

$$y_{n+1} = \text{NB}(\mathbf{d}, y_n).$$

Thus:

Theorem 5.1 (Order of GARK methods, [SG15]). *A GARK method is of order r iff*

$$\mathbf{d}(u) = \frac{1}{\gamma(u)}$$

for all $u \in \text{NT}$ with $1 \leq \rho(u) \leq r$.

We sketch the main moments of the proof. The mapping $\mathbf{d} : \text{NT} \rightarrow \mathbb{R}$ depends on the GARK method and is also defined in a recursive manner using the internal stages of the method. One has

$$\begin{aligned} Y_i^{\{l\}} &= \text{NB}(\mathbf{d}_i^{\{l\}}, y_n) \\ h\mathcal{F}^{\{m\}}(Y_i^{\{m\}}) &= \text{NB}(\mathbf{g}_i^{\{m\}}, y_n), \end{aligned}$$

hence

$$\mathbf{d}(u) = \sum_{l=1}^N \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} \mathbf{g}_i^{\{l\}}(u), \quad u \in \text{NT} - \{\emptyset\},$$

and, similarly,

$$\mathbf{d}_i^{\{l\}}(u) = \sum_{m=1}^N \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} \mathbf{g}_j^{\{m\}}(u).$$

Using these in a recursive manner, one finds that, for $u = [u_1, \dots, u_l]^{[\nu]}$,

$$\mathbf{g}_i^{\{m\}}(u) = \delta_{\nu,m} \sum_{n_1, \dots, n_l} \sum_{j_1, \dots, j_l} a_{i,j_1}^{\{m,n_1\}} \dots a_{i,j_l}^{\{m,n_l\}} \mathbf{g}_{j_1}^{\{n_1\}}(u_1) \dots \mathbf{g}_{j_l}^{\{n_l\}}(u_l),$$

where $\delta_{\nu,m} = 1$ for $\nu = m$ and zero otherwise, implying that $\mathbf{g}_i^{\{m\}}(u) = 0$ whenever $u = \emptyset$ is the empty tree or u has root $\nu \neq m$. When $u = \tau^{[m]}$, then $\mathbf{g}_i^{\{m\}}(u) = 1$.

In this paper, we proceed in a manner similar to [Bor01]. We introduce the following notation:

$$(17) \quad \mathcal{A}^{[u]} = \mathbb{1}^{\{l\}} \quad \text{for } u = \tau^{[l]},$$

$$(18) \quad \mathcal{A}^{[u]} = (A^{\{l,\nu_1\}} \mathcal{A}^{[u_1]}) \odot \dots \odot (A^{\{l,\nu_m\}} \mathcal{A}^{[u_m]}) \quad \text{for } u = [u_1, \dots, u_m]^{[l]}$$

where ν_1, \dots, ν_m are the root colors of the subtrees u_1, \dots, u_m respectively and \odot is the componentwise vector multiplication. Thus, if $u = [u_1, \dots, u_m]^{[l]}$, then

$$\mathbf{d}(u) = \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} \mathcal{A}_i^{[u]} = b^{\{l\}T} \mathcal{A}^{[u]}.$$

Denoting by NT_l the set of N-trees with root l and matching for all the roots $l \in \{1, \dots, N\}$, the numerical method can be written as

$$y_{n+1} = y_n + \sum_{k=1}^r h^k \sum_{l=1}^N \sum_{\substack{u \in \text{NT}_l \\ \rho(u)=k}} \frac{1}{\sigma(u)} b^{\{l\}T} \mathcal{A}^{[u]} F(u) + O(h^{r+1}).$$

Performing a similar ordering for the trees in the exact solution, the order conditions can be written elegantly as

$$(19) \quad b^{\{l\}T} \mathcal{A}^{[u]} = \frac{1}{\gamma(u)}, \quad u \in \text{NT}_l, \quad l = 1, \dots, N,$$

for trees of order $\rho(u) = 1, \dots, r$.









RK-tree u	Order $\rho(u)$	$\gamma(u)$	GARK order condition	$\in \{1, \dots, N\}$
	1	1	$b^{\{l\}T} \mathbb{1}^{\{l\}} = 1$	$\forall l$
	2	2	$b^{\{l\}T} A^{\{l,m\}} \mathbb{1}^{\{m\}} = \frac{1}{2}$	$\forall l, m$
	3	3	$b^{\{l\}T} ((A^{\{l,m\}} \mathbb{1}^{\{m\}}) \odot (A^{\{l,n\}} \mathbb{1}^{\{n\}})) = \frac{1}{3}$	$\forall l, m, n$
	3	6	$b^{\{l\}T} A^{\{l,m\}} A^{\{m,n\}} \mathbb{1}^{\{n\}} = \frac{1}{6}$	$\forall l, m, n$
	4	4	$b^{\{l\}T} ((A^{\{l,m\}} \mathbb{1}^{\{m\}}) \odot (A^{\{l,n\}} \mathbb{1}^{\{n\}}) \odot (A^{\{l,u\}} \mathbb{1}^{\{u\}})) = \frac{1}{4}$	$\forall l, m, n, u$
	4	8	$b^{\{l\}T} ((A^{\{l,m\}} A^{\{m,n\}} \mathbb{1}^{\{n\}}) \odot (A^{\{l,u\}} \mathbb{1}^{\{u\}})) = \frac{1}{8}$	$\forall l, m, n, u$
	4	12	$b^{\{l\}T} A^{\{l,m\}} ((A^{\{m,n\}} \mathbb{1}^{\{n\}}) \odot (A^{\{m,u\}} \mathbb{1}^{\{u\}})) = \frac{1}{12}$	$\forall l, m, n, u$
	4	24	$b^{\{l\}T} A^{\{l,m\}} A^{\{m,n\}} A^{\{n,u\}} \mathbb{1}^{\{u\}} = \frac{1}{24}$	$\forall l, m, n, u$

TABLE 1. Order conditions for GARK methods up to order 4. The symbol \odot denotes componentwise vector multiplication.

