SYMPLECTIC GARK METHODS FOR PARTITIONED HAMILTONIAN SYSTEMS

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Abstract. Generalized Additive Runge-Kutta schemes have shown to be a suitable tool for solving ordinary differential equations with additively partitioned right-hand sides. This work develops symplectic GARK schemes for additively partitioned Hamiltonian systems. In a general setting, we derive conditions for symplecticness, as well as symmetry and time-reversibility. We show how symplectic and symmetric schemes can be constructed based on schemes which are only symplectic, or only symmetric. Special attention is given to the special case of partitioned schemes for Hamiltonians split into multiple potential and kinetic energies. Finally we show how symplectic GARK schemes can leverage different time scales and evaluation costs for different potentials, and provide efficient numerical solutions by using different order for these parts.

Key words. Generalized additive Runge-Kutta methods, Symplectic schemes, symmetric schemes, Partitioned symplectic GARK schemes

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1. Introduction. In many applications, initial value problems of ordinary differential equations are given as additively partitioned systems of the form:

\[ y' = f(y) = \sum_{m=1}^{N} f^{(m)}(y), \quad t \geq t_0, \quad y(t_0) = y_0, \]

where the right-hand side \( f : \mathbb{R}^d \rightarrow \mathbb{R}^d \) is split into \( N \) different parts with respect to, for example, stiffness, nonlinearity, dynamical behavior, and evaluation cost.

One step of a GARK method applied to (1.1) advances the solution \( y_0 \) at \( t_0 \) to the solution \( y_1 \) at \( t_1 = t_0 + h \) as follows:

\[
\begin{align*}
Y^{(q)}_i &= y_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a^{(q,m)}_{i,j} f^{(m)}(y^{(m)}_j), \\
y_1 &= y_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{(q)}} b^{(q)}_i f^{(q)}(y^{(q)}_i).
\end{align*}
\]

The general-structure additive Runge-Kutta (GARK) framework, developed in [22], allows to construct multimethods that apply a different Runge-Kutta scheme,
with possibly different time steps, to discretize each component of (1.1). The GARK framework explicitly reveals the structure of the multmethod in form of the numerical discretizations of individual components and coupling terms. The GARK formalism allowed to construct new schemes such as implicit-implicit, multirate methods of high order, multirate infinitesimal step schemes, and partitioned Rosenbrock methods. In addition, it was shown that all classical splitting-based implicit time integration schemes can be understood as GARK methods.

Hamiltonian dynamics is fundamental to many fields in science and engineering. Symplectic integrators are special schemes for the numerical solution of Hamiltonian systems that preserve the geometric properties of the flow of the differential equation. Higher order symplectic integrators are typically constructed by “operator splitting”, and symmetrically alternating fractional steps. Explicit symplectic schemes for partitioned Hamiltonians are also based on splitting the potential and kinetic energies.

In this paper we discuss the GARK numerical solutions of split Hamiltonian systems, where each component of the system may correspond to a Hamiltonian subsystem or not. The main contributions of this work are as follows. (i) Symplecticness, symmetry, and order conditions for GARK schemes applied to partitioned Hamiltonian systems are derived. (ii) The GARK formalism allows to consider very general partitions of Hamiltonian systems (e.g., splitting the Hamiltonian or splitting only the potential energy) of type \( f(y) = J \nabla H(y) \) with an arbitrary, but skew-symmetric matrix \( J = -J^T \). (iii) The GARK approach allows to integrate each component of the Hamiltonian with a different method, e.g., a high order method for the fast component and a low order method for the slow component. (iv) We construct symmetric and symplectic partitioned methods starting from partitioned symmetric (but non-symmetric) schemes, or starting from symplectic (but non-symmetric) methods. This is discussed in Section 4.4. We show that explicit symplectic and symmetric partitioned GARK schemes are composition schemes.

The paper is organized as follows. Section 2 reviews Hamiltonian systems, partitioned forms, and GARK schemes for the integration of partitioned systems. Section 3 introduces general symplectic GARK schemes. We derive conditions on the coefficients for symplecticity, which reduce the number of order conditions of GARK schemes drastically, and discuss symmetry and time-reversibility. If the Hamiltonians are split with respect to the potentials or kinetic parts and potentials, respectively, partitioned versions of symplectic GARK schemes are tailored to exploit this structure. Section 4 introduces these schemes, with a discussion of symplecticity conditions, order conditions, symmetry and time-reversibility, as well as GARK discrete adjoints. Section 5.2 discusses how symplectic GARK schemes can exploit the multirate potential given by potentials of different activity levels. Numerical tests for a coupled oscillator are given. Section 6 concludes with a summary.

2. Partitioned Hamiltonian systems and GARK schemes. A Hamiltonian system is given by the ODE initial value problem

\[
y' = J \nabla H(y), \quad y(t_0) = y_0, \quad \text{with} \quad y = \begin{bmatrix} p \\ q \end{bmatrix}, \quad J = \begin{bmatrix} 0_{dp \times dp} & -I_{dp \times dq} \\ I_{dp \times dp} & 0_{dq \times dq} \end{bmatrix},
\]

where \( d_p = d_q = d/2, \) \( q \in \mathbb{R}^{dq} \) denote the generalized coordinates, \( p \in \mathbb{R}^{dp} \) the conjugate momenta, and \( H : \mathbb{R}^{dp} \times \mathbb{R}^{dq} \to \mathbb{R} \) is a twice continuously differentiable function.
Hamiltonian function. The Hamiltonian flow $y(t) = \varphi_t(y_0)$, i.e., the solution to (2.1), is characterized by the following properties:

- The Hamiltonian is an invariant of the flow:

$$\frac{d}{dt} H(\varphi_t(y_0)) = 0. \quad (2.2)$$

- The Hamiltonian is invariant with respect of changing the sign of momenta, $H(p, q) = H(-p, q)$. This can be formalized as follows:

$$H = H \circ \rho \quad \text{where} \quad \rho = \begin{bmatrix} -I_{d_p \times d_p} & 0_{d_p \times d_q} \\
0_{d_q \times d_p} & I_{d_q \times d_q} \end{bmatrix}. \quad (2.3)$$

Consequently, the Hamiltonian equation of motion (2.1) are $\rho$-reversible, i.e., $\rho \circ (\nabla H) = -\nabla (H \circ \rho)$.

- The Hamiltonian flow is time-reversible:

$$\rho \circ \varphi_t \circ \rho \circ \varphi_t(y_0) = y_0 \iff \rho \circ \varphi_t = \varphi_{-t} \circ \rho, \quad (2.4)$$

where the second equivalent equation is due to the symmetry $\varphi_t \circ \varphi_{-t}(y_0) = y_0$ of the flow.

- The Hamiltonian flow is symplectic:

$$(\frac{\partial \varphi_t(y_0)}{\partial y_0})^\top J^{-1} \left( \frac{\partial \varphi_t(y_0)}{\partial y_0} \right) = J^{-1}, \quad (2.5)$$

and thus volume-preserving

$$\det \left( \frac{\partial \varphi_t(y_0)}{\partial y_0} \right) = 1. \quad (2.6)$$

In geometric integration, we demand the mapping $y_0 \mapsto \Phi_t(y_0)$ defining the numerical approximation $\Phi_t(y_0) \approx \varphi_t(y_0)$ to be time-reversible and symplectic as well:

$$(2.7a) \quad \rho \circ \Phi_t \circ \rho \circ \Phi_t(y_0) = y_0,$$

$$(2.7b) \quad \left( \frac{\partial \Phi_t(y_0)}{\partial y_0} \right)^\top J^{-1} \left( \frac{\partial \Phi_t(y_0)}{\partial y_0} \right) = J^{-1}. \quad (2.7b)$$

**Remark 1.** If we replace $J$ in (2.1) by an arbitrary regular skew-symmetric matrix, the invariance of the Hamiltonian (2.2) and the symplecticeness (2.5) of the flow (here the proof of Theorem 2.4 in [12] directly generalizes to regular skew-symmetric matrices) still hold, as well as volume-preservation (2.6). In this case, however, the unknowns $q$ and $p$ might lose their meaning as generalized coordinates and positions of classical mechanics, and time-reversibility (2.4) loses its significance.

**2.1. GARK schemes for Hamiltonian systems.** Consider a general splitting of the right-hand side of the type

$$y' = \sum_{m=1}^{N} f^{(m)}(y). \quad (2.8)$$
One step of a GARK method (1.2) applied to (2.8) advances the solution \((y_0)\) at \(t_0\) to the solution \((y_1)\) at \(t_1 = t_0 + h\) as follows:

\[
\begin{align*}
(Y_{i}^{q}) & = y_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s(m)} a_{i,j}^{m,q} k_{j}^{m}, \quad q = 1, \ldots, N, \\
k_{i}^{m} & := f_{i}^{m} \left( Y_{i}^{m} \right), \\
y_1 = y_0 + h \sum_{q=1}^{N} b_{i}^{q} k_{i}^{(q)}. 
\end{align*}
\]

The corresponding generalized Butcher tableau is:

\[
\begin{align*}
\begin{bmatrix}
A^{(1,1)} & \cdots & A^{(1,N)} \\
\vdots & \ddots & \vdots \\
A^{(N,1)} & \cdots & A^{(N,N)}
\end{bmatrix}
\begin{bmatrix}
b_1^{T} \\
\vdots \\
b_N^{T}
\end{bmatrix}
= 
\begin{bmatrix}
A_{GARK}^{(1,1)} & \cdots & A_{GARK}^{(1,N)} \\
\vdots & \ddots & \vdots \\
A_{GARK}^{(N,1)} & \cdots & A_{GARK}^{(N,N)}
\end{bmatrix}
\begin{bmatrix}
b_1^{(1)} \\
\vdots \\
b_1^{(N)}
\end{bmatrix}. 
\end{align*}
\]

In contrast to traditional additive methods [14] different stage values are used with different components of the right hand side. The methods \((A^{(q,q)}, b^{(q)})\) can be regarded as stand-alone integration schemes applied to each individual component \(q\). The off-diagonal matrices \(A^{(q,m)}\), \(m \neq q\), can be viewed as a coupling mechanism among components.

We define the abscissae associated with each tableau as \(c^{(q,1)} = \cdots = c^{(q,N)} =: c^{(q)}, \quad q = 1, \ldots, N\).

A particular splitting case is offered by partitioned Hamiltonian systems, which are characterized by a Hamiltonian function \(H(y)\) split into \(N\) individual Hamiltonians:

\[
H(y) = \sum_{m=1}^{N} H^{(m)}(y).
\]

Consequently, the equations of motion are a partitioned system (2.8) where each component function corresponds to one individual Hamiltonian:

\[
y' = J \nabla H(y) = \sum_{m=1}^{N} f^{(m)}(y), \quad f^{(m)}(y) := J \nabla H^{(m)}(y).
\]

An efficient numerical integration scheme needs to exploit the different properties of the \(N\) individual Hamiltonians, such as slow dynamics with expensive evaluation costs versus fast dynamics with cheap evaluation costs, while preserving time-reversibility and symplecticity. One class of numerical schemes tailored to exploiting different right-hand side component properties are partitioned GARK schemes: one step of a GARK method (1.2) applied to (2.12) advances the solution \((y_0)\) at \(t_0\) to the solution \((y_1)\) at \(t_1 = t_0 + h\) as given in (2.9), with (2.9b) replaced by

\[
k_{i}^{(m)} = J \nabla H^{(m)}(Y_{i}^{(m)}),
\]
An example of a system with skew-symmetric, but singular $J$ is given next.

**Example 1** (Splitting of Hamiltonian for a two mass oscillator).

Consider the following one-dimensional mechanical system consisting of two masses and three linear springs shown in Fig. 2.1. It has the Hamiltonian

\[
H = \frac{1}{2} \left( \frac{p_1^2}{m_1} + \frac{p_2^2}{m_2} + K_1 q_1^2 + K(q_1 - q_2)^2 + K_2 q_2^2 \right).
\]

If we split the system into two subsystems consisting of elements $(K_1, m_1, K)$ and $(m_2, K_2)$, the $H$ is split into the two Hamiltonians $H_1$ and $H_2$ of the subsystems with

\[
H_1(p_1, q_1, q_1 - q) = \frac{1}{2} \left( \frac{p_1^2}{m_1} + K_1 q_1^2 + K(q_1 - q)^2 \right), \quad H_2(p_2, q_2) = \frac{1}{2} \left( \frac{p_2^2}{m_2} + K_2 q_2^2 \right),
\]

respectively, where $q$ is a port variable that defines the coupling parameter from the first to the second system; for the coupling configuration above $q = q_2$. Now the dynamics can be defined by two coupled port-Hamiltonian systems (see [4]), which yields in condensed form with $x = (x_1, x_2)^T$, $x_1 = (p_1, q_1, q_1 - q)^T$ and $x_2 = (p_2, q_2)^T$:

\[
\dot{x} = J \cdot \nabla H(x), \quad J = \begin{bmatrix} J_1 & B \\ -B^T & J_2 \end{bmatrix},
\]

with $\nabla$ denoting the derivative with respect to $x$ and

\[
J_1 = \begin{bmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad J_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.
\]

A Hamiltonian splitting is given by

\[
f^{(1)}(x_1, x_2) = \begin{bmatrix} J_1 & B \\ -B^T & J_2 \end{bmatrix} \nabla H_1(x_1), \quad f^{(2)}(x_1, x_2) = \begin{bmatrix} J_1 & B \\ -B^T & J_2 \end{bmatrix} \nabla H_2(x_2).
\]

