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SPECIALIZED PARTITIONED ADDITIVE RUNGE–KUTTA METHODS FOR SYSTEMS OF OVERDETERMINED DAES WITH HOLONOMIC CONSTRAINTS*

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Abstract. We consider a general class of systems of overdetermined differential-algebraic equations (ODAEs). We are particularly interested in extending the application of the symplectic Gauss methods to Hamiltonian and Lagrangian systems with holonomic constraints. For the numerical approximation to the solution to these ODAEs, we present specialized partitioned additive Runge–Kutta (SPARK) methods, and in particular the new class of (s, s)-Gauss–Lobatto SPARK methods. These methods not only preserve the constraints, symmetry, symplecticness of the flow, and variational nature of the trajectories of holonomically constrained Hamiltonian and Lagrangian systems, but they also have an optimal order of convergence $2s$.

Key words. differential-algebraic equations, Gauss coefficients, Hamiltonian systems, holonomic constraints, Lagrangian systems, Lobatto coefficients, Runge–Kutta methods, symplecticness, variational integrators

AMS subject classifications. 65L05, 65L06, 65L80, 70F20, 70H03, 70H05, 70H45

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1. Introduction.

Gauss methods for Hamiltonian systems are known to be symplectic [7, 8, 19, 25, 28]. For Lagrangian systems these methods are also known to be of a variational nature [21]. The main objective of this paper is to present extensions of Gauss methods to Hamiltonian and Lagrangian systems with holonomic constraints. For these systems we have found extensions of Gauss methods preserving symplecticness, the manifold of constraints, the variational nature of trajectories, and having an optimal order of convergence. When applied to nonstiff ordinary differential equations (ODEs), Gauss methods have a maximal order of convergence in the class of Runge–Kutta (RK) methods [3, 8]. However, for index 3 differential-algebraic equations (DAEs) such as Hamiltonian systems with holonomic constraints, standard Gauss methods either are divergent or have a very low order of convergence when the underlying differentiated constraints are not taken into account [5]. Gauss methods have thus not been considered of much practical interest for the numerical solution of high index DAEs. Recently, optimal methods based on Gauss coefficients have been obtained for index 2 DAEs [18] and have stirred renewed interest in Gauss methods for DAEs.

In this paper we consider a general class of systems of overdetermined differential-algebraic equations (ODAEs), including a unified formulation of Hamiltonian and Lagrangian systems with holonomic constraints. To approximate numerically the solution to these systems of ODAEs, we present the new class of specialized partitioned additive Runge–Kutta (SPARK) methods. We make great use of the structure of the ODAEs. The new class of (s, s)-Gauss–Lobatto SPARK methods extends to these ODAEs the application of Gauss methods to ODEs. These symmetric methods are

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shown to be superconvergent of order $2s$ and constraint preserving. Moreover, for Hamiltonian and Lagrangian systems with holonomic constraints these methods are shown to be symplectic and to satisfy a discrete variational principle.

The paper is organized as follows. In section 2 we introduce the equations of Hamiltonian and Lagrangian systems with holonomic constraints. We state some of their relations and main properties. A unified formulation of Hamiltonian and Lagrangian systems is presented and generalized to a larger class of systems of ODAEs. In section 3 we introduce the new class of SPARK methods. Examples of SPARK methods are given. In section 4 we characterize symplectic SPARK methods and show their variational nature. In section 5 we give results about existence, uniqueness, local error, and global convergence of SPARK methods. Finally, in section 6 some numerical experiments are given to illustrate our theoretical results. A short conclusion is given in section 7.

Regarding notation, we denote by x' the total derivative of x with respect to the independent variable t. For a function $f(x, y)$, we denote by $f_x(x, y)$ its partial derivative with respect to x.

2. Hamiltonian and Lagrangian systems with holonomic constraints. In this section we introduce the equations of Hamiltonian and Lagrangian systems with holonomic constraints. For these systems some important relations and properties are stated [1, 4, 20]. A unified and generalized formulation of Hamiltonian and Lagrangian systems is presented.

2.1. Hamiltonian systems with holonomic constraints. The Hamiltonian system with Hamiltonian $H : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}$ and holonomic constraints $g : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ $(m < n)$ is given by

$$q' = H_p^T(q, p), \tag{2.1a}$$

$$p' = -H_q^T(q, p) - g_q^T(q)\lambda, \tag{2.1b}$$

$$0 = g(q). \tag{2.1c}$$

Differentiating (2.1c) once with respect to the independent variable t, we obtain $g_q(q)q' = 0$, and from (2.1a) this leads to

$$0 = g_q(q)H_p^T(q, p). \tag{2.1d}$$

We assume that $g_q(q)$ is of full row rank m and that the Hessian matrix

$$H_{pp}^T(q, p) \text{ is invertible.} \tag{2.2}$$

For example, $H_{pp}^T(q, p)$ is generally assumed to be (strictly) positive definite. Equations (2.1a,b,c) are DAEs of index 3 in Hessenberg form [2, 6, 9, 12, 15]. The whole system (2.1) can be considered as a system of index 2 ODAEs. For consistent initial values, i.e., for $(q_0, p_0) \in V$, where

$$V := \left\{(q, p) \in \mathbb{R}^n \times \mathbb{R}^n \mid 0 = g(q),\ 0 = g_q(q)H_p^T(q, p)\right\}, \tag{2.3}$$

we have existence and uniqueness of a solution.

2.2. Lagrangian systems with holonomic constraints