We note that if the diagonal methods $(A^{\{l,l\}}, b^{\{l\}}, c^{\{l\}})$ have order $r^{\{l\}}$, then the corresponding order conditions for $l = m = n = u = \dots$ (all the indices equal) are satisfied up to order $r^{\{l\}}$, as they are the same as the underlying order conditions for the RK method. Moreover, for consistency, it is also reasonable to require that

$$(20) \quad A^{\{l,m\}} \mathbb{1}^{\{m\}} = c^{\{l\}}, \quad \forall l, m.$$

This condition is automatically satisfied for $m = l$, as long as the underlying RK method $(A^{\{l,l\}}, b^{\{l\}}, c^{\{l\}})$ is consistent. Using the consistency condition (20), one recovers exactly the order condition listed in [SG15].

Definition 5.1 (Simplifying conditions for GARK methods, [Tan18]). *Simplifying conditions for GARK methods: for $l, m = 1, \dots, N$, where N is the number of methods,*

(21)

$$B^{\{l\}}(r^{\{l\}}) : \quad \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} (c_i^{\{l\}})^{k-1} = \frac{1}{k}, \quad k = 1, \dots, r^{\{l\}}$$

(22)

$$C^{\{l,m\}}(\eta^{\{l,m\}}) : \quad \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} (c_j^{\{m\}})^{k-1} = \frac{(c_i^{\{l\}})^k}{k}, \quad i = 1, \dots, s^{\{l\}}, \quad k = 1, \dots, \eta^{\{l,m\}}.$$

(23)

$$D^{\{l,m\}}(\zeta^{\{l,m\}}) : \quad \sum_{i=1}^{s^{\{l\}}} b_i^{\{l\}} (c_i^{\{l\}})^{k-1} a_{i,j}^{\{l,m\}} = \frac{b_j^{\{m\}}}{k} (1 - (c_j^{\{m\}})^k), \quad j = 1, \dots, s^{\{m\}}, \quad k = 1, \dots, \zeta^{\{l,m\}}.$$

Note that $C^{\{l,m\}}(1)$ is the same as (20), required for consistency. The above conditions are generalization of the corresponding B, C, D conditions for RK methods, which are recovered when $N = 1$. The B condition (21) implies that the quadrature formula with weights $b_i^{\{l\}}$ and nodes $c_i^{\{l\}}$ has order $p^{\{l\}}$ and, provided that the diagonal methods are consistent so that (20) holds, it

is equivalent to state that the order conditions for the bushy trees like $u = \begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \bullet \quad \bullet \end{array}$ with k vertices ($\gamma(u) = k$) are automatically satisfied up to $p^{\{l\}}$. The C condition (22) is related to the notion of the *stage order* of the method, that is the order of approximation at the internal stages. The D condition (23) is a simplifying condition, that guarantees the order conditions for trees of type

$u = \begin{array}{c} \bullet \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \bullet \quad \bullet \quad \bullet \quad \bullet \end{array}$ are also satisfied.

The theorem below generalizes an important theorem due to Butcher, who used the RK simplifying assumptions B, C, D to obtain an estimate of the order of the underlying method.

Theorem 5.2 (Simplifying Assumption Theorem, [Tan18]). *If $B^{\{l\}}(r^{\{l\}})$, $C^{\{l,m\}}(\eta^{\{l,m\}})$, $D^{\{l,m\}}(\zeta^{\{l,m\}})$ are satisfied for $l, m = 1, \dots, N$, then the order of the GARK method is at least*

$$\min\{r, 2\eta + 2, \xi + 1, \eta + \zeta + 1\},$$

where $r = \min_l \{r^{\{l\}}\}$, $\eta = \min_{l,m} \{\eta^{\{l,m\}}\}$, $\zeta = \min_{l,m} \{\zeta^{\{l,m\}}\}$ and $\xi = \min_{l,m} \{\eta^{\{l,m\}} + \zeta^{\{l,m\}}\}$.

Definition (5.1) and Theorem (5.2) are originally stated for $N = 2$ but extension to a general N -terms case is immediate.

6. SOME TECHNIQUES TO CONSTRUCT THE TRANSFER MATRICES $A^{\{l,m\}}$, FOR $l \neq m$

As the variational methods discussed in this paper are a more general case of the methods proposed in [Zan], we generalize the approach in [Zan] for the construction of the coefficients and use rather the order conditions to establish the order of the resulting GARK method.

Assume the primary (diagonal) methods, $(A^{\{m,m\}}, b^{\{m\}}, c^{\{m\}})$, $m = 1, \dots, N$, are given. Denote by $\mathcal{L}_k^{\{m\}}(t) = \prod_{j=1, j \neq k}^{s^{\{m\}}} \frac{t - c_j^{\{m\}}}{c_k^{\{m\}} - c_j^{\{m\}}}$ the k th Lagrange interpolating polynomial based on the $c^{\{m\}}$ nodes that we assume to be distinct. We wish to construct $A^{\{l,m\}}$, corresponding to the $c^{\{l\}}$ nodes (also distinct).

6.1. Collocation. An obvious choice of the coefficients is by a technique similar to *collocation*, i.e. by taking

$$(24) \quad a_{i,j}^{\{l,m\}} = \int_0^{c_i^{\{l\}}} \mathcal{L}_j^{\{m\}}(\tau) d\tau, \quad l \neq m.$$

If $c^{\{l\}} = c^{\{m\}}$ then $A^{\{l,m\}}$ is the matrix of the collocation RK method based on the quadrature $(b^{\{l\}}, c^{\{l\}})$. However, in general, $A^{\{l,m\}} \neq A^{\{m,m\}}$, unless $(A^{\{m,m\}}, b^{\{m\}}, c^{\{m\}})$ is itself a collocation RK method.