One may also split $J$ instead of the Hamiltonian $H$ and obtain either a non-Hamiltonian (component-wise) splitting by

\[
f^{(1)}(x_1, x_2) = \begin{bmatrix} J_1 & B \\ 0 & 0 \end{bmatrix} \cdot \nabla H(x), \quad f^{(2)}(x_1, x_2) = \begin{bmatrix} 0 & 0 \\ -B^T & J_2 \end{bmatrix} \cdot \nabla H(x),
\]

Fig. 2.1: The two masses oscillator.
or a (non-)Hamiltonian splitting with respect to subsystems and coupling parts

\[
\begin{align*}
 f^{(1)}(x_1, x_2) &= \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix} \cdot \nabla H(x), \\
 f^{(2)}(x_1, x_2) &= \begin{bmatrix} 0 & B \\ -B^\top & 0 \end{bmatrix} \cdot \nabla H(x).
\end{align*}
\]

**Remark 2.** Note that the skew-symmetric matrix \( J \) in (2.14) is singular. Nevertheless, it fulfills a symplectic structure as we can see as follows: as the Hamiltonian is quadratic, (2.14) can be written as \( \dot{x} = JQx \) with \( Q \) positive-definite, which can be transformed into \( \dot{w} = \tilde{J}w \) with \( w := Q^{1/2}x \) and \( \tilde{J} = Q^{1/2}JQ^{1/2} \). Consider now the variational equations \( \dot{\Phi} = JQ\Phi, \Phi(0) = I_{5 \times 5} \) and \( \dot{\Psi} = \tilde{J}\Psi, \Psi(0) = I_{5 \times 5} \) of the original and transformed system, resp. Defining \( J^+ \) as the Drazin inverse of \( J \) and \( \tilde{J}^+ \) as the Drazin inverse of \( \tilde{J} \), we get on the one hand

\[
\begin{align*}
 \frac{d}{dt} \left( \Psi^\top \tilde{J}^+ \Psi \right) &= (\Psi^\top \tilde{J}^+ \Psi + \Psi^\top \tilde{J}^+ \Psi) \\
 &= (\tilde{J}\Psi)^\top \tilde{J}^+ \Psi + \Psi^\top \tilde{J}^+ (\tilde{J}\Psi) \\
 &= \Psi^\top (\tilde{J}^+ \tilde{J}^+ + \tilde{J}^+ \tilde{J}) \Psi \\
 &= \Psi^\top \left( -\tilde{J} \tilde{J}^+ + \tilde{J}^+ \tilde{J} \right) \Psi \\
 &= 0,
\end{align*}
\]

i.e., \( \Psi^\top \tilde{J}^+ \Psi = \tilde{J}^+ \) is a quadratic invariant. On the other hand we have with \( \Psi = Q^{1/2}\Phi \)

\[
\Psi^\top \tilde{J}^+ \Psi = (Q^{1/2}\Phi)^\top (Q^{1/2}JQ^{1/2})^+ (Q^{1/2}\Phi) = \Phi^\top Q^{1/2}Q^{-1/2}J^+ Q^{-1/2}Q^{1/2} \Phi = \Phi^\top J^+ \Phi,
\]

which shows that \( \Phi^\top J^+ \Phi = J^+ \) is a quadratic invariant, too. Summing up, for a singular skew-symmetric matrix \( J \) the symplectic structure given by (2.5) holds, if one replaces \( J^{-1} \) by the Drazin inverse of \( J \).

3. Symplectic GARK schemes – the general case. In this section we consider the general case of GARK schemes (2.9) applied to a Hamiltonian system (2.1) based on a general splitting (2.8).

Several matrices are defined from the coefficients of (1.2) for \( m, \ell = 1, \ldots, N \):

\[
\begin{align*}
(3.1a) \quad & B^{(m)} := \text{diag}(b^{(m)}) \in \mathbb{R}^{s^{(m)} \times s^{(m)}}, \\
(3.1b) \quad & B^{(m, \ell)} := A^{(\ell, m)}^\top B^{(\ell)} + B^{(m)} A^{(m, \ell)} - b^{(m)} b^{(\ell)}^\top \in \mathbb{R}^{s^{(m)} \times s^{(\ell)}}, \\
(3.1c) \quad & P := [P^{(m, \ell)}]_{1 \leq \ell, m \leq N} \in \mathbb{R}^{s \times s}, \quad \text{where} \quad s := \sum_{m=1}^{N} s^{(m)}.
\end{align*}
\]

The matrix \( P \in \mathbb{R}^{s \times s} \) is symmetric since \( P^{(\ell, m)} = P^{(m, \ell)^\top} \). It was shown in [22] that the GARK method is algebraically stable iff the matrix \( P \) is non-negative definite. Using the Butcher tableau (2.10) the matrix (3.1c) is constructed as:

\[
(3.2) \quad B_{\text{GARK}} := \text{diag}(b_{\text{GARK}}), \quad \text{P} = A_{\text{GARK}}^\top B_{\text{GARK}} + B_{\text{GARK}} A_{\text{GARK}} - b_{\text{GARK}} b_{\text{GARK}}^\top.
\]
We have the following property that generalizes the characterization of symplectic Runge Kutta schemes \[13\].

**Theorem 3.1** (Symplectic GARK schemes). *Consider a GARK scheme \([2.13]\)* applied to an Hamiltonian splitting \([2.12]\), and its matrix \(P\) defined by \((3.1c)\). The GARK scheme is symplectic if and only if \(P = 0_{s \times s}\), which is equivalent to:

\[
P^{\{m, \ell\}} = A^{\{\ell, m\}}^T B^{\{\ell\}} + B^{\{m\}} A^{\{m, \ell\}} - b^{\{m\}} b^{\{\ell\}}^T = 0_{s^{(m)} \times s^{(\ell)}},
\]

\[\forall \, \ell, m = 1, \ldots, N.\]

**Proof.** The proof is based on symplectic NB-series introduced in \([1]\), and is similar to the proof for Runge-Kutta, partitioned Runge-Kutta methods \([26]\) and ARK schemes \([1]\).

N-trees \([1]\) are a generalization of P-trees from the case of component partitioning to the general case of right-hand side partitioning \((1.1)\). The set \(T_N\) of N-trees consists of all Butcher trees with colored vertices; each vertex is assigned one of \(N\) different colors corresponding to the \(N\) components of the partition. Similar to regular Butcher trees each vertex is also assigned a label. The order \(\rho(u)\) is the number of nodes of \(u \in T_N\).

The empty N-tree is denoted by \(\emptyset\). The N-tree with a single vertex of color \(m\) is denoted by \(\tau_{\{m\}}\). The N-tree \(u \in T_N\) with \(\rho(u) > 1\) and a root of color \(m\) can be represented as \(u = \{u_1, \ldots, u_r\}_m\), where \(\{u_1, \ldots, u_r\}\) are the non-empty subtrees (N-trees) arising from removing the root of \(u\). The elementary differential associated with the N-tree \(u\) and evaluated at \(y\) is:

\[
F(u)(y) := \begin{cases} y, & u = \emptyset; \\ \sum_{t \in T_N} \sum_{\ell, m} a(\ell, m) \frac{h^{t(t)}}{\sigma(t)} F(t)(y(t)), & u = [u_1, \ldots, u_r]_m. 
\end{cases}
\]

An NB-series is a formal power expansion:

\[
NB(a, y(t)) := \sum_{t \in T_N} a(t) \frac{h^{t(t)}}{\sigma(t)} F(t)(y(t)),
\]

where \(a : T_N \rightarrow \mathbb{R}\) is a mapping that assigns a real number to each N-tree; with some abuse of nomenclature we call the mappings NB-series as well. It can be shown that the stage vectors and the solution of the GARK scheme \(2.13\) can be written as NB-series:

\[
\begin{align*}
k^{(m)}_i &= NB(\theta^{(m)}_i, y_0), & \theta^{(m)} = [\theta^{(m)}_1 \ldots \theta^{(m)}_{s(m)}]^T; \\
y_1 &= NB(a, y_0).
\end{align*}
\]

The Butcher product \(u \bullet v\) of the NT-trees \(u, v\) is defined as follows:

\[
\begin{align*}
\{u_1, \ldots, u_r\}_m, & \quad u_1 \bullet v := \begin{cases} u, & v = \emptyset; \\ v, & u = \tau_{\{m\}}, \\
\{v_1, \ldots, v_p\}_n, & \quad \{u_1, \ldots, u_r, v\}_m, \quad \text{otherwise.}
\end{cases}
\end{align*}
\]

Consider the NB-series associated with a partitioning where each component is Hamiltonian. In Araujo et al \([1]\) it is shown that the NB-series \(a\) is symplectic (for the special case of \(J\) given by \([2.1]\)) iff for each pair \(u, v \in T_N \setminus \{\emptyset\}\) it holds that

\[
a(u \bullet v) + a(v \bullet u) = a(u) a(v).
\]
This result also holds for an arbitrary regular skew-symmetric matrix $J$, as the argumentation in [1] is based only on the skew-symmetry of $J$, and not on the special structure of $J$ in the Hamiltonian dynamics case (2.1).

Consider the non-empty NT-trees $u$ and $v$ in (3.7) and define:

\[(3.9)\quad U := g^{(m)}(u_1) \times \cdots \times g^{(m)}(u_r), \quad V := g^{(n)}(v_1) \times \cdots \times g^{(n)}(v_p),\]

where $\times$ denotes the element-by-element product of vectors. From (2.13) we have the following expressions for the corresponding NB-series:

\[a(u) = b^{(m)}(U) = \sum_{i=1}^{s^{(m)}} b_{i}^{(m)} U_i, \quad a(v) = b^{(n)}(V) = \sum_{j=1}^{s^{(n)}} b_{j}^{(n)} V_j,\]

\[a(u \cdot v) = b^{(m)}(U \times A^{(m,n)} V) = \sum_{i=1}^{s^{(m)}} \sum_{j=1}^{s^{(n)}} b_{i}^{(m)} U_i A_{i,j}^{(m,n)} V_j,\]

\[a(v \cdot u) = b^{(n)}(V \times A^{(n,m)} U) = \sum_{j=1}^{s^{(n)}} \sum_{i=1}^{s^{(m)}} b_{j}^{(n)} V_j A_{j,i}^{(n,m)} U_i,\]

After reordering the coefficients, the symplecticness condition (3.8) reads:

\[(3.10)\quad \sum_{i=1}^{s^{(m)}} \sum_{j=1}^{s^{(n)}} \left( b_{i}^{(m)} A_{i,j}^{(m,n)} + (A_{i,j}^{(n,m)})^{\top} b_{j}^{(n)} - b_{i}^{(m)} b_{j}^{(n)} \right) U_i V_j = 0,
\]

which is equivalent to $P^{(m,n)} = 0$. □

**Corollary 3.2.** A GARK scheme (2.9) based on a general splitting (2.8) is symplectic iff (3.3) and

\[(3.11)\quad b^{(\mu)} = b^{(\sigma)}, \quad s^{(\mu)} = s^{(\sigma)}, \quad \forall \mu, \sigma = 1, \ldots, N
\]

hold.

**Proof.** This follows directly from Araujo et al [1]: for a general splitting, the NB-series $a$ is symplectic iff in addition to (3.8) the following condition holds: $a(u) = a(v)$ for each pair of nonempty N-trees $u, v$ that differ only in the color of their roots. □

**Remark 3.** Additive Runge-Kutta schemes applied to a general splitting can always be rewritten as a single symplectic Runge-Kutta method for the non-decomposed system, see [2]. However this is not the case for symplectic GARK schemes, as shown in Example 3.

**3.1. Order conditions.** As shown in [22], the order conditions for a GARK method (1.2) are obtained from the order conditions of ordinary Runge–Kutta methods. The usual labeling of the Runge-Kutta coefficients (subscripts $i, j, k, \ldots$) is accompanied by a corresponding labeling of the different partitions (superscripts
m, s, t, . . .). The conditions for orders one to four are as follows:

\begin{align}
(3.12a) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{1}^{(m)} = 1, \quad \forall m, \quad \text{(order 1)} \\
(3.12b) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{c}^{(m,\ell)} = \frac{1}{2}, \quad \forall m, \ell, \quad \text{(order 2)} \\
(3.12c) & \quad \mathbf{b}^{(m)\top} \cdot \left( \mathbf{c}^{(m,\ell)} \times \mathbf{c}^{(m,s)} \right) = \frac{1}{2}, \quad \forall m, \ell \leq s, \quad \text{(order 3)} \\
(3.12d) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{A}^{(m,\ell)} \cdot \mathbf{c}^{(\ell,s)} = \frac{1}{6}, \quad \forall m, \ell, s, \quad \text{(order 3)} \\
(3.12e) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{c}^{(m,\ell)} = \frac{1}{4}, \quad \forall m, \ell s \leq t, \quad \text{(order 4)} \\
(3.12f) & \quad \mathbf{b}^{(m)\top} \cdot \left( \mathbf{c}^{(m,\ell)} \times \mathbf{c}^{(m,s)} \times \mathbf{c}^{(m,t)} \right) = \frac{1}{8}, \quad \forall m, \ell s \leq t, \quad \text{(order 4)} \\
(3.12g) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{A}^{(m,\ell)} \cdot \left( \mathbf{c}^{(\ell,s)} \times \mathbf{c}^{(\ell,t)} \right) = \frac{1}{12}, \quad \forall m, \ell s \leq t, \quad \text{(order 4)} \\
(3.12h) & \quad \mathbf{b}^{(m)\top} \cdot \mathbf{A}^{(m,\ell)} \cdot \mathbf{A}^{(\ell,s)} \cdot \mathbf{c}^{(s,t)} = \frac{1}{24}, \quad \forall m, \ell s t. \quad \text{(order 4)}
\end{align}

Here, the standard matrix and vector multiplication is denoted by dot (e.g., $\mathbf{b}^\top \cdot \mathbf{c}$ is a dot product), whereas the cross denotes component-wise multiplication (e.g., $\mathbf{b} \times \mathbf{c}$ is a vector of element-wise products). For internally consistent schemes these order conditions simplify considerably. Moreover, for symplectic GARK schemes many of the order conditions [3.12] are redundant.