This collocation construction is equivalent to the construction for some SPARK methods in [Jay98] and GARK methods in [Tan18] developed in the DAEs context.

Example: Consider $A^{\{1,1\}}$ to be a Gauss-Legendre RK and $A^{\{2,2\}}$ to be a Lobatto IIIA method, both of order 4. The corresponding GARK based on collocation is:

$$\begin{array}{c|cccccc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} & \frac{1}{6} - \frac{1}{108}\sqrt{3} & \frac{1}{3} + \frac{4}{27}\sqrt{3} & \frac{1}{108}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{6} + \frac{1}{108}\sqrt{3} & \frac{1}{3} - \frac{4}{27}\sqrt{3} & -\frac{1}{108}\sqrt{3} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} + \frac{1}{8}\sqrt{3} & \frac{1}{4} - \frac{1}{8}\sqrt{3} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

Its symplectic conjugate methods is

$$\begin{array}{c|ccccc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} & \frac{1}{6} & \frac{1}{3} - \frac{1}{6}\sqrt{3} & 0 \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{6} & \frac{1}{3} + \frac{1}{6}\sqrt{3} & 0 \\ 0 & \frac{1}{36}\sqrt{3} & -\frac{1}{36}\sqrt{3} & \frac{1}{6} & -\frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{4} + \frac{1}{9}\sqrt{3} & \frac{1}{4} - \frac{1}{9}\sqrt{3} & \frac{1}{6} & \frac{1}{3} & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{5}{6} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

6.2. Interpolation. Another choice is *interpolation* for the l -variables using an interpolating polynomial based on the method $A^{\{m,m\}}$ for the m variables. Interpolating the results given by the m method on the $c^{\{l\}}$ nodes gives

$$(25) \quad A^{\{l,m\}} = \mathcal{L}^{\{m\}}(c^{\{l\}})A^{\{m,m\}},$$

where $\mathcal{L}^{\{m\}}(c^{\{l\}})$ is the $s^{\{l\}} \times s^{\{m\}}$ matrix with element (i, j) given as $\mathcal{L}_j^{\{m\}}(c_i^{\{l\}})$. If $c^{\{l\}} = c^{\{m\}}$, $\mathcal{L}^{\{m\}}(c^{\{l\}}) = I$, and $A^{\{l,m\}} = A^{\{m,m\}}$.

Example: Let $A^{\{1,1\}}, A^{\{2,2\}}$ as above. The corresponding GARK based on interpolation is:

$$\begin{array}{c|ccccc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} & \frac{1}{6} - \frac{1}{36}\sqrt{3} & \frac{1}{3} - \frac{1}{9}\sqrt{3} & -\frac{1}{36}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{6} + \frac{1}{36}\sqrt{3} & \frac{1}{3} + \frac{1}{9}\sqrt{3} & \frac{1}{36}\sqrt{3} \\ 0 & \frac{1}{12}\sqrt{3} & -\frac{1}{12}\sqrt{3} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} + \frac{1}{12}\sqrt{3} & \frac{1}{4} - \frac{1}{12}\sqrt{3} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{2} + \frac{1}{12}\sqrt{3} & \frac{1}{2} - \frac{1}{12}\sqrt{3} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

Similarly, its symplectic conjugate is

$$\begin{array}{c|ccccc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} & \frac{1}{6} - \frac{1}{36}\sqrt{3} & \frac{1}{3} - \frac{1}{9}\sqrt{3} & -\frac{1}{36}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{6} + \frac{1}{36}\sqrt{3} & \frac{1}{3} + \frac{1}{9}\sqrt{3} & \frac{1}{36}\sqrt{3} \\ 0 & \frac{1}{12}\sqrt{3} & -\frac{1}{12}\sqrt{3} & \frac{1}{6} & -\frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{4} + \frac{1}{12}\sqrt{3} & \frac{1}{4} - \frac{1}{12}\sqrt{3} & \frac{1}{6} & \frac{1}{3} & 0 \\ 1 & \frac{1}{2} + \frac{1}{12}\sqrt{3} & \frac{1}{2} - \frac{1}{12}\sqrt{3} & \frac{1}{6} & \frac{5}{6} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

The methods in § 6.1-6.2 all have order 4, as it can be checked directly from the order conditions in Section 5.

6.3. Consistency and simplifying conditions for transfer matrices by collocation and interpolation. In this section we assume the diagonal methods $(A^{\{l,l\}}, b^{\{l\}}, c^{\{l\}})$, $l = 1, \dots, N$, given, and study how the construction of the transfer matrices, by collocation or interpolation, contributes to the simplifying assumptions.

Proposition 6.1. *Assume that the diagonal methods are consistent. Then the matrices $A^{\{l,m\}}$ in (24) and (25) satisfy $A^{\{l,m\}} \mathbb{1}^{\{m\}} = c^{\{l\}}$, and so do the corresponding $\widehat{A}^{\{l,m\}}$, as well as*

$$(26) \quad A^{\{l,m\}} = \tau_1 A_{\text{interp}}^{\{l,m\}} + \tau_2 A_{\text{colloc}}^{\{l,m\}} + \tau_3 \widehat{A}_{\text{interp}}^{\{l,m\}} + \tau_4 \widehat{A}_{\text{colloc}}^{\{l,m\}}, \quad \tau_1 + \dots + \tau_4 = 1.$$