Remark 4 (Redundancy of order conditions for symplectic GARK schemes). Assume that the symplectic GARK method has a solution with NB-series coefficients $\mathbf{a}$, and that it satisfies all conditions up to order $k$:

$$a(u) = \frac{1}{\gamma(u)} \quad \forall u : \rho(u) \leq k.$$  

Symplecticness equation [3.8] implies

$$a(u \cdot v) + a(v \cdot u) = \frac{1}{\gamma(u) \gamma(v)}, \quad \forall u, v : \rho(u), \rho(v) \leq k.$$  

Since $\rho(u \cdot v) = \rho(v \cdot u) = k + 1$, equation (3.13) involves two order $k + 1$ conditions; if one is satisfied, then the other is satisfied as well. Specifically, assuming that $a(u \cdot v) = 1/\gamma(u \cdot v)$ we have

$$a(u \cdot v) = \frac{1}{\gamma(u \cdot v)} = \frac{\rho(u)}{\rho(u) + \rho(v)} \frac{1}{\gamma(u) \gamma(v)} \quad \Rightarrow \quad \frac{\rho(u)}{\rho(u) + \rho(v)} = \frac{1}{\gamma(u \cdot v)}.$$  

For $v = \tau_{\{\ell\}}$ and $u = [u_1, \ldots, u_r]_{\{m\}}$, $\rho(u) = k < p$, we have

$$u \cdot v = [u_1, \ldots, u_r, \tau_{\{\ell\}}]_{\{m\}}, \quad v \cdot u = [[u_1, \ldots, u_r]_{\{m\}}]_{\{\ell\}},$$

with $\rho(u \cdot v) = \rho(v \cdot u) = k + 1 \leq p$. Equation (3.13) yields:

$$a([u_1, \ldots, u_r, \tau_{\{\ell\}}]_{\{m\}}) + a([[u_1, \ldots, u_r]_{\{m\}}]_{\{\ell\}}) = a(\tau_{\{\ell\}}) a([u_1, \ldots, u_r]_{\{m\}}),$$

which implies the order $k + 1$ relation

$$b^{(m)\top} (U \times c^{(m,\ell)}) + b^{(\ell)\top} A^{(\ell,m)} U = \frac{1}{\gamma([u_1, \ldots, u_r]_{\{m\}})}.$$
where $U$ is defined in (3.9).

This redundancy of order conditions discussed in Remark 4 yields the following reduction.

**Theorem 3.3 (Reduced order conditions for symplectic GARK schemes).** For symplectic GARK schemes the number of order conditions is reduced due to redundancy:

- **Order two.** Assuming that the order two condition

  \[
  b^{(m)\tau} c^{(m,\ell)} + b^{(\ell)\tau} c^{(\ell,m)} - 1 = 0, \tag{3.15}
  \]

  which yields for $\ell = m$ the order two conditions

  \[
  b^{(m)\tau} c^{(m,m)} = \frac{1}{2},
  \]

  Assuming that the order two condition

  \[
  b^{(m)\tau} c^{(m,\ell)} = \frac{1}{2}
  \]

  holds for $\ell < m$, (3.15) yields the order two condition for $\ell > m$. This condition is automatically fulfilled for internally consistent schemes.

  **Order three.** Using (3.14) with $v = \tau_{\ell}$ and $u = \tau_{(s)}^{(m)}$, we get $U = c^{(m,s)}$, and:

  \[
  b^{(m)\tau} (c^{(m,s)} \times c^{(m,\ell)}) + b^{(\ell)\tau} A^{(\ell,m)} c^{(m,m)} = \frac{1}{2}. \tag{3.16}
  \]

  Thus the order three condition (3.12c) (for a set of partitions $m, s, \ell$) yields the corresponding order condition (3.12d), and vice versa:

  \[
  b^{(\ell)\tau} (c^{(\ell,m)} \times c^{(\ell,s)}) = \frac{1}{3} \iff b^{(m)\tau} A^{(m,\ell)} c^{(s,s)} = \frac{1}{6}. \tag{3.17}
  \]

  Since (3.12c) consists of $(N^3 + N^2)/2$ order conditions, the total number of order three conditions becomes $(N^3 + N^2)/2$ for symplectic GARK schemes.

  **Order four.** Using the redundancy relation (3.14) with $u = \tau_{(l)}^{(s)}$, we get $U = A^{(m,s)} c^{(m,s)}$, and the following relation:

  \[
  b^{(m)\tau} (A^{(m,s)} c^{(s,l)} \times c^{(m,l)}) + b^{(\ell)\tau} A^{(\ell,m)} A^{(m,\ell)} c^{(s,l)} - \frac{1}{6} = 0. \tag{3.18}
  \]

  If an order condition (3.12f) is satisfied (for a set of partitions $m, s, \ell, t$) then so is the corresponding order condition (3.12h), and vice-versa.

  Using the redundancy relation (3.14) with $u = [\tau_{(s)}, \tau_{(l)}]_{(\ell)}$, we get $U = c^{(\ell,s)} \times c^{(\ell,t)}$, and the following relation:

  \[
  b^{(\ell)\tau} (c^{(\ell,s)} \times c^{(\ell,t)} \times c^{(\ell,m)}) + b^{(m)\tau} A^{(m,\ell)} (c^{(\ell,s)} \times c^{(\ell,t)}) - \frac{1}{3} = 0. \tag{3.19}
  \]
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If an order condition (3.12e) is satisfied then so is the corresponding order condition (3.12g), and vice-versa. (3.12e) consists of \((N^4 + 3N^3 + 2N^2)/6\) order conditions, while the equivalent order condition (3.12g) consists of \((N^4 + N^3)/2\) equations. Since \((N^4 + 3N^3 + 2N^2)/6 \leq (N^4 + N^3)/2 \forall N \in \mathbb{N}\), (3.12e) and (3.12g) reduce to \((N^4 + 3N^3 + 2N^2)/6\) conditions in case of symplectic GARK schemes.

For \(v = [\tau_{(s)}]_{(\ell)}\) and \(u = [\tau_{(t)}]_{(m)}\) we have

\[
\begin{align*}
&u \bullet v = [\tau_{(t)}]_{(\ell)} [\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)} [\tau_{(s)}]_{(m)} \\
v \bullet u &= [\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)} [\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)}
\end{align*}
\]

and thus (3.13) leads to

\[
a([\tau_{(t)}]_{(\ell)} [\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)} [\tau_{(s)}]_{(m)}) + a([\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)} [\tau_{(s)}]_{(\ell)} [\tau_{(t)}]_{(m)}) = a([\tau_{(t)}]_{(m)}) a([\tau_{(s)}]_{(\ell)}),
\]

which implies the following relation between order four conditions (3.12f):

\[
b^{(m)} \tau (c^{(m, \ell)} \times A^{(m, \ell)} c^{(\ell, s)} \times A^{(\ell, m)} c^{(m, \ell)}) = \frac{1}{\gamma([\tau_{(t)}]_{(m)})} \frac{1}{\gamma([\tau_{(s)}]_{(\ell)})} = \frac{1}{4},
\]

Setting \(t = \ell\) and \(m = s\), the second redundancy relation (3.19) yields the \(N^2\) order four conditions

\[
b^{(\ell)} \tau (c^{(\ell, \ell)} \times A^{(\ell, \ell)} c^{(\ell, \ell)}) - \frac{1}{8} = 0
\]

as part of (3.12f). If in addition

\[
b^{(\ell)} \tau (c^{(\ell, m)} \times A^{(\ell, t)} c^{(t, s)}) - \frac{1}{8} = 0
\]

holds for \(\ell + m \leq t + s\), then the overall \(N^2(N^2 - 1)/2\) conditions are equivalent to (3.12f). Assuming now that these \(N^2(N^2 - 1)/2\) conditions hold, (3.17) yields the \(N^4\) order conditions (3.12h). □

**Remark 5.** Theorem (3.3) contains all reductions implied by symplecticness, as follows:

- for order two, there is only one symplecticness condition: \(a(u \bullet v)\) defines an order two condition, if both \(u\) and \(v\) contain one node.
- for order three, there is only one symplecticness condition: \(a(u \bullet v)\) defines an order three condition, if \(u\) and \(v\) contain one and node and two nodes, resp.
- for order four, there are only three symplecticness conditions: \(a(u \bullet v)\) defines an order four condition, if \(u\) and \(v\) contain one and three nodes and two and two nodes, resp., which gives \(2 + 1 = 3\) conditions.

Overall, symplecticness yields 5 conditions reducing the number of order conditions, which have all been discussed in Theorem (3.3).

**Corollary 3.4** (Reduced number of order conditions for internally consistent symplectic GARK schemes). If the symplectic GARK scheme is internally consistent, then

- order 2: the order two conditions (3.12b) are automatically fulfilled;
- order 3: if the scheme has at least order two, only the order conditions (3.12e) (\(N\) equations) have to be fulfilled;
- order 4: if the scheme has at least order three, then only the order four conditions (3.12c) (\(N\) equations) and (3.12g) for \(m < s\) (\(N(N - 1)/2\) equations) have to be fulfilled.
Proof. The proposition for internally consistent schemes follows directly from the results above in theorem 3.3.

Order two. From (3.15), we get the N order two conditions (3.12b).

Order three. Here the order conditions (3.16) reduce to the N order conditions (3.12c).

Order four. If the N(N − 1)/2 order conditions
\[ b^{(t)\top} (c^{(t)} \times A^{(t,t)c^{(t)}}) = \frac{1}{8} \]
for \( \ell < t \) hold, then the \( N^2 \) order conditions (3.12a) are fulfilled, and as before the \( N^3 \) order conditions (3.12b) are fulfilled, the \( N^2 \) order conditions (3.12a) hold. \( \Box \)

3.2. Symmetry and time-reversibility. Remark 6 (Time-reversed GARK method). Let \( P^{(n)} \in \mathbb{R}^{s(n) \times s^{(n)}} \) be the permutation matrix that reverses the order of the entries of a vector. In matrix notation the time-reversed GARK method is:

\[
\begin{align*}
(3.20a) \quad b^{(m)} &= P^{(m)} b^{(m)} \quad \Leftrightarrow \quad b^{(m)}_j = b^{(m)}_{s(m)+1-j}, \quad \forall j; \\
(3.20b) \quad A^{(\ell,m)} &= 1^{(\ell)} b^{(m)\top} - P^{(\ell)} A^{(\ell,m)} P^{(m)} \\
& \quad \Leftrightarrow \quad a^{(\ell,m)}_{i,j} = b^{(m)}_j - a^{(\ell,m)}_{s(\ell)+1-i,s(m)+1-j}, \quad \forall i,j.
\end{align*}
\]

The general Butcher tableau (2.10) of the time-reversed GARK method is:

\[ b_{\text{GARK}} = P b_{\text{GARK}}, \quad A_{\text{GARK}} = 1_{s \times 1} b_{\text{GARK}}^\top - P A_{\text{GARK}} P, \]

where \( P := \text{blkdiag}(P^{(m)}) \in \mathbb{R}^{s \times s} \).

Definition 3.5 (Symmetric GARK schemes). The GARK scheme (2.9) is symmetric if it is invariant with respect to time reversion (3.20):

\[
\begin{align*}
(3.21a) \quad b^{(m)} = b^{(m)} & \quad \Leftrightarrow \quad b^{(m)}_j = b^{(m)}_{s(m)+1-j}, \quad \forall j; \\
(3.21b) \quad A^{(\ell,m)} &= A^{(\ell,m)} \\
& \quad \Leftrightarrow \quad a^{(\ell,m)}_{i,j} = b^{(m)}_j - a^{(\ell,m)}_{s(\ell)+1-i,s(m)+1-j}, \quad \forall i,j.
\end{align*}
\]

Using (3.20c), the symmetry condition (3.21) can be written compactly as

\[ b_{\text{GARK}} = P b_{\text{GARK}}, \quad A_{\text{GARK}} = 1_{s \times 1} b_{\text{GARK}}^\top - P A_{\text{GARK}} P. \]

Note that (3.21b) implies (3.21a). From (3.20b) and (3.21b),

\[ P^{(\ell)} A^{(\ell,m)} P^{(m)} + A^{(\ell,m)} = P^{(\ell)} A^{(\ell,m)} P^{(m)} + A^{(\ell,m)} = 1^{(\ell)} b^{(m)\top}, \]

and multiplying this equation from left with \( P^{(\ell)} \) and from the right with \( P^{(m)} \) yields

\[ P^{(\ell)} A^{(\ell,m)} P^{(m)} + A^{(\ell,m)} = 1^{(\ell)} b^{(m)\top} P^{(m)}, \]

which implies \( P^{(m)} b^{(m)} = b^{(m)} \).