Proof. For the collocation-coefficients: taking the i th component, $\sum_j a_{i,j}^{\{l,m\}} = \sum_j \int_0^{c_i^{\{l\}}} \mathcal{L}_j^{\{m\}}(\tau) d\tau = c_i^{\{l\}}$, by exchanging the order of sum and integration and using the fact that $\sum_j \mathcal{L}_j^{\{m\}}(t) = 1$. For the interpolation-type coefficients, $A^{\{l,m\}} \mathbb{1}^{\{m\}} = \mathcal{L}^{\{m\}}(c^{\{l\}})A^{\{m,m\}} \mathbb{1}^{\{m\}} = \mathcal{L}^{\{m\}}(c^{\{l\}})c^{\{m\}}$, because of the assumption $A^{\{m,m\}} \mathbb{1}^{\{m\}} = c^{\{m\}}$. The last passage, $\mathcal{L}^{\{m\}}(c^{\{l\}})c^{\{m\}} = c^{\{l\}}$ follows

from the the fact that $\sum_{i=1}^m \mathcal{L}_i^{\{m\}}(t)c_i^{\{m\}} = t$ (identity function), hence evaluations in the $c^{\{l\}}$ does the trick. For $\widehat{A}^{\{l,m\}}$ both in the collocation and interpolation case, it follows from the consistency of the method, which is a consequence of Theorem 7.2 in Section 7 below. The statement for (26) it follows immediately from the same property of the individual matrices and the type of the combination. \square

The consequence of the above result is that any choice (26), with transfer coefficients constructed as in this section, will give a consistent GARK method.

In [Zan] we developed some results specific to the case with $V^{\{1\}}(q,p) = p$, $V^{\{2\}}(q,p) = 0$, $F^{\{1\}} = F^{\{1\}}(q)$, $F^{\{2\}} = F^{\{2\}}(q)$. The following results generalize those findings with the notation of this paper.

Lemma 6.2. *Assume that $A^{\{l,m\}}$ ($m \neq l$) is constructed either by interpolation or collocation. Then*

$$(27) \quad C^{\{l,m\}}(\eta^{\{l,m\}}) : \quad \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} (c_j^{\{m\}})^{k-1} = \frac{(c_i^{\{l\}})^k}{k}, \quad i = 1, \dots, s^{\{l\}},$$

for $k = 1, \dots, \min\{\eta^{\{m,m\}}, s^{\{m\}} - 1\}$ in the interpolation setting and $k = 1, \dots, s^{\{m\}} - 1$ in the collocation setting.

Proof. The proof is essentially the same as in [Zan]. We simplify it and put it in the formalism of GARK methods. Consider the interpolation setting first.

$$\begin{aligned} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} (c_j^{\{m\}})^{k-1} &= \sum_{j=1}^{s^{\{m\}}} \sum_{n=1}^{s^{\{m\}}} \mathcal{L}_n^{\{m\}}(c_i^{\{l\}}) a_{n,j}^{\{m,m\}} (c_j^{\{m\}})^{k-1} = \sum_{n=1}^{s^{\{m\}}} \mathcal{L}_n^{\{m\}}(c_i^{\{l\}}) \sum_{j=1}^{s^{\{m\}}} a_{n,j}^{\{m,m\}} (c_j^{\{m\}})^{k-1} \\ &= \sum_{n=1}^{s^{\{m\}}} \mathcal{L}_n^{\{m\}}(c_i^{\{l\}}) \frac{(c_n^{\{m\}})^k}{k} \quad \text{from } C^{\{m,m\}}(\eta^{\{m,m\}}), \quad k = 1, \dots, \eta^{\{m,m\}} \\ &= \frac{(c_i^{\{l\}})^k}{k} \quad k = \min\{\eta^{\{m,m\}}, s^{\{m\}} - 1\} \end{aligned}$$

where last passage follows from the fact that $\sum_{n=1}^{s^{\{m\}}} \mathcal{L}_n^{\{m\}}(t)f_n$ is the interpolating polynomial based on $s^{\{m\}}$ nodes and is exact for polynomials up to degree $s^{\{m\}} - 1$.

Next, for the collocation setting,

$$\begin{aligned} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{l,m\}} (c_j^{\{m\}})^{k-1} &= \sum_{j=1}^{s^{\{m\}}} \int_0^{c_i^{\{l\}}} \mathcal{L}_j^{\{m\}}(\tau) (c_j^{\{m\}})^{k-1} d\tau = \int_0^{c_i^{\{l\}}} \sum_{j=1}^{s^{\{m\}}} \mathcal{L}_j^{\{m\}}(\tau) (c_j^{\{m\}})^{k-1} d\tau \\ &= \int_0^{c_i^{\{l\}}} \tau^{k-1} d\tau = \frac{(c_i^{\{l\}})^k}{k}, \quad k = 1, \dots, s^{\{m\}} - 1 \end{aligned}$$

where the third passage follows from the fact that the unique interpolant to $(c_i^{\{m\}})^{k-1}$ with nodes $c_i^{\{m\}}$ is the function τ^{k-1} . \square

Corollary 6.2.1. *Let $A_{\text{interp}}^{\{l,m\}}$ and $A_{\text{coll}}^{\{l,m\}}$ be the coefficients of the secondary method based on interpolation and collocation. Then the method*

$$A^{\{l,m\}} = \tau_1 A_{\text{interp}}^{\{l,m\}} + \tau_2 A_{\text{coll}}^{\{l,m\}}, \quad \tau_1 + \tau_2 = 1,$$

satisfies $C^{\{l,m\}}(\eta^{\{l,m\}})$, where $\eta^{\{l,m\}} = \min\{\eta^{\{m,m\}}, s^{\{m\}} - 1\}$, for any $\tau \in \mathbb{R}$.

There is no immediate way to extend the above results to the symplectic conjugate method. However, if the conjugate method also satisfies $C^{\{l,m\}}(\eta^{\{l,m\}})$, then so does $A^{\{l,m\}} = \tau_1 A_{\text{interp}}^{\{l,m\}} + \tau_2 A_{\text{coll}}^{\{l,m\}} + \tau_3 \widehat{A}_{\text{interp}}^{\{l,m\}} + \tau_4 \widehat{A}_{\text{coll}}^{\{l,m\}}$ when $\tau_1 + \dots + \tau_4 = 1$.

The $D^{\{l,m\}}$ properties are more difficult to generalize [Tan18]. However, it is reasonable to expect that, with both transfer matrix as in § 6.1-6.2, the resulting method will have order equal to the minimum of the order of the diagonal methods. This is not obvious for superconvergent diagonal methods (like Gauss-Legendre, Lobatto, etc.) but the constructions in § 6.1-6.2 seem to indicate that it is generally true. The same was observed for some methods with transfer matrices constructed by collocation in [Tan18].

7. ORDER OF THE VARIATIONAL GARK METHODS

We have seen that Lagrangian (variational) formalism leads automatically to partitioned symplectic GARK methods (13) which can be written as the (redundant) GARK method (15). Checking the GARK order condition for the full (15) is a cumbersome task. However, since the method (13) is symplectic, many of the order conditions are superfluous. In fact, because of the *symplectic conjugacy* of the methods, we claim that it is sufficient to look at the order condition of the GARK method for the q (or for the p) variables only. The order conditions for the conjugate method and the application of the GARK method and its symplectic conjugate to a Lagrangian/Hamiltonian system will follow by virtue of the symplectic conjugacy.

Theorem 7.1. *Let (A, b, c) be a RK method of order r with $b_i \neq 0$. Then its symplectic conjugate method (\widehat{A}, b, c) has also order r .*

Proof. We wish to show that the method (\widehat{A}, b, c) applied to a differential equation $\dot{p} = f(p)$, with f sufficiently differentiable, has also order r . It is sufficient to prove the result when p and f are scalar functions. We introduce $H(q, p) = g(p) - f(p)q$ with $g(q)$ a function to be determined. We see that $\dot{p} = -\frac{\partial H}{\partial q}$, in turn we let $\dot{q} = \frac{\partial H}{\partial p} = g'(p) - f'(p)q$. The system is thus a Hamiltonian system. We choose the function $g(p)$ so that $\frac{\partial}{\partial p}(g'(p) - f'(p)q) \neq 0$, hence

$$\dot{q} = g'(p) - f'(p)q$$

is invertible, therefore we can write $p = h(q, \dot{q})$. We then construct the Lagrangian $L(q, \dot{q}) = p\dot{q} - H(q, p)$, which is now a function of (q, \dot{q}) since $p = h(q, \dot{q})$. By construction, this Lagrangian is such that

$$p = \frac{\partial}{\partial \dot{q}} L(q, \dot{q}), \quad \dot{p} = \frac{\partial}{\partial q} L(q, \dot{q}) = f(p).$$

We next apply the method (A, b, c) of order r to the q variables, resulting in an approximation of order r for the solution of the system. Because of the variational derivation, this is equivalent to applying the method (\widehat{A}, b, c) to the p variables, therefore this must also have order r , as the p variables are only a result of the Legendre transform. \square

The result above generalizes to GARK methods:

Theorem 7.2 (Order of symplectic conjugate partitioned GARK methods). *Consider a GARK method (2) $(A^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$, $l, m = 1, \dots, N$ of order r with weights $b_i^{\{m\}} \neq 0$, for $i = 1, \dots, s^{\{m\}}$, $m = 1, \dots, N$. Then the GARK method $(\widehat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$, $l, m = 1, \dots, N$ with coefficients $\widehat{A}^{\{l,m\}}$ as in (11) has also order r , and so has the application of the symplectic pair $(A^{\{l,m\}}, \widehat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$ to a Lagrangian or Hamiltonian system (split in Hamiltonian terms).*

Proof. It is similar to the proof above. Let $\dot{p} = f(p) = \sum_{m=1}^N F^{\{m\}}(p)$ and let $H(q, p) = \sum_{m=1}^N H^{\{m\}}(q, p)$ where $H^{\{m\}}(q, p) = g^{\{m\}}(p) - F^{\{m\}}(p)q$. We set

$$\dot{q} = \sum_{m=1}^N (g^{\{m\}\prime}(p) - F^{\{m\}\prime}(p)q) = \dot{Q}_1 + \cdots + \dot{Q}_N.$$

Once again, we choose the $g^{\{m\}}(p)$ so that $\dot{Q}_m = g^{\{m\}\prime}(P_m) - F^{\{m\}\prime}(P_m)q$ is invertible, so that $P_m = h_m(q, \dot{Q}_m)$. Similarly, we construct the Lagrangian $L(q, \dot{q}) = \sum_{m=1}^N (P_m \dot{Q}_m - H^{\{m\}}(q, P_m)) = \sum_{m=1}^N L^{\{m\}}(q, \dot{q})$. By construction, we have $\frac{\partial}{\partial q} L^{\{m\}}(q, \dot{q}) = F^{\{m\}}(p)$ and by the same argument as above, the application of the GARK method of order r to the split Lagrangian $\sum_{m=1}^N L^{\{m\}}(q, \dot{q})$, implies that the symplectic conjugate method has also the same order, as it is just a consequence of the Legendre transformation. \square

Example 7.1. Consider $f(p) = p + p^2 = F^{\{1\}}(p) + F^{\{2\}}(p)$. We take $H(q, p) = \sum_{m=1,2} H^{\{m\}}(q, p)$ as above. To make the \dot{Q}_i invertible, we can choose $g^{\{1\}}(p) = \frac{1}{2}p^2$ and $g^{\{2\}} = 0$. This results in $P_1 = \dot{Q}_1 + q$ and $P_2 = -\frac{\dot{Q}_2}{2q}$. The Lagrangian is constructed as $L(q, \dot{q}) = \sum_{m=1,2} (P_m \dot{Q}_m - H^{\{m\}}(q, P_m))$, corresponding to $L^{\{1\}}(q, \dot{q}) = \frac{1}{2}(\dot{q} + q)^2$ and $L^{\{2\}}(q, \dot{q}) = -\frac{\dot{q}^2}{4q}$. This is the Lagrangian splitting corresponding to the partitioned symplectic GARK method. Using the GARK method of order r on the q variables will automatically result in the symplectic conjugate method on the p variables, and this must also be of order r .