Remark 7 (Symplecticness of time-reversed GARK methods). Using (3.2) and (3.20c) we have:

\[
(3.23) \quad P = (A_{\text{GARK}})^\top B_{\text{GARK}} + B_{\text{GARK}} A_{\text{GARK}} - b_{\text{GARK}} b_{\text{GARK}}^\top = b_{\text{GARK}} b_{\text{GARK}}^\top + b_{\text{GARK}} b_{\text{GARK}}^\top - 2 b_{\text{GARK}} b_{\text{GARK}}^\top - P P P.
\]
Consider a symplectic GARK method (3.3) with $P = 0$. The symplecteness condition $P = 0$ for the time-reversed scheme (3.20) reads:

$$b_{\text{GARK}} b_{\text{GARK}}^T + b_{\text{GARK}} b_{\text{GARK}}^T = 2 b_{\text{GARK}} b_{\text{GARK}}^T.$$ 

Multiply this equation from the right by a vector of ones $1_s \times 1$, and divide both sides by $N$. We conclude that a necessary and sufficient condition for symplecticness of the time-reversed scheme is that all weight vectors are palindromic:

$$b_{\text{GARK}} = b_{\text{GARK}} \iff b\{m\} = P\{m\} b\{m\} = b\{m\}, \quad m = 1, \ldots, N.$$

With the help of time-reversed symplectic GARK methods one can derive symmetric and symplectic GARK methods:

**Theorem 3.6.** Consider a GARK scheme $(A_{\text{GARK}}, b_{\text{GARK}})$ that is symplectic and has palindromic weights, $b\{m\} = P\{m\} b\{m\} = b\{m\}$ for all $m$. The GARK scheme defined by applying one step with the GARK scheme, followed by one step with its time-reversed GARK scheme, is defined by the Butcher tableau (2.10) (3.24)

$$\begin{bmatrix} A_{\text{GARK}} & 0_{s \times s} \\ 1_{s \times 1} b_{\text{GARK}}^T & A_{\text{GARK}}^T b_{\text{GARK}}^T \end{bmatrix}$$

and is both symmetric and symplectic.

**Proof.** According to remark 7, the time-reversed scheme is symplectic, too, and so is (3.24) as composition of two symplectic schemes. Symmetry is given by the fact that we have a composition of a scheme with its time-reversed scheme. □

**Remark 8.** Consider a GARK method (with possibly some weights equal to zero). Multiplying the symmetry equation (3.20c) by $b_{\text{GARK}}^T$ from the left leads to:

$$b_{\text{GARK}}^T A_{\text{GARK}} P = b_{\text{GARK}} b_{\text{GARK}}^T - b_{\text{GARK}} A_{\text{GARK}}.$$

and from the symplecteness equation (3.2) we have:

$$b_{\text{GARK}} b_{\text{GARK}}^T - b_{\text{GARK}} A_{\text{GARK}} = A_{\text{GARK}}^T b_{\text{GARK}}.$$

Therefore, for symmetric and symplectic methods it holds that:

$$b_{\text{GARK}}^T A_{\text{GARK}} P = A_{\text{GARK}}^T b_{\text{GARK}} \iff b\{\ell\} a\{\ell,m\}_{s+1-i,s+1-j} = b\{m\} a\{m,\ell\}_{j,i}.$$

This condition together with symmetry implies symplecticness, and vice versa, together with symplecticness it implies symmetry.

$$\{\text{symmetric}\} \cap \{\text{symplectic}\} \iff \text{symmetric} \cap (3.25) \iff (3.25) \cap \text{symplectic}.$$

When dealing with Hamiltonian systems, time-reversibility of a scheme $\Phi_h$ (2.7a) is a desirable property. In the following we show that the symmetry of a GARK scheme (2.7a) ensures its time-reversibility, if each component is $\rho$-reversible.

**Theorem 3.7 (Symmetric GARK schemes are time-reversible).** A symmetric GARK scheme is time-reversible. A symmetric GARK scheme (2.9) is $\rho$-reversible, provided that all individual components are $\rho$-reversible:

$$\rho \circ f^{(m)}(y) = -f^{(m)}(\rho \circ y), \quad m = 1, \ldots, N.$$
Proof. Apply the GARK step (2.13) to the initial values \( \rho(y_0) \) with step size \(-h\) to obtain:

\[
\begin{align*}
Y^{(q)}_i &= \rho(y_0) + (-h) \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a_{i,j}^{(q,m)} f^{(m)}(Y^{(m)}_j), \\
y_1 &= \rho(y_0) + (-h) \sum_{q=1}^{N} \sum_{i=1}^{s^{(q)}} b_i^{(q)} f^{(q)}(Y^{(q)}_i).
\end{align*}
\]

As the partitions of the Hamiltonian are \( \rho \)-reversible, \( \rho \circ f^{(m)}(Y^{(m)}_j) = -f^{(m)}(\rho(Y^{(m)}_j)) \) renaming the internal variables \( \tilde{Y}^{(m)}_i := \rho^{-1}(Y^{(m)}_i) \) leads to the scheme:

\[
\begin{align*}
\rho(\tilde{Y}^{(q)}_i) &= \rho(y_0) + (-h) \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a_{i,j}^{(q,m)} f^{(m)}(\rho(\tilde{Y}^{(m)}_j)) \\
&= \rho(y_0) + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a_{i,j}^{(q,m)} \rho \circ f^{(m)}(\tilde{Y}^{(m)}_j), \\
y_1 &= \rho(y_0) + h \sum_{q=1}^{N} \sum_{i=1}^{s^{(q)}} b_i^{(q)} \rho \circ f^{(q)}(\tilde{Y}^{(q)}_i),
\end{align*}
\]

which yields for \( \rho \) linear and regular (see, for example, the mapping given in (2.3)),

\[
\begin{align*}
\tilde{Y}^{(q)}_i &= y_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a_{i,j}^{(q,m)} f^{(m)}(\tilde{Y}^{(m)}_j), \\
y_1 &= \rho \left( y_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{(q)}} b_i^{(q)} \rho \circ f^{(q)}(\tilde{Y}^{(q)}_i) \right),
\end{align*}
\]

which immediately shows that (2.7a) holds for the GARK scheme (2.9).  

Remark 9. For a Hamiltonian splitting (2.12) with \( y = (p,q)^\top \), we have

\[
\rho \circ f^{(m)}(p,q) = \begin{pmatrix}
H_q^{(m)}(p,q) \\
H_p^{(m)}(p,q)
\end{pmatrix} = \begin{pmatrix}
H_q^{(m)}(p,-q) \\
-H_p^{(m)}(p,-q)
\end{pmatrix} = -f^{(m)}(\rho \circ (p,q)),
\]

i.e., all components define \( \rho \)-reversible flows. Hence the GARK method (2.9) is time-reversible.

We finish this section with two examples of symmetric and/or symplectic schemes for \( N = 2 \) partitions.

Example 2 (A symplectic implicit-implicit scheme). Consider the GARK
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scheme \([2.9]\) defined by the generalized Butcher tableau \([2.10]\)

\[
\begin{array}{c|c|cc}
A^{(1,1)} & A^{(1,2)} \\
\hline
A^{(2,1)} & A^{(2,2)} \\
\hline
b^{(1)^T} & b^{(2)^T}
\end{array}
\]

\[
\begin{array}{c|c|cc}
\frac{1}{5} & 0 & 0 & 0 \\
\hline
\frac{1}{4} & \frac{3}{8} & \frac{2}{3} & 0 \\
\hline
\frac{1}{4} & 0 & \frac{1}{2} & 0 \\
\hline
\frac{1}{4} & \frac{3}{8} & \frac{2}{3} & \frac{1}{6}
\end{array}
\]

This scheme is symplectic for a Hamiltonian splitting according to Theorem 3.1 and of second order. However, the scheme is neither internally consistent nor symmetric.

**Example 3** (A symplectic and symmetric implicit-implicit GARK).

An example of a symmetric and symplectic GARK method of order two for a general splitting \([1.1]\) (the component subsystems are not necessarily Hamiltonian, i.e., \([2.12]\) may not hold), based on the Verlet scheme in the coupling parts, is given by the following Butcher tableau \([2.10]\)

\[
\begin{array}{c|c|cc}
A^{(1,1)} & A^{(1,2)} \\
\hline
A^{(2,1)} & A^{(2,2)} \\
\hline
b^{(1)^T} & b^{(2)^T}
\end{array}
\]

\[
\begin{array}{c|c|cc}
\frac{1}{4} & \alpha & a_{1,1} & a_{1,2} \\
\hline
\frac{1}{2} - \alpha & \frac{1}{2} & a_{2,1} & a_{2,2} \\
\hline
\frac{1}{2} - a_{1,1} & \frac{1}{2} - a_{2,1} & \frac{1}{4} & \beta \\
\hline
\frac{1}{2} - a_{1,2} & \frac{1}{2} - a_{2,2} & \frac{1}{2} - \beta & \frac{1}{4}
\end{array}
\]

where \(\alpha, \beta, a_{1,1}, \ldots, a_{2,2}\) are free real parameters with \(a_{1,1} + a_{2,2} = 1/2\) and \(a_{1,2} + a_{2,1} = 1/2\).

**Remark 10.** This GARK scheme has the following properties:

- it is decoupled for \(\alpha = \beta = 0\) provided that \(A^{(1,2)} \times A^{(2,1)^T} = 0\) holds, when it becomes a DIRK-DIRK scheme;
- it is internally consistent, if the four conditions \(1/4 + \alpha = a_{1,1} + a_{1,2}, 3/4 - \alpha = a_{2,1} + a_{2,2}, 1/4 + \beta = 1 - a_{1,1} - a_{2,1}, 3/4 - \beta = 1 - a_{1,2} - a_{2,2}\) are satisfied;
- in general, if \(A^{(1,2)} \times A^{(2,1)^T} = 0\) does not hold, it is NOT a composition scheme;

**Remark 11.** Whereas in the case of additive Runge-Kutta schemes the component sums \(f^{(1)}(P_i, Q_i) + f^{(2)}(P_i, Q_i) = f(P_i, Q_i)\) equal the total right-hand side, we have in the GARK case different arguments and the components do not add to the total right-hand side in general. Consequently, the symplectic GARK is not equivalent to a single RK scheme applied to the non-partitioned system. This is also the case in Example 3. For the choice \(\alpha = \beta = a_{1,1} = a_{1,2} = 0\) and \(a_{2,1} = a_{2,2} = 1/2\) the GARK scheme \([2.9]\) reads with \(f_i^{(m)} := f^{(m)}(Y_i^{(m)})\):
Then, the modified system (3.27) is Hamiltonian with shadow
the equivalence class
\(u\)
Similar to investigations for B-series and P-series [12], we select representatives from (3.27) \(\dot{\tilde{y}}\) to the modified system \(y\) terms of backward error analysis, the numerical solution can be regarded as the exact \(y\) whose numerical solution \(H\) show [12] that the modified equation of symplectic numerical integration schemes, applied to the Hamiltonian system (2.1), is also Hamiltonian. Consequently, the \(H\) shadow Hamiltonian
scheme preserves a nearby \(\text{shadow Hamiltonian}\). Consider the GARK scheme (2.9) whose numerical solution \(y_1 = \Phi_h(y_0)\), written as NB-series, is given by (3.6). In terms of backward error analysis, the numerical solution can be regarded as the exact solution to the modified system
\[
\dot{y} = \sum_{t \in T_N} b(t) \frac{h^{\rho(t)-1}}{\sigma(t)} F(t)(\tilde{y}),
\]
with elementary differentials \(F(t)(y)\) defined recursively via (3.4). Defining the set of all splittings
\[
\text{SP}(t) := \{ \theta \in \text{OST}(t) \mid t \setminus \theta \text{ consists of a single element} \},
\]
with \(\text{OST}(t)\) being the set of ordered subtrees, the real coefficients \(b(t)\) are recursively defined by \(b(\emptyset) = 0, b(\tau_{(m)}) = 1\) and
\[
b(t) = a(t) - \sum_{j=\rho(t)}^{\rho(t)-1} \frac{\partial}{\partial b_j} b(t) \quad \text{for} \quad t \in T_N.
\]
Here, \(\partial b_j^{-1}\) denotes the \((j-1)\)-th iterate of the Lie derivative
\[
\partial b \epsilon(t) = \sum_{\theta \in \text{SP}(t)} \epsilon(\theta) b(t \setminus \theta).
\]
For a given smooth Hamiltonian function \(H : \mathbb{R}^d \to \mathbb{R}\) and for \(t \in T_N\), the elementary Hamiltonian \(H(t) : \mathbb{R}^d \to \mathbb{R}\) is given by
\[
H(\tau_{(m)})(y) = H^{(m)}(y),
\]
\[
H(t)(y) = H^{(m)\rho(t)}(y)(F(t_1)(y),\ldots,F(t_r)(y)), \quad t = [t_1,\ldots,t_r]_{(m)}.
\]
Similar to investigations for B-series and P-series [12], we select representatives from the equivalence class \(u \circ v \sim v \circ u\), resulting in the set
\[
T_N^* = \{ \tau_{(1)},\ldots,\tau_{(N)} \} \cup \left\{ t \in T_N \mid t \text{ cannot be written as } t = u \circ v \text{ with } u < v, \text{ also not if the color of the root is changed} \right\}.
\]
Then, the modified system (3.27) is Hamiltonian with shadow
\[
(3.28) \quad \tilde{H}(y) = \sum_{k=1}^{\infty} h^{k-1} H_k(y), \quad \text{with} \quad H_k(y) = \sum_{t \in T_N^*, \rho(t) = k} \frac{b(t)}{\sigma(t)} H(t)(y).
\]
EXAMPLE 4. Consider the symplectic and symmetric implicit-implicit GARK scheme given by the Butcher tableau \(3.26\) with \(a_{1,2} = a_{2,2} = 0\) and \(a_{1,1} = a_{2,1} = \frac{1}{2}\). The scheme preserves the shadow Hamiltonian
\[
\dot{H} = H + h^2 \left( \frac{\alpha^2}{2} - \frac{\alpha}{4} - \frac{1}{96} \right) \mathcal{H}[\{\tau(1), \tau(1)\}(1)] - \frac{1}{12} h^2 \mathcal{H}[\{\tau(1), \tau(2)\}(1)]
\]
\[
- \frac{1}{24} \mathcal{H}[\{\tau(2), \tau(2)\}(1)] + \left( \frac{\beta^2}{2} - \frac{\beta}{4} - \frac{1}{96} \right) \mathcal{H}[\{\tau(2), \tau(2)\}(2)]
\]
\[
+ \left( \frac{1}{24} - \frac{\beta}{2} \right) \mathcal{H}[\{\tau(2), \tau(1)\}(2)] + \mathcal{O}(h^4).
\]

4. Partitioned GARK schemes for separable Hamiltonian systems. In this section we consider schemes for separable Hamiltonians \(H(q, p) = T(p) + V(q)\). We discuss two types of partitioned Hamiltonians, first when both the potential part \(V(q)\) and kinetic part \(T(p)\) are split, and second when only the potential is split.

4.1. Partitioned symplectic GARK schemes for kinetic and potential splitting. We consider systems where both the potential and the kinetic parts are split:
\[
H(p, q) = \sum_{m=1}^{N} \left( T^{(m)}(p) + V^{(m)}(q) \right),
\]
we consider the \(2N - \text{way}\) partitioned Hamiltonian \(2.11\)
\[
H(p, q) = \sum_{m=1}^{2N} H^{(m)}(p, q) \quad \text{with} \quad \begin{cases} H^{(m)}(p, q) = T^{(m)}(p), & m = 1, \ldots, N, \\ H^{(m+N)}(p, q) = V^{(m)}(q), & m = 1, \ldots, N. \end{cases}
\]
The GARK scheme \(2.13\) applied to a system with splitting \(4.1\) reads:
\[
\bar{P}^{(q)}_i = p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(N+m)}} \tilde{a}_{i,j}^{(q, N+m)} \bar{k}^{(N+m)}_j,
\]
\[
\bar{Q}^{(q)}_i = q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} \tilde{a}_{i,j}^{(q, m)} \bar{r}^{(m)}_j,
\]
\[
P_1 = p_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{(N+q)}} \bar{b}_i^{(N+q)} \tilde{r}_i^{(q)},
\]
\[
q_1 = q_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{(N+q)}} \bar{b}_i^{(N+q)} \tilde{r}_i^{(q)},
\]
\[
\bar{k}^{(N+m)}_i = -V^{(m)}(q) \langle \bar{Q}^{(N+m)}_i \rangle,
\]
\[
\bar{r}^{(m)}_i = T^{(m)}(p) \langle \bar{P}^{(m)}_i \rangle.
\]
The stage vectors \(\bar{Q}^{(q)}_i\) and \(\bar{P}^{(N+q)}_i\) are not needed for any \(q = 1, \ldots, N\). Using the notation \(P^{(m)}_i := \bar{P}^{(m)}_i\), \(Q^{(m)}_i := \bar{Q}^{(N+m)}_i\), \(s(q) := s^{(N+q)}\), and
\[
\tilde{A}^{(\ell, m)} := \tilde{A}^{(\ell, N+m)}, \quad A^{(\ell, m)} := \tilde{A}^{(N+\ell, m)}, \quad \tilde{b}^{(m)} := \tilde{b}^{(N+m)}, \quad b^{(m)} := b^{(m)},
\]
for $m = 1, \ldots, N$, the partitioned GARK scheme (4.2) reads:

\[(4.3a)\]  
\[P_i^{(q)} = p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{N} \hat{a}_{i,j}^{(q,m)} k_j^{(m)}, \quad Q_i^{(q)} = q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{N} a_{i,j}^{(q,m)} \ell_j^{(m)},\]

\[(4.3b)\]  
\[p_1 = p_0 + h \sum_{q=1}^{N} \hat{b}_{i}^{(q)} k_i^{(q)}, \quad q_1 = q_0 + h \sum_{q=1}^{N} b_{i}^{(q)} \ell_i^{(q)},\]

\[(4.3c)\]  
\[k_i^{(m)} = -V_{q_i}^{(m)}(Q_i^{(m)}), \quad \ell_i^{(m)} = T_p^{(m)}(P_i^{(m)}).\]

This scheme can also be analyzed in the framework presented in this section. The corresponding generalized Butcher tableau (2.10) is:

\[
\begin{array}{c|cc}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
\hline
\hat{A}^{(1,1)} & \cdots & \hat{A}^{(1,N)} \\
\vdots & \ddots & \vdots \\
\hat{A}^{(N,1)} & \cdots & \hat{A}^{(N,N)} \\
\end{array}
\]

\[(4.4)\]  
\[
\begin{pmatrix}
0 \\
A \\
b^+ \\
\end{pmatrix}
= \begin{pmatrix}
\hat{A}^{(1,1)} & \cdots & \hat{A}^{(1,N)} \\
\vdots & \ddots & \vdots \\
\hat{A}^{(N,1)} & \cdots & \hat{A}^{(N,N)} \\
\end{pmatrix}
\begin{pmatrix}
b^{(1)t} \\
\cdots \\
b^{(N)t} \\
\end{pmatrix}
\]

Corollary 4.1 (Symplecticity). **The necessary and sufficient conditions for the symplecticity of the GARK scheme (4.2) are $P^{(\ell,m)} = 0$ for $\ell \in \{1, \ldots, N\}$ and $m \in \{N + 1, \ldots, 2N\}$. Using notation (4.4), the necessary and sufficient condition (3.3) for symplecticness is:**

\[(4.5)\]  
\[\hat{A}^{(\ell,m)} B^{(\ell)} + \hat{B}^{(m)} A^{(m,\ell)} - b^{(m)} b^{(\ell)t} = 0, \quad \ell, m = 1, \ldots, N.\]

**Proof.** From (4.2) we see that $\tilde{k}_i^{(\ell)} = 0$ and $\tilde{\ell}_i^{(N+\ell)} = 0$ for $\ell = 1, \ldots, N$. Consequently, using the partition

\[g_i^{(m)} = \begin{bmatrix} g_{k_i}^{(m)} \\ g_{l_i}^{(m)} \end{bmatrix}, \quad 1 \leq m \leq 2N,
\]

in the proof of Theorem 3.1 gives:

\[
\begin{pmatrix}
k_i^{(t)} \\
\ell_i^{(t)} \\
\end{pmatrix} = [NB(g_{l_i}^{(m)}; [q_0, p_0])], \quad 1 \leq t \leq N.
\]

Hence we have for the non-empty NT trees $u = [u_1, \ldots, u_r]_{(m)}$ and $v = [v_1, \ldots, v_p]_{(n)}$

\[1 \leq s \leq N : \quad U := \begin{bmatrix} 0 & \cdots & 0 \\ g_{k}^{(m)}(u_1) & \cdots & g_{k}^{(m)}(u_r) \end{bmatrix}, \quad V := \begin{bmatrix} 0 & \cdots & 0 \\ g_{l}^{(n)}(v_1) & \cdots & g_{l}^{(n)}(v_r) \end{bmatrix},
\]

\[N + 1 \leq s \leq 2N : \quad U := \begin{bmatrix} g_{k}^{(m)}(u_1) & \cdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \cdots & g_{k}^{(m)}(u_r) \end{bmatrix}, \quad V := \begin{bmatrix} g_{k}^{(n)}(v_1) & \cdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \cdots & g_{k}^{(n)}(v_r) \end{bmatrix},
\]

and thus $U_i V_j \neq 0$ for $m \leq N, n > N$ or $m > N, n \leq N$. Hence (3.10) implies $P^{(\ell,m)} = 0$ for $\ell \in \{1, \ldots, N\}$ and $m \in \{N + 1, \ldots, 2N\}$. □
Remark 12 (Dimensions). Equation (4.5) implies \( \hat{s}^{(m)} = s^{(m)} \) for all \( m \).

Consider the \( \hat{B}^{(\ell)} \) weights to be degrees of freedom, with \( \hat{B}^{(\ell)} \) regular. The symplecticness equation (4.5) can be solved for \( \hat{A}^{(\ell,m)} \) to obtain:

\[
\hat{A}^{(\ell,m)} = 1^{(\ell)} \hat{b}^{(m)\top} - B^{(\ell)-1} A^{(m,\ell)\top} \hat{b}^{(m)},
\]

(4.6)

\[
\Rightarrow \quad \hat{c}^{(\ell,m)} = 1^{(\ell)} - B^{(\ell)-1} d^{(\ell,m)} \quad \text{with} \quad d^{(\ell,m)} := A^{(m,\ell)\top} \hat{b}^{(m)},
\]

\[
\Leftrightarrow \quad d^{(\ell,m)} = b^{(\ell)} \times (1^{(\ell)} - \hat{c}^{(\ell,m)}).
\]

We note that if the weights are equal, \( b = \hat{b} \), then \( \hat{A}^{(\ell,m)} \) is fixed via (4.6) by the choice of the base methods \((A^{(m,\ell)}, b^{(\ell)})\):

\[
\hat{A}^{(\ell,m)} = 1^{(\ell)} b^{(m)\top} - B^{(\ell)-1} A^{(m,\ell)\top} B^{(m)}.
\]

Remark 13. The Runge-Kutta \( D(1) \) simplifying assumption extends to GARK \( D^{(m,\ell)}(1) \) simplifying assumption \([28]\), which for our method reads:

\[
\begin{align*}
A^{(m,\ell)\top} \hat{b}^{(m)} &= b^{(\ell)} \times (1 - \hat{c}^{(\ell,m)}), \\
\hat{A}^{(m,\ell)\top} b^{(m)} &= \hat{b}^{(\ell)} \times (1 - c^{(\ell,m)}).
\end{align*}
\]

(4.8)

If the symplecticness condition (4.5) holds then both (4.8) equations are fulfilled. This can be seen by multiplying (4.5) with a vector of ones from the left and from the right.

4.2. GARK discrete adjoints. GARK discrete adjoints were developed in \([18]\).

As in the case of standard Runge-Kutta methods \([19]\), if all the weights are nonzero, \( b_i^{(q)} \neq 0 \), one can reformulate the discrete GARK adjoint as another GARK method to advance (in reverse time) the adjoint variables \( \lambda_n \):

\[
\begin{align*}
\lambda_n &= \lambda_{n+1} + h \sum_{j=1}^{N} b_j^{(q)} \ell_{n,j}^{(q)}, \\
\Lambda_{n,i}^{(q)} &= \lambda_{n+1} + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} a_{i,j}^{(q,m)} \ell_{n,j}^{(m)}, \quad i = s^{(q)}, \ldots, 1, \\
\ell_{n,i}^{(q)} &= f_{Y_{n,i}}^{(q)}(Y_{n,i}) \cdot \Lambda_{n,i}^{(q)}, \\
b_i^{(q)} &= \bar{b}_i^{(q)}, \quad \hat{a}_{i,j}^{(q,m)} = \frac{b_j^{(m)} a_{j,i}^{(m,q)}}{\bar{b}_i^{(q)}},
\end{align*}
\]

(4.9a)

(4.9b)

(4.9c)

(4.9d)

Reverting the time \( h \to -h \) the method (4.9) reads:

\[
\begin{align*}
\Lambda_{n,i}^{(q)} &= \lambda_n + h \sum_{m=1}^{N} \sum_{j=1}^{s^{(m)}} \hat{a}_{i,j}^{(q,m)} \ell_{n,j}^{(m)}, \\
\lambda_{n+1} &= \lambda_n + h \sum_{q=1}^{N} \sum_{j=1}^{s^{(q)}} \hat{b}_j^{(q)} \ell_{n,j}^{(q)}, \\
\hat{a}_{i,j}^{(q,m)} &= \hat{b}_j^{(m)} - \bar{a}_{i,j}^{(m,q)} = b_j^{(m)} - \frac{b_j^{(m)} a_{j,i}^{(m,q)}}{\bar{b}_i^{(q)}}, \quad \hat{b}_j^{(q)} = \bar{b}_j^{(q)} = b_j^{(q)},
\end{align*}
\]

(4.10)
which is called the formal discrete adjoint GARK method. In matrix notation the coefficients read

\[
\hat{A}^{(q,m)} = 1^{(q)} b^{(m)\top} - B^{(q)-1} A^{(m,q)\top} B^{(m)}, \quad \hat{b}^{(q)} = b^{(q)},
\]

and is equivalent to the symplecticness condition \((4.7)\) for partitioned GARK schemes. The matrix \(\hat{A}^{(q,m)}\) given by \((4.11)\) is called the symplectic conjugate of \(A^{(q,m)}\). If \(A^{(q,m)} = \hat{A}^{(q,m)}\) holds for all \(q, m\) the GARK method is called self-adjoint. We have the following result.

**Lemma 4.2.** Symplecticity and self-adjointness of a GARK scheme \((b^{(m)}, A^{(m,n)})\) with \(b^{(m)} \neq 0\) are equivalent properties.

**Proof.** For nonzero weights the symplecticness condition \((3.3)\) is equivalent to

\[
P^{(q,m)} = 0_{s(q) \times s(m)} \iff A^{(q,m)} = 1^{(q)} b^{(m)\top} - B^{(q)-1} A^{(m,q)\top} B^{(m)},
\]

and therefore is equivalent to self-adjointness using \((4.11)\). \(\blacksquare\)

It was shown in \([18]\) that the order of the discrete adjoint method \((4.9), (4.10)\) coincides with the order of the base GARK scheme when computing solution derivatives, i.e., \(\lambda_n = (d\Phi/dy_n)^\top\) for some functional \(\Phi\) defined on the solution \(\{y_i\}\). This is true if in \((4.9c)\) the Jacobians \(J_y^{(q)\top}(Y_{n,i}^{(q)})\) are evaluated at the forward GARK stages. However, this is not true for the formal discrete adjoint GARK \((4.10)\) regarded as a general GARK integration scheme.

**Remark 14.** Zanna \([30]\) has shown that integrating the states \(Q_{1}^{(m)}\) with a GARK scheme, and the co-states \(P_{1}^{(m)}\) with the discrete adjoint of the GARK method \((4.9)\) results in a symplectic numerical method. This result generalizes the results of Sanz-Serna \([23]\) for RK methods to GARK methods.