As a consequence of Theorem 7.2, when considering symplectic conjugate partitioned GARK methods $(A^{\{l,m\}}, \hat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$ applied to a Lagrangian or Hamiltonian system², it is sufficient to study the order of only one of the GARK methods $(A^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$ (or $(\hat{A}^{\{l,m\}}, b^{\{m\}}, c^{\{l\}})$).

8. SPECIAL CASES FOR $N = 2$

We consider two main special cases, the first one when

$$L(q, \dot{q}) = L^{\{1\}}(q, \dot{q}) + L^{\{2\}}(q), \quad H(q, p) = H^{\{1\}}(q, p) + H^{\{2\}}(q)$$

that we call a *semi-separable* case, and the fully *separable* case

$$L(q, \dot{q}) = \frac{1}{2}\dot{q}^T \dot{q} - U(q), \quad H(q, p) = \frac{1}{2}p^T p + U(q),$$

for a potential function U . Some examples of the semi-separable case are mechanical systems in which the mass matrix depends on the generalized variable q , while $L^{\{2\}}(q) = -U(q)$, with U a potential depending on the generalized variable q only. Other example are the case of systems with *holonomic* constraints or stiff systems [Jay98, Tan18, Zan]. In the separable case, we assume that the mass matrix is constant and invertible, and, without loss of generality, we set it equal to I .

8.1. The semi-separable case. The variational derivation is the same as in [Zan], see also Section 3. Let

$$L(q, \dot{q}) = L^{\{1\}}(q, \dot{q}) + L^{\{2\}}(q).$$

One has

$$\begin{aligned} P_j^{\{1\}} &= \frac{\partial L^{\{1\}}}{\partial \dot{q}}(Q_j^{\{1\}}, \dot{Q}_j^{\{1\}}) & \dot{P}_j^{\{1\}} &= \frac{\partial L^{\{1\}}}{\partial q}(Q_j^{\{1\}}, \dot{Q}_j^{\{1\}}) \\ P_j^{\{2\}} &= \frac{\partial L^{\{2\}}}{\partial \dot{q}}(Q_j^{\{2\}}) = 0 & \dot{P}_j^{\{2\}} &= \frac{\partial L^{\{2\}}}{\partial q}(Q_j^{\{2\}}) \end{aligned}$$

²Split in Hamiltonian parts.

The constraint condition reads

$$b_j^{\{1\}} P_j^{\{1\}} = b_j^{\{1\}} \lambda - h \sum_{i=1}^{s^{\{1\}}} b_i^{\{1\}} a_{i,j}^{\{1,1\}} \dot{P}_j^{\{1\}} - h \sum_{i=1}^{s^{\{2\}}} b_i^{\{2\}} a_{i,j}^{\{1,2\}} \dot{P}_j^{\{2\}}.$$

As there is no $P^{\{2\}}$, the above relation *requires only* $b_j^{\{1\}}$ to be nonzero, $j = 1, \dots, s^{\{1\}}$. The symplecticity conditions are

$$\widehat{A}^{\{1,i\}} = (\mathbb{1}^{\{1,i\}} - (B^{\{1\}})^{-1} (A^{\{i,1\}})^T B^{\{i\}}), \quad i = 1, 2.$$

Since $P^{\{2\}}$ is not defined, the \dot{q} variables are recovered simply by inverting the Legendre transform $P_j^{\{1\}} = \frac{\partial L^{\{1\}}}{\partial \dot{q}}(Q_j^{\{1\}}, \dot{Q}_j^{\{1\}})$, implying that the q variable is only direct function of $P^{\{1\}}$, and therefore there is no need for $A^{\{l,2\}}$, for $l = 1, 2$. Eventually, the tables can be completed by choosing an appropriate $A^{\{2,2\}}$ compatible with the nodes $c^{\{2\}}$ and the weights $b^{\{2\}}$. Such matrix $A^{\{2,2\}}$ can also be useful in constructing the $A^{\{2,1\}}$ coefficients, if, for instance, one uses the methods proposed in Section 6. The method, in a partitioned GARK formalism reads

$$Q : \begin{array}{c|c} c^{\{1\}} & A^{\{1,1\}} \\ c^{\{2\}} & A^{\{2,1\}} \\ \hline & b^{\{1\}} \end{array}, \quad P : \begin{array}{c|cc} c^{\{1\}} & \widehat{A}^{\{1,1\}} & \widehat{A}^{\{1,2\}} \\ \hline & b^{\{1\}} & b^{\{2\}} \end{array},$$

where, in the Hamiltonian formalism introduced earlier,

$$\begin{aligned} V^{\{1\}}(Q_j^{\{1\}}, P_j^{\{1\}}) &= \dot{Q}_j^{\{1\}}, & V^{\{2\}} &= 0, \\ F^{\{1\}}(Q_j^{\{1\}}, P_j^{\{1\}}) &= \dot{P}_j^{\{1\}} & F^{\{2\}}(Q_j^{\{2\}}) &= \dot{P}_j^{\{2\}}, \end{aligned}$$

the first line being obtained by inverting the Legendre transform for $\dot{Q}_j^{\{1\}}$. In the Hamiltonian formalism, the methods read