### 4.3. Order conditions.

In this section we consider a partitioned GARK scheme \((4.3), (4.4)\) satisfying the symplecticness condition \((4.5)\), and study the order conditions when applied to solve a partitioned system of the form \((4.1)\).

**Remark 15.** The choice of setting the coefficients \(A^{(m,n)}\) and \(A^{(N+m,N+n)}\) for \(1 \leq m, n \leq N\) to zero (or any other value) in \((4.4)\) follows the fact that they do not contribute to the order conditions since the associated elementary differentials are identically equal to zero. To see this, consider general \(N\)-trees of the form

\[
v = [[t_1],[m_1], \ldots, [t_M],[m_M],[r_1],[t_{i+1}+N], \ldots, [r_L],[t_{L+N}]]\}
\]

The associated order condition involves \(A^{(n,m)}\) and \(A^{(n,i,i+N)}\), and the corresponding elementary differential is:

\[
F(v) = \begin{cases}
\frac{\partial M+L f_{1}^{(n)}}{\partial q_{1}} (p_{1}) \equiv 0 \quad &\text{for } 1 \leq n \leq N \text{ and } M \geq 1, \\
\frac{\partial M+L f_{2}^{(n)}}{\partial q_{1}} (p_{1}) \equiv 0 \quad &\text{for } N+1 \leq n \leq 2N \text{ and } L \geq 1.
\end{cases}
\]

The only non-zero elementary differentials correspond to \(N\)-trees where any \(q\)-node has only \(p\)-children, and vice-versa.

The order conditions (up to order four) for a symplectic partitioned GARK scheme
(4.3)–(4.4) are obtained directly from Theorem 3.3

(4.12a) \[ b^{(m)_T} \cdot 1^{(m)} = 1, \quad \forall m, \]  
(4.12b) \[ \hat{b}^{(m)_T} \cdot 1^{(m)} = 1, \quad \forall m, \]  
(4.12c) \[ \hat{b}^{(m)_T} \cdot c^{(m,\ell)} = \frac{1}{2}, \quad \forall m, \ell, \]  
(4.12d) \[ b^{(m)_T} \cdot \left( \hat{c}^{(m,\ell)} \times \hat{c}^{(m,s)} \right) = \frac{1}{3}, \quad \forall m, \forall \ell \leq s, \]  
(4.12e) \[ \hat{b}^{(m)_T} \cdot \left( c^{(m,\ell)} \times c^{(m,s)} \right) = \frac{1}{3}, \quad \forall m, \forall \ell \leq s, \]  
(4.12f) \[ b^{(m)_T} \cdot \left( \hat{c}^{(m,\ell)} \times c^{(m,s)} \times \hat{c}^{(m,t)} \right) = \frac{1}{4}, \quad \forall m, \forall \ell \leq s \leq t, \]  
(4.12g) \[ \hat{b}^{(m)_T} \cdot \left( c^{(m,\ell)} \times c^{(m,s)} \times c^{(m,t)} \right) = \frac{1}{4}, \quad \forall m, \forall \ell \leq s \leq t, \]  
(4.12h) \[ \hat{b}^{(m)_T} \cdot \left( c^{(m,\ell)} \times A^{(m,s)} \cdot \hat{c}^{(s,\ell)} \right) = \frac{1}{8}, \quad \forall m, \ell, s, t. \]  

Remark 16. Using (4.6), these order conditions can be rewritten in terms of \( d^{(m,\ell)} \) by substituting \( c^{(m,\ell)} = 1^{(m)} - B^{(m,\ell)} d^{(m,\ell)} \):

\[
\begin{align*}
(4.12d) & \iff b^{(\ell)_T} \cdot \left( B^{(\ell)-1} d^{(\ell,s)} \times B^{(\ell)-1} d^{(\ell,t)} \right) = \frac{1}{3}, \\
(4.12e) & \iff b^{(\ell)_T} \cdot \left( B^{(\ell)-1} d^{(\ell,s)} \times B^{(\ell)-1} d^{(\ell,t)} \times B^{(\ell)-1} d^{(\ell,s)} \right) = \frac{1}{4}, \\
(4.12h) & \iff \hat{b}^{(m)_T} \cdot \left( c^{(m,s)} \times A^{(m,\ell)} B^{(\ell)-1} d^{(\ell,\ell)} \right) = \frac{5}{24}.
\end{align*}
\]

For \( N = 1 \) and \( b^{(1)} = \hat{b}^{(1)} \), these order conditions coincide with the order conditions given by Hager [11, Table 1] (neglecting the superscripts for simplicity):

\[
\begin{align*}
\sum_i b_i = 1, \quad & \sum_i d_i = \frac{1}{2}, \quad \sum_i \frac{d_i^2}{b_i} = \frac{1}{3}, \quad \sum_i b_i c_i^3 = \frac{1}{3}, \\
\sum_i \frac{d_i^3}{b_i} = \frac{1}{4}, \quad & \sum_i b_i c_i^3 = \frac{1}{4}, \quad \sum_i \frac{b_i c_i^3 a_{i,j} d_j}{b_j} = \frac{5}{24}.
\end{align*}
\]

Note that the remaining order conditions in Hager (the first order three condition and the second, third, fourth, fifth and eighth order four conditions in [11, Table 1]) are redundant due to the symplecticity of the partitioned scheme.

Lemma 4.3 (The same weights case). Let us now assume that \( s^{(\ell)} = \hat{s}^{(\ell)} \) and \( b^{(\ell)} = \hat{b}^{(\ell)} \) holds for all \( \ell = 1, 2, \ldots, N \). If the base GARK scheme \( (b^{(m)}, A^{(m,\ell)}) \) has order four, then the symplectic partitioned scheme (4.3)–(4.4) has at least order two. In addition, we have:

- The partitioned GARK scheme has order three if condition (4.12d) holds.
- In addition, the partitioned GARK scheme has order four, if conditions (4.12f) and (4.12h) hold. These are automatically fulfilled for symmetric schemes.

Example 5. The Verlet algorithm (the two-stage Lobatto IIIA–IIIB pair of order 2) is of the form (4.4) with \( N = 1 \):

\[
\begin{align*}
\begin{array}{c|ccc}
\hat{c} & \hat{A} & \hat{b}^T \\
\hline
0 & 0 & 0 \\
1 & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}
& \quad 
\begin{array}{c|ccc}
\hat{c} & A & \hat{b}^T \\
\hline
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}
\end{align*}
\]
Similarly, the three-stage Lobatto IIIA–IIIB pair of order 4 has the form (4.4)

\[
\begin{pmatrix}
0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{5}{6} & 1 & -\frac{1}{6} \\
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0
\end{pmatrix},
\begin{pmatrix}
0 & 1 & 0 & 0 \\
\frac{1}{2} & 1 & 0 & 0
\end{pmatrix}
\]

(4.14)  \( \hat{c} \) \( \hat{A} \) = \( \begin{pmatrix}
1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{pmatrix} \), \( c \) \( A \) = \( \begin{pmatrix}
1 & \frac{1}{6} & \frac{5}{6} & 0 \\
\frac{1}{6} & \frac{5}{6} & 0 & 0
\end{pmatrix} \).

4.4. Symmetry and time-reversibility. The symmetry and time-reversible results for GARK schemes can be adapted to partitioned GARK schemes as follows.

**Theorem 4.4** (Symmetric partitioned GARK schemes). The partitioned GARK scheme (4.3) is symmetric (3.22) if the following conditions hold:

(4.15a) \( b^{(m)} = b^{(m)} \), \( \hat{b}^{(m)} = \hat{b}^{(m)} \),

(4.15b) \( A^{(\ell,m)} = A^{(\ell,m)} \), \( \hat{A}^{(\ell,m)} = \hat{A}^{(\ell,m)} \)

In other words, a partitioned GARK scheme is symmetric, iff both the base GARK scheme and its discrete adjoint scheme are symmetric.

**Proof.** The time-reversed tableau (3.20c) of the partitioned method (4.4) is:

\[
\left( \begin{array}{c|c|c}
0_{s \times s} & 1 \hat{b}^T - \mathcal{P} \hat{A} \mathcal{P} & 0_{s \times s} \\
\mathcal{P} b^T & 0_{s \times s} & \mathcal{P} b^T \\
\end{array} \right) = \left( \begin{array}{c|c|c}
A & 0_{s \times s} \\
B & \mathcal{P} b^T \\
\end{array} \right) = \left( \begin{array}{c|c|c}
\hat{A} & 0_{s \times s} \\
\hat{b} & \mathcal{P} b^T \\
\end{array} \right).
\]

The diagonal blocks in the time-reversed scheme (4.16) are set to 0 as they do not have any effect in the computation. □

**Lemma 4.5** (Symmetry of partitioned GARK schemes). Consider a GARK scheme \( (b^{(m)}, A^{(m,\ell)}) \) that is symmetric (3.21). Then its discrete adjoint scheme \( (\hat{b}^{(m)}, \hat{A}^{(m,\ell)}) \) is also symmetric, and so is the partitioned GARK scheme \( (b^{(m)}, A^{(m,\ell)}, \hat{A}^{(m,\ell)}) \) given by (4.3)–(4.4) with \( \hat{b}^{(m)} = b^{(m)} \).

**Proof.** We only have to show that \( A^{(\ell,m)} = \hat{A}^{(\ell,m)} \) implies \( \hat{A}^{(\ell,m)} = \hat{A}^{(\ell,m)} \).

From (3.20b), the symmetry of the GARK scheme is:

\[
A^{(\ell,m)} = \hat{A}^{(\ell,m)} = 1^{(\ell)} b^{(m)\top} - \mathcal{P}^{(\ell)} A^{(m,\ell)} \mathcal{P}^{(m)}.
\]

From (3.20b), (4.11), and the symmetry of the GARK scheme assumption, the time reversed discrete adjoint matrix is:

\[
\hat{A}^{(\ell,m)} = 1^{(\ell)} b^{(m)\top} - \mathcal{P}^{(\ell)} \hat{A}^{(\ell,m)} \mathcal{P}^{(m)}
\]

\[
= 1^{(\ell)} b^{(m)\top} - \mathcal{P}^{(\ell)} \left( 1^{(\ell)} b^{(m)\top} - B^{(\ell) - 1} A^{(m,\ell)} B^{(m)} \right) \mathcal{P}^{(m)}
\]

\[
= B^{(\ell) - 1} A^{(m,\ell)} B^{(m)}
\]

\[
= B^{(\ell) - 1} \left( B^{(\ell)} 1^{(m)\top} - \mathcal{P}^{(\ell)} A^{(m,\ell)} \mathcal{P}^{(m)} \right) B^{(m)}
\]

\[
= 1^{(\ell)} b^{(m)\top} - B^{(\ell) - 1} A^{(m,\ell)} B^{(m)}
\]

\[
= \hat{A}^{(\ell,m)}.
\]
4.4.1. Construction of symmetric and symplectic methods starting from a symmetric scheme. Lemma 4.5 provides an easy way to construct partitioned GARK schemes of order four, which are both symmetric and symplectic. One starts with a symmetric GARK scheme \( (b^{[m]}, A^{(m,ℓ)}) \) and constructs the symplectic partitioned GARK scheme \( (b^{[m]}, A^{(m,ℓ)}, \hat{A}^{(m,ℓ)}) \). This scheme is symmetric by Lemma 4.5. If condition \( (4.12d) \) holds the partitioned scheme has order three, and therefore order four is ensured by symmetry.

Remark 17. Consider a partitioned GARK scheme that is both symplectic and symmetric. The symmetry condition \( (4.15b) \) together with the symplecticness condition \( (4.5) \) give

\[
A^{(ℓ,m)} = 1^{(ℓ)} b^{[m]T} - P^{(ℓ)} A^{(ℓ,m)} P^{(m)} = 1^{(ℓ)} \hat{b}^{[m]T} - B^{(ℓ)} - 1 \hat{A}^{(m,ℓ)} T B^{[m]},
\]

\[
\hat{A}^{(ℓ,m)} = 1^{(ℓ)} \hat{b}^{[m]T} - P^{(ℓ)} \hat{A}^{(ℓ,m)} P^{(m)} = 1^{(ℓ)} b^{[m]T} - \hat{B}^{(ℓ)} - 1 A^{(m,ℓ)} T B^{[m]}.
\]

and condition \( (3.25) \) reads

\[
\hat{A}^{(m,ℓ)T} B^{[m]} = B^{(ℓ) T} P^{(ℓ)} A^{(ℓ,m)} P^{(m)} + b^{(ℓ)} (\hat{b}^{[m]T} - b^{[m]T}),
\]

\[
A^{(m,ℓ)T} B^{[m]} = \hat{B}^{(ℓ) T} P^{(ℓ)} \hat{A}^{(ℓ,m)} P^{(m)} + \hat{b}^{(ℓ)} (b^{[m]T} - \hat{b}^{[m]T}).
\]

The last terms vanish when \( b^{[m]} = \hat{b}^{[m]} \).

4.4.2. Construction of symmetric and symplectic methods starting from a symplectic scheme. Remark 7 can also be applied to the time-reversed scheme \( 4.20c \), i.e., it is symplectic, iff the underlying partitioned GARK scheme is symplectic and all weights are palindromic: \( b^{[m]} = \hat{b}^{[m]} \) and \( \hat{b}^{[m]} = \hat{b}^{[m]} \) for all \( m \). Similar to Theorem 3.6, we have the following result.

Theorem 4.6. Consider a partitioned GARK scheme \( 4.4 \) that is symplectic and has palindromic weights, \( b^{[m]} = \hat{b}^{[m]} \) and \( \hat{b}^{[m]} = \hat{b}^{[m]} \) for all \( m \). Applying one step with the partitioned GARK scheme, followed by one step with its time-reversed partitioned GARK scheme \( 4.16 \), defines a new GARK scheme with the Butcher tableau

\[
\begin{array}{c|cc}
0_{s \times s} & \frac{1}{2} \hat{A} & 0_{s \times s} \\
\frac{1}{2} A & 0_{s \times s} & 0_{s \times s} \\
\hline
\frac{1}{2} b^{T} & \frac{1}{2} b^{T} & \frac{1}{2} \hat{A} \\
\frac{1}{2} \hat{b}^{T} & \frac{1}{2} \hat{b}^{T} & 0_{s \times s} \\
\frac{1}{2} b^{T} & \frac{1}{2} b^{T} & \frac{1}{2} \hat{b}^{T} \\
\frac{1}{2} \hat{b}^{T} & \frac{1}{2} \hat{b}^{T} & \frac{1}{2} b^{T}
\end{array}
\]

which is both symmetric and symplectic.

Proof. See proof of Theorem 3.6. Note that the coefficients are divided by two in order to recover the standard form over one step.

Remark 18. Also note that \( 4.18 \) is not a partitioned GARK scheme of the form \( 4.4 \).
4.5. Partitioned GARK schemes for potential splitting. We now consider
the often encountered case where only the potential is split:

\[
H(p, q) = T(p) + V(q) \quad \text{with} \quad V(q) = \sum_{m=2}^{N} V^{(m)}(q),
\]
and where we have the following partitioned Hamiltonian (2.11)

\[
H(p, q) = \sum_{m=1}^{N} H^{(m)}(p, q) \quad \text{with} \quad H^{(m)}(p, q) = \begin{cases} T(p), & m = 1, \\
V^{(m)}(q), & m = 2, \ldots, N. \end{cases}
\]

We note that the potential split system (4.19) is a special case of a partitioned system (4.1) with \(V^{(1)}(q) = 0\) and \(T^{(m)}(p) = 0\) for \(m = 2, \ldots, N\).

The partitioned GARK scheme (4.3) applied to the potential splitting (4.19) reads:

\[
P^{(1)}_i = p_0 + h \sum_{m=2}^{N} \sum_{j=1}^{s^{(m)}} a^{{(1,m)}}_{i,j} k^m_j, \quad Q^{(1)}_i = q_0 + h \sum_{j=1}^{s^{(1)}} a^{{(q,1)}}_{i,j} l^{(1)}_j,
\]

\[
p_1 = p_0 + h \sum_{m=2}^{N} \sum_{q=2}^{s^{(m)}} \hat{a}^{(m)}_{i,q} k^m_i, \quad q_1 = q_0 + h \sum_{i=1}^{s^{(1)}} \hat{a}^{(1)}_{i,1} l^{(1)}_i,
\]

\[
k^m_i = -V^m(q^{(m)}_i), \quad l^{(m)}_i = T^m_p(p^{(m)}_i).
\]

One notes that the stage vectors \(P^{(q)}_i\) for \(q = 2, \ldots, N\) and \(Q^{(1)}_i\) are not needed for this type of splitting. The corresponding generalized Butcher tableau (2.10) is:

\[
\begin{array}{c|ccc}
0 & \mathbf{A}^{(1,2)} & \cdots & \mathbf{A}^{(1,N)} \\
\mathbf{A}^{(2,1)} & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots \\
\mathbf{A}^{(N,1)} & 0 & 0 \\
\mathbf{b}^{(1)T} & \mathbf{b}^{(2)T} & \cdots & \mathbf{b}^{(N)T} \\
\end{array}
\]

The generalized momenta are obtained by integrating each potential \(V^{(m)}\) with a Runge-Kutta scheme \((\mathbf{b}^{(m)}, \mathbf{A}^{(1,m)})\) for \(m = 2, \ldots, N\). The generalized positions are obtained by integrating the kinetic energy with a Runge-Kutta scheme \((\mathbf{b}^{(1)}, \mathbf{A}^{(m,1)})\) for \(m = 2, \ldots, N\). All other coupling coefficients are zero.

As the partitioned GARK scheme (4.20) is a special case of (4.3), Theorem 4.1 yields the symplecticity conditions (4.5):

\[
P^{(1,m)} = \mathbf{A}^{(m,1)T} \mathbf{b}^{(m)} + \mathbf{B}^{(1)} \mathbf{A}^{(1,m)} - \mathbf{b}^{(1)} \mathbf{b}^{(m)T} = 0, \quad m = 2, \ldots, N,
\]
and can be solved for \(\mathbf{A}^{(1,m)}\) when all entries of \(\mathbf{b}^{(1)}\) are nonzero (4.6):

\[
\mathbf{A}^{(1,m)} := 1^{(1)} \mathbf{b}^{(m)T} - B^{(1)-1} A^{(m,1)T} \mathbf{b}^{(m)}, \quad m = 2, \ldots, N.
\]

In the symplectic case, each \(\mathbf{A}^{(1,m)}\) is uniquely defined in terms of the Runge Kutta scheme \((\mathbf{b}^{(1)}, \mathbf{A}^{(m,1)})\) and the weight vector \(\mathbf{b}^{(m)}\).
The order conditions up to order four are obtained directly from (4.12) (refer to Theorem 3.3):

\[ b^{(1)\top} \cdot 1^{(1)} = 1, \]  

\[ \hat{b}^{(m)\top} \cdot 1^{(m)} = 1, \quad \forall m > 1, \]  

\[ \hat{b}^{(m)\top} \cdot c^{(m,1)} = \frac{1}{2}, \quad \forall m > 1, \]  

\[ b^{(1)\top} \cdot (\tilde{c}^{(1,\ell)} \times \tilde{c}^{(1,s)}) = \frac{1}{3}, \quad \forall \ell, s > 1, \ell \leq s, \]  

\[ \hat{b}^{(m)\top} \cdot (c^{(m,1)} \times c^{(m,1)}) = \frac{1}{3}, \quad \forall m > 1, \]  

\[ b^{(1)\top} \cdot (\hat{c}^{(1,\ell)} \times \hat{c}^{(1,s)} \times \hat{c}^{(1,t)}) = \frac{1}{4}, \quad \forall \ell, s, t > 1, \ell \leq s \leq t, \]  

\[ \hat{b}^{(m)\top} \cdot (c^{(m,1)} \times c^{(m,1)} \times c^{(m,1)}) = \frac{1}{4}, \quad \forall m > 1, \]  

\[ b^{(1)\top} \cdot (\hat{c}^{(1,\ell)} \times \hat{A}^{(1,s)} \cdot c^{(s,1)}) = \frac{1}{8}, \quad \forall \ell, s > 1, \]  

\[ \hat{b}^{(m)\top} \cdot (c^{(m,1)} \times A^{(m,1)} \cdot c^{(1,t)}) = \frac{1}{8}, \quad \forall m, t > 1. \]  

**Remark 19.** For \( N = 2 \) and \( s^{(1)} = s^{(2)} \) the scheme (4.21) is equivalent to a traditional Partitioned RK scheme with Butcher tableau:

\[ \begin{array}{c|c}
A & \hat{A} \\
b^{\top} & b^{\top}
\end{array} \quad \text{with} \quad \begin{cases}
A = A^{(2,1)}, & \hat{A} = \hat{A}^{(1,2)} = 1 b^{\top} - B^{-1} A^{(2,1)} \hat{B}, \\
b = b^{(1)}, & \hat{b} = b^{(2)}.
\end{cases} \]

**4.6. Explicit partitioned GARK schemes.** One idea for constructing explicit symmetric and symplectic GARK schemes is to define a two-step scheme: take a first step with an explicit symplectic partitioned GARK scheme, and then a second step with its time-reversed scheme (see Section 4.4.2). However, the resulting symplectic and symmetric scheme might not fall into the class of partitioned GARK schemes, as discussed in the proof of Theorem 4.6.

In the following we will consider ideas how to construct explicit schemes that define partitioned GARK schemes.

**Explicit symplectic partitioned GARK schemes.** Partitioned GARK schemes (4.4) are explicit iff they fulfill the condition [22]

\[ S^{(\ell,m)} := \hat{A}^{(\ell,m)} \times A^{(m,\ell)} = 0 \quad \forall \ell, m = 1, \ldots, N, \]

where \(|\cdots|\) takes element-wise absolute values, and \(\times\) is the element-wise product.

For symplectic partitioned GARK schemes (4.4) schemes with non-vanishing weights \(b^{(\ell)}\) and \(\hat{b}^{(m)}\), equation (4.16)

\[ \hat{a}^{(\ell,m)}_{i,j} = \hat{a}^{(m)}_j \left( 1 - a^{(m,\ell)}_{j,i} / b^{(\ell)}_i \right), \]

together with condition (4.24) lead to:

\[ \hat{a}^{(\ell,m)}_{i,j} = \hat{b}^{(m)}_j \left( 1 - a^{(m,\ell)}_{j,i} \right) \text{ and } a^{(m,\ell)}_{j,i} = b^{(\ell)}_i x^{(m,\ell)}_{j,i}, \quad x^{(m,\ell)}_{j,i} \in \{0,1\}, \]
for all \( i = 1, \ldots, s^{(\ell)}; \ j = 1, \ldots, s^{(m)} \), or in compact notation with \( x := (x_{i,j})_{i,j} \) and \( \tilde{x} := (1 - x_{i,j})_{i,j} \):

\[
A^{(m,\ell)} = x^{(m,\ell)} \cdot B^{(\ell)}, \quad \tilde{A}^{(\ell,m)} = \tilde{x}^{(\ell,m)} \cdot \tilde{B}^{(m)}.
\]

The scheme (4.3) then reads:

\[
P_1^{(m)} = p_0 + h \sum_{\ell=1}^{N} \sum_{j=1}^{s^{(\ell)}} a_{i,j}^{(m,\ell)} k_j^{(\ell)} = p_0 + h \sum_{\ell=1}^{N} \sum_{j=1}^{s^{(\ell)}} x_{i,j}^{(\ell,m)} \tilde{a}_{j}^{(\ell)} k_j^{(\ell)},
\]

\[
q_i^{(m)} = q_0 + h \sum_{\ell=1}^{N} \sum_{j=1}^{s^{(\ell)}} a_{i,j}^{(m,\ell)} \tilde{a}_j^{(\ell)} = q_0 + h \sum_{\ell=1}^{N} \sum_{j=1}^{s^{(\ell)}} x_{i,j}^{(\ell,m)} b_j^{(\ell)} \tilde{a}_j^{(\ell)},
\]

\[
P_1 = p_0 + h \sum_{\ell=1}^{N} \sum_{i=1}^{s^{(\ell)}} \tilde{a}_i^{(\ell)} k_i^{(\ell)},
\]

\[
q_1 = q_0 + h \sum_{\ell=1}^{N} \sum_{i=1}^{s^{(\ell)}} b_i^{(\ell)} \tilde{a}_i^{(\ell)}.
\]

After reordering the rows and columns such as to reflect the order in which stages are computed, we have the following cases.

1. If we compute all the stages \( i = 1, \ldots, s^{(m)} \) for partition \( m \) before moving on to partition \( m + 1 \), then:
   - both \( A^{(m,\ell)} \) and \( \tilde{A}^{(m,\ell)} \) are zero for \( m < \ell \);
   - they are full matrices for \( m > \ell \), with \( A^{(m,\ell)} = 1^{(m)} b^{(\ell)T} \) and \( \tilde{A}^{(m,\ell)} = 1^{(m)} \tilde{b}^{(\ell)T} \);
   - are lower triangular for \( m = \ell \) with \( a_{i,i}^{(m,m)} \cdot \tilde{a}_{i,i}^{(m,m)} = 0 \) for explicitness.

2. If we compute stage \( i \) for each partition \( m = 1, \ldots, N \) before moving on to stage \( i + 1 \), then each of the coefficient matrices has to be lower triangular such as to preserve explicitness. This implies \( x_{i,j}^{(m,\ell)} = 0 \) and \( 1 - x_{i,j}^{(m,\ell)} = 0 \) for \( i < j \), therefore \( x_{i,j}^{(m,\ell)} = 1 \) for \( i > j \). We have the following structures when \( s^{(m)} \geq s^{(\ell)} \):

\[
A^{(m,\ell)} = \begin{bmatrix}
q_0 & 0 & \cdots & 0 \\
\vdots & q_0^{(m)} & \cdots & \vdots \\
0 & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & q_0^{(m)}
\end{bmatrix}, \quad \tilde{A}^{(\ell,m)} = \begin{bmatrix}
\tilde{q}_0 & 0 & \cdots & 0 \\
\vdots & \tilde{q}_0^{(\ell)} & \cdots & \vdots \\
0 & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & \tilde{q}_0^{(\ell)}
\end{bmatrix}.
\]

The last \( s^{(m)} - s^{(\ell)} - 1 \) stages of \( A^{(m,\ell)} \) are redundant (equal to each other) and the last \( s^{(m)} - s^{(\ell)} - 1 \) columns of \( \tilde{A}^{(m,\ell)} \) are zero. To avoid redundancy, it makes sense to only consider \( s^{(m)} = s^{(\ell)} + 1 \) if \( x_{s^{(\ell)},s^{(\ell)}} = 0 \), and \( s^{(m)} = s^{(\ell)} \) if \( x_{s^{(\ell)},s^{(\ell)}} = 1 \). For \( s^{(m)} \leq s^{(\ell)} \) we get

\[
A^{(m,\ell)} = \begin{bmatrix}
q_0 & 0 & \cdots & 0 \\
\vdots & q_0^{(m)} & \cdots & \vdots \\
0 & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & q_0^{(m)}
\end{bmatrix}, \quad \tilde{A}^{(\ell,m)} = \begin{bmatrix}
\tilde{q}_0 & 0 & \cdots & 0 \\
\vdots & \tilde{q}_0^{(\ell)} & \cdots & \vdots \\
0 & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & \tilde{q}_0^{(\ell)}
\end{bmatrix}.
\]
Similar to the first case, the last \( s^{(\ell)} - s^{(m)} - 1 \) stages of \( \hat{A}^{(m, \ell)} \) are redundant (equal to each other) and the last \( s^{(\ell)} - s^{(m)} - 1 \) columns of \( A^{(m, \ell)} \) are zero. To avoid redundancy, it makes again sense to only consider \( s^{(\ell)} = s^{(m)} + 1 \) if \( x_{s^{(\ell)}, s^{(\ell)}} = 1 \), and \( s^{(m)} = s^{(\ell)} \) if \( x_{s^{(\ell)}, s^{(\ell)}} = 0 \).