$$\begin{aligned} Q_i^{\{1\}} &= q_0 + h \sum_{j=1}^{s^{\{1\}}} a_{i,j}^{\{1,1\}} V^{\{1\}}(Q_j^{\{1\}}, P_j^{\{1\}}) \\ Q_i^{\{2\}} &= q_0 + h \sum_{j=1}^{s^{\{1\}}} a_{i,j}^{\{2,1\}} V^{\{1\}}(Q_j^{\{1\}}, P_j^{\{1\}}) \\ q_1 &= q_0 + h \sum_{i=1}^{s^{\{1\}}} b_i^{\{1\}} V^{\{1\}}(Q_i^{\{1\}}, P_i^{\{1\}}) \\ P_i^{\{1\}} &= p_0 + h \sum_{j=1}^{s^{\{1\}}} \widehat{a}_{i,j}^{\{1,1\}} F^{\{1\}}(Q_j^{\{1\}}, P_j^{\{1\}}) + h \sum_{j=1}^{s^{\{2\}}} \widehat{a}_{i,j}^{\{1,2\}} F^{\{2\}}(Q_j^{\{2\}}) \\ p_1 &= p_0 + h \sum_{i=1}^{s^{\{1\}}} b_i^{\{1\}} F^{\{1\}}(Q_i^{\{1\}}, P_i^{\{1\}}) + h \sum_{i=1}^{s^{\{2\}}} b_i^{\{2\}} F^{\{2\}}(Q_i^{\{2\}}) \end{aligned}$$

8.2. The fully separable case. Proceeding as above,

$$\begin{aligned} P_j^{\{1\}} &= \frac{\partial L^{\{1\}}}{\partial \dot{q}}(\dot{Q}_j^{\{1\}}) & \dot{P}_j^{\{1\}} &= 0 \\ P_j^{\{2\}} &= 0 & \dot{P}_j^{\{2\}} &= \frac{\partial L^{\{2\}}}{\partial q}(Q_j^{\{2\}}). \end{aligned}$$

The constraint condition reads

$$b_j^{\{1\}} P_j^{\{1\}} = b_j^{\{1\}} \lambda - h \sum_{i=1}^{s^{\{2\}}} b_i^{\{2\}} a_{i,j}^{\{1,2\}} \dot{P}_j^{\{2\}},$$

where, as before, we require the $b_j^{\{1\}}$ to be nonzero. In the Hamiltonian setting, taking

$$\dot{Q}_i^{\{1\}} = V^{\{1\}}(P_i^{\{1\}}), \quad \dot{P}_i^{\{2\}} = F^{\{2\}}(Q_i^{\{2\}}),$$

the system reads

$$\begin{aligned} Q_i^{\{2\}} &= q_0 + h \sum_{j=1}^{s^{\{1\}}} a_{i,j}^{\{2,1\}} V^{\{1\}}(P_j^{\{1\}}), \\ q_1 &= q_0 + h \sum_{i=1}^{s^{\{1\}}} b_i^{\{1\}} V^{\{1\}}(P_i^{\{1\}}) \\ P_i^{\{1\}} &= p_0 + h \sum_{j=1}^{s^{\{2\}}} \hat{a}_{i,j}^{\{1,2\}} F^{\{2\}}(Q_j^{\{2\}}) \\ p_1 &= p_0 + h \sum_{i=1}^{s^{\{2\}}} b_i^{\{2\}} F^{\{2\}}(Q_i^{\{2\}}). \end{aligned}$$

The scheme has tableau

$$Q : \frac{c^{\{2\}}}{b^{\{1\}}} \left| \begin{array}{c} A^{\{2,1\}} \\ b^{\{1\}} \end{array} \right., \quad P : \frac{c^{\{1\}}}{b^{\{2\}}} \left| \begin{array}{c} \hat{A}^{\{1,2\}} \\ b^{\{2\}} \end{array} \right.$$

and the matrices need not be square, as in the usual setting. For instance one could choose the symplectic method

$$(28) \quad Q : \begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} + \frac{1}{8}\sqrt{3} & \frac{1}{4} - \frac{1}{8}\sqrt{3} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad P : \begin{array}{c|ccc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{6} & \frac{1}{3} - \frac{1}{6}\sqrt{3} & 0 \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{6} & \frac{1}{3} + \frac{1}{6}\sqrt{3} & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

see Section 6 (collocation example). We observe that it is allowed to use different weights $b^{\{1\}}$ and $b^{\{2\}}$ for the Q and the P part respectively. The symplecticity condition is

$$\hat{A}^{\{1,2\}} = (\mathbb{1}^{\{1,2\}} - (B^{\{1\}})^{-1} (A^{\{2,1\}})^T) B^{\{2\}},$$

which coincides with the well known sufficient symplecticity condition for PRK for the separable case,

$$b_i^{\{1\}} b_j^{\{2\}} = b_i^{\{1\}} \hat{a}_{i,j}^{\{1,2\}} + b_j^{\{2\}} a_{j,i}^{\{2,1\}},$$

[EH06, SSC94, AMSS97]. Note, however, that there must be some form of compatibility as the weights of the q -part must be compatible with the nodes of the p -part and viceversa. The rectangular scheme (28) is essentially implicit only in the Q_2 stage only, it has order four, as it follows from our error analysis, shares many of the benefits of Gauss-Legendre and Gauss-Lobatto methods, in addition to being slightly computationally less expensive than both the underlying methods methods.

In the general setting (non-separable) the weights used in the GARK method for the Q and P part must be the same set of weights, as it is clear from the variational derivation in Section 3.

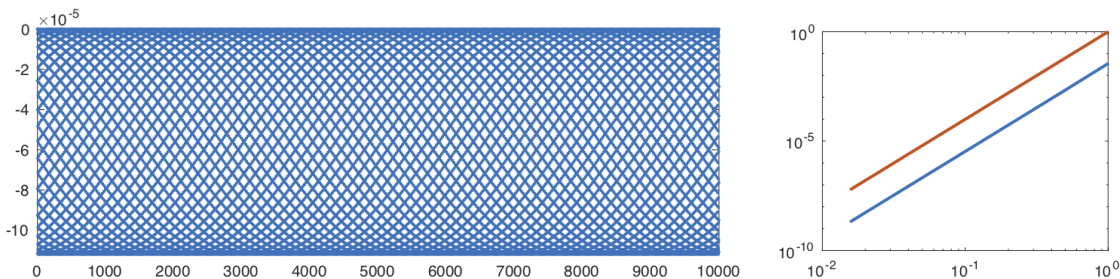


FIGURE 1. Error in the total energy (left) in $[0, 10^4]$ with stepsize $h = \frac{1}{2}$ and log-log order plot (right) for the unconventional method (28) applied to the harmonic oscillator. The red line is the reference line for order four.

9. CONCLUSIONS AND FURTHER REMARKS

We have presented a variational framework that allows for the treatment of different Lagrangian terms by different RK methods. The framework uses GARK methods and leads to symplectic partitioned numerical methods that can be put in a GARK formalism. Since the methods for the q and p variables are conjugate by virtue of the symplectic condition imposed by the Legendre transform, we have shown that the order analysis needs only be carried out on one of the methods, thus significantly simplifying the analysis task. Further, we have proposed two ways of constructing transfer coefficients $A^{\{l,m\}}$, which, in turn, allow for an infinite family of coefficients satisfying the same order conditions. The main idea is to use as diagonal methods one's favourite methods, with good properties, and to derive transfer conditions that share these properties and possibly other desirable properties, by tuning the free parameters, see for instance [Zan].

We have also discussed in more detail the special case $N = 2$, for semiseparable and separable problems. For the separable case, we have given an example of an unconventional scheme, constructed from Gauss–Legendre and Gauss–Lobatto, with rectangular matrices. The method is symplectic, fourth order, and essentially only implicit in one variable.

The following topics were not addressed in this paper, as they are more natural in a Hamiltonian setting rather than Lagrangian setting.

- The case of zero weights, as we have assumed $b_i^{\{m\}} \neq 0$, $i = 1, \dots, s^{\{m\}}$, for all $m = 1, \dots, N$.
- The case of redundant stages. In several proofs we use the uniqueness and the order of Lagrange interpolation, and for this purpose we have assumed $c_i^{\{m\}} \neq c_j^{\{m\}}$, $i \neq j$, $i, j = 1, \dots, s^{\{m\}}$, for all $m = 1, \dots, N$. When some of the nodes coincide, extra conditions on derivatives might be required.
- The number of order conditions for an arbitrary symplectic partitioned GARK method for Hamiltonian vector fields. If it is desirable to derive *all* the coefficients of a symplectic partitioned GARK method for both the q and p variables imposing symplecticity of the vector field, there is a reduction in number of total order conditions due to the fact that the underlying vector field is not arbitrary, hence some of the order conditions fall out and need not be satisfied, see also [AMSS97].

These three topics are more relevant in the context of the derivation of new coefficients (also for the diagonal methods) directly from the order conditions, rather than using one's favourite diagonal methods, that already has some desirable properties, as it has been the main focus of this paper.

ACKNOWLEDGEMENTS

The author would like to thank the Isaac Newton Institute for Mathematical Sciences, Cambridge, for support and hospitality during the programme “Geometry, Compatibility and Structure

Preservation in Computational Differential Equations” where work on this paper was undertaken. This work was supported by EPSRC grant no. EP/R014604/1.

REFERENCES

- [AMSS97] A. L. Araújo, A. Murua, and J. M. Sanz-Serna. Symplectic methods based on decompositions. *SIAM J. Numer. Anal.*, 34(5):1926–1947, 1997.
- [Bor01] F. Bornemann. Runge–Kutta methods, trees and maple. on a simple proof of Butcher’s Theorem and the automatic generation of Order Conditions. *Selçuk Journal of Applied Mathematics*, 2(1), 2001. <http://acikerisimarsiv.selcuk.edu.tr:8080/xmlui/handle/123456789/3403>.
- [CS83] G. J. Cooper and A. Sayfy. Additive Runge–Kutta methods for stiff ordinary differential equations. *Math. Comp.*, 40(161):207–2018, 1983.
- [EH06] G. Wanner E. Hairer, C. Lubich. *Geometric Numerical Integrtion, Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics. Springer, 2006.
- [Jay98] L. Jay. Structure preservation for constrained dynamics with super partitioned additive Runge–Kutta methods. *SIAM J. Sci. Comput.*, 20(2):416–446, 1998.
- [MW01] J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numerica*, 10:357514, 2001.
- [OBJM11] S. Ober-Blöbaum, O. Junge, and J. E. Marsden. Discrete mechanics and optimal control: An analysis. *ESAIM: COCV*, 17(2):322–352, 2011.
- [SG15] A. Sandu and M. Günther. A generalized-structure approach to additive Runge–Kutta methods. *SIAM J. Num. Anal.*, 53(1):17–42, 2015.
- [SSC94] J. M. Sanz-Serna and M. P. Calvo. *Numerical Hamiltonian Problems*. AMMC 7. Chapman & Hall, 1994.
- [Tan18] G. M. Tanner. *Generalized additive Runge–Kutta methods for stiff ODEs*. PhD thesis, University of Iowa, 2018.
- [WOBL16] T. Wenger, S. Ober-Blöbaum, and S. Leyendecker. Variational integrators of mixed order for dynamical systems with multiple time scales and split potentials. In G. Stefanou M. Papadrakakis, V. Papadopoulos and V. Plevris, editors, *ECCOMAS Congress 2016*, 2016.
- [WOBL17] T. Wenger, S. Ober-Blöbaum, and S. Leyendecker. Construction and analysis of higher order variational integrators for dynamical systems with holonomic constraints. *Advances in Computational Mathematics*, 43(5):1163–1195, Oct 2017.
- [Zan] A. Zanna. Symplectic P-stable additive Runge–Kutta methods. arXiv:1909.11017.