**Remark 20.** For \( |s^{(m)} - s^{(\ell)}| \geq 2 \) the redundant stages may arise not only at the end for the last \( |s^{(m)} - s^{(\ell)}| - 1 \) stages, but also before. The corresponding matrices are then no longer tridiagonal, but have a step form, i.e., if one element in a row is zero, all elements above are zero, too.

One example for such a setting will be given in Example 7 for the matrices \( \hat{A}^{(1,3)} \) and \( A^{(3,1)} \).

**Explicit symplectic and symmetric partitioned GARK schemes.** If, in addition, the scheme is also symmetric then condition (5.21) leads to

\[
\begin{align*}
\hat{a}_{i,j}^{(m, \ell)} + a_{s^{(m)}+1-j, s^{(\ell)}+1-i}^{(m, \ell)} & = b_{i}^{(\ell)}, \\
\hat{a}_{i,j}^{(\ell, m)} + a_{s^{(\ell)}+1-i, s^{(m)}+1-j}^{(\ell, m)} & = \hat{b}_{j}^{(m)},
\end{align*}
\]

Since \( a_{j,i}^{(m, \ell)} \) can take either values 0 or \( b_{i}^{(\ell)} \), \( a_{s^{(m)}+1-j, s^{(\ell)}+1-i}^{(m, \ell)} \) takes the complementary values \( \hat{b}_{s^{(\ell)}+1-i}^{(m)} \) or 0, respectively. All possible solutions of equation (4.25) have the form:

\[
\begin{align*}
\hat{a}_{i,j}^{(\ell, m)} & = \hat{b}_{j}^{(m)} (1 - x_{j,i}^{(m, \ell)}), \\
\hat{a}_{s^{(\ell)}+1-i, s^{(m)}+1-j}^{(\ell, m)} & = \hat{b}_{s^{(m)}+1-j}^{(m)} x_{j,i}^{(m, \ell)}, \\
\hat{a}_{j,i}^{(m, \ell)} & = b_{i}^{(\ell)} x_{j,i}^{(m, \ell)}, \\
\hat{a}_{s^{(m)}+1-j, s^{(\ell)}+1-i}^{(m, \ell)} & = \hat{b}_{s^{(\ell)}+1-i}^{(m)} (1 - x_{j,i}^{(m, \ell)}),
\end{align*}
\]

We finish with two examples for symplectic and symmetric GARK schemes.

**Example 6 (Yoshida [29]).** The classical fourth order symplectic and symmetric scheme of Yoshida can be written as a partitioned GARK scheme with \( N = 1 \) and

\[
\begin{align*}
A^{(1,1)} &= \begin{bmatrix}
\frac{d_1}{2} & 0 & 0 & 0 \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & 0 & 0 \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2} & 0 \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2}
\end{bmatrix}, & \quad \widehat{A}^{(1,1)} &= \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & d_1 & 0 & 0 \\
0 & d_1 & d_2 & 0 \\
0 & d_1 & d_2 & d_1
\end{bmatrix},
\end{align*}
\]

\[
b = \begin{bmatrix}
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2} & \frac{d_1}{2}
\end{bmatrix}^\top, & \quad \widehat{b} = [d_1, d_2, d_1]^\top, & \quad d_1 = \frac{1}{2 - 2^{\frac{1}{2}}}, & \quad d_2 = -2^{\frac{1}{2}} \cdot d_1.
\]

**Example 7 (Extension of Yoshida’s scheme [29]).** An explicit partitioned symmetric and symplectic scheme of type (4.20) for potential splitting with \( N = 3 \) is given
by the following extension of Yoshida’s fourth order scheme \cite{29}:

\[
\begin{bmatrix}
0 & 0 & 0 & 0 \\
\frac{d_1}{2} & 0 & 0 & \frac{1}{2} \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & 0 & 0 \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2} & 0 \\
\frac{d_1}{2} & \frac{d_1 + d_2}{2} & \frac{d_1 + d_2}{2} & \frac{d_1}{2}
\end{bmatrix}
\]

Note that this scheme has order four for \(H_1(p, q) = T(p) + V_1(q)\) and order two for \(H_2(p, q) = V_2(q)\). This multi-order character of the scheme is tailored to exploiting a fast dynamics and cheap evaluation costs in \(H_1\), and a slow dynamics and expensive evaluation costs in \(H_2\).

5. Numerical examples. We finish with two examples for symplectic and time-reversible GARK schemes: the \(\text{kdv}\) equation as an example for a general skew-symmetric matrix \(J\) discussed in Section 3, and a mathematical pendulum as an example for multirate potential in a potential splitting discussed in Section 4.

5.1. Symplectic integration with non-symplectic partitions. We consider symplectic time integration for the Korteweg-de Vries (KdV) equation \cite{3,6}, a non-dissipative nonlinear hyperbolic equation with smooth solutions:

\[
\begin{align*}
    u' &= \alpha \left( u^3 \right)_x + \rho \, u_x + \nu \, u_{xxx} = V'(u)_x + \nu \, u_{xxx}, \\
    V(u) &= \frac{\alpha}{3} u^3 + \frac{\rho}{2} u^2, \quad u(t=0,x) = 6 \, \text{sech}(x)^2, \quad \alpha = -3, \quad \rho = 1, \quad \nu = -1,
\end{align*}
\]

and periodic boundary conditions \(u(0,t) = u(10,t)\). The initial condition leads to the formation of two solitons traveling at different speeds \cite{6}, as seen in Figure 5.1a. The discrete Hamiltonian leads to a symplectic semi-discretization in space:

\[
H(u) = \Delta x \sum_i \left( V(u_i) - \frac{\nu}{2} \left( \frac{u_{i+1} - u_i}{\Delta x} \right)^2 \right), \quad u'_i = \frac{1}{2 \Delta x} \left( \frac{\partial H}{\partial u_{i+1}} - \frac{\partial H}{\partial u_{i-1}} \right),
\]

which can be written as a generalized Hamiltonian system with

\[
u' = J \cdot \nabla H(u)
\]

and the skew-symmetric matrix \(J\) given by

\[
J = \begin{bmatrix}
0 & 1 \\
-1 & \ddots & \ddots \\
& \ddots & \ddots & 1 \\
& & -1 & 0
\end{bmatrix} - e_1 e_n^T + e_n e_1^T, \quad n := 10/\Delta x.
\]
We integrate the system (5.3) with ode15s in Matlab, the symplectic implicit midpoint scheme, and with the symplectic GARK-IMIM scheme (3.26) using different partitions:

\[
(5.4) \quad f^{(1)}(u) = \begin{cases} J\nabla H_1(u), & (A) \\ J\nabla H_2(u), & (B) \\ J\nabla(H_1(u) + H_2(u)), & (C) \end{cases}
\]

with

\[
(5.5) \quad H_1(u) = \Delta x \sum_i \frac{\sigma}{2} u_i^2, \quad H_2(u) = \Delta x \sum_i \frac{\alpha}{3} u_i^3.
\]

A fixed time step \( \Delta t = 10^{-3} \) is used. Results are shown in Figure 5.1. For all partitions (5.4) the GARK scheme is symplectic and thus preserves a nearby shadow Hamiltonian. Consequently, the error in the Hamiltonian oscillates around the true value as it can be seen in Figure 5.1b.

\[
\begin{array}{c}
\text{Time} \\
\hline
0 & 1 & 2 & 3 & 4
\end{array}
\quad
\begin{array}{c}
\text{Hamiltonian relative error} \\
\hline
10^{-10} & 10^{-5} & 10^0
\end{array}
\]

(a) Solution at different times
(b) Hamiltonian error evolution

Fig. 5.1: Numerical results for the KdV system (5.2) solved with different time integration methods.

### 5.2. Symplectic and time-reversible GARK schemes for Hamiltonians with multirate potential.

Consider a Hamiltonian \( H(p, q) = T(p) + V(q) \), where the potential can be split into two parts \( V(q) = V_1(q) + V_2(q) \). Assuming that \( V_1 \) is characterized by a fast dynamics and cheap evaluation costs, and \( V_2 \) by a slow dynamics and expensive evaluation costs, respectively. Then the Hamiltonian can be partitioned into two parts \( H_1(p, q) + H_2(p, q) \) (with \( H_1(p, q) := T(p) \), \( H_2(p, q) := V_1(q) \)) and \( H_3(p, q) = V_2(q) \) with fast/slow dynamics and cheap/expensive evaluation costs, respectively.

As an example of such a system with multiscale behaviour we consider a mathematical pendulum of constant length \( \ell \) that is coupled to a damped oscillator with a horizontal degree of freedom, as illustrated in Figure 5.2. The system consists of two rigid bodies: the first mass \( m_{\text{pend}} \) is connected to a second mass \( m_{\text{osc}} \) by a soft spring with stiffness \( k \). Neglecting the friction of the spring, the system is Hamiltonian.
The minimal set of coordinates $q^\top = (q_1, q_2) := (\alpha, x_1)$ and generalized momenta $p^\top = (p_1, p_2)$ uniquely describe the position and momenta of both bodies. The Hamiltonian of the system is given by:

$$H(p, q) = H_1(p, q) + H_2(p, q)$$

with the fast Hamiltonian

$$H_1(p, q) = T(p) + V_1(q),$$
$$T(p) = \frac{1}{2m_{osc}} p_2^2 + \frac{1}{2m_{pend}} \left( \frac{p_1}{\ell} \right)^2,$$
$$V_1(q) = -m_{pend} g \ell \cos(q_1),$$

and the slow Hamiltonian

$$H_2(p, q) = V_2(q) = \frac{1}{2} k (q_2 - \ell \sin(q_1))^2.$$  

The equations of motion are then given by the second-order ODE system

$$\begin{pmatrix} m_{pend} \ell & 0 \\ 0 & m_{osc} \end{pmatrix} \ddot{q} = \begin{pmatrix} -m_{pend} g \sin(\alpha) + \cos(\alpha) F \\ -F \end{pmatrix} =: f(q),$$

where the following abbreviation stands for the spring force:

$$F = k (x_1 - \ell \sin(\alpha)).$$

Figure 5.3 shows the numerical results obtained for this benchmark for the GARK extension of Yoshida’s fourth order scheme derived in Example 7 and, for comparison, Yoshida’s fourth order method from Example 6. Note that per integration step Yoshida’s scheme needs three function evaluations of both $V_1$ and $V_2$, whereas the extension needs three for $V_1$, but only two for $V_2$. Figure 5.3 shows the achieved accuracy compared to the number of $V_2$ evaluations assuming that the evaluation costs of $V_2$ are 10,000 times higher than the ones of $V_1$. In this case, the extension clearly outperforms the basic scheme of Yoshida. This situation in typical for many problems with a fast but cheap and slow but expensive force as in Lattice Quantum Chromodynamics, for example, with a cheap gauge field with fast dynamics and an expensive fermionic force with slow dynamics 7.
Fig. 5.3: Numerical results for parameters $m_{\text{pend}} = m_{\text{osc}} = \ell = 1$, $k = 5 \cdot 10^{-6}$, and 10000 times higher evaluation costs for $V_2$: absolute error in the Hamiltonian $H$ for Yoshida and the Yoshida extension vs. computation time.

6. Conclusions. This paper derives partitioned symplectic schemes in the GARK framework, which allows for arbitrary splittings of the Hamiltonian into different Hamiltonian subsystems, which works also in the case of a more general Hamiltonian flow $f(y) = J \nabla H(y)$ with an arbitrary, but skew-symmetric matrix $J = -J^\top$. The derived symplecticity conditions reduce drastically the number of GARK order conditions. We show that symmetric GARK schemes are time-reversible and construct symmetric and time-reversible GARK schemes based on composing a symplectic GARK scheme and its time-reversed scheme. A special attention is given to partitioned symplectic GARK schemes, which can be tailored to a specific splitting w.r.t. potentials or potentials and kinetic parts, resp. We show that symplecticity and self-adjointness are equivalent, and show how the coupling matrices $A^{(\ell,m)}$ and $\hat{A}^{(\ell,m)}$ can be chosen such as to construct explicit schemes. Using different discretization orders for different parts of the splitting defines one way to exploit the multiscale behavior of different potentials $V_1$ and $V_2$ of a Hamiltonian, where $V_1$ is characterized by a fast dynamics and cheap evaluation costs, and $V_2$ by a slow dynamics and expensive evaluation costs, respectively. Numerical tests for a coupled oscillator confirm the theoretical results.

Future work will be to derive efficient symplectic GARK schemes tailored for couplings arising in port-Hamiltonian modeling on the one hand, and to generalize symplectic GARK schemes to multirate symplectic GARK schemes, which use different step sizes for different partitions to exploit the multirate potential. Another task will be to generalize this Abelian setting to a Non-Abelian setting used in lattice QCD, for example, where the equations of motion are defined on Lie groups and their associated Lie algebras.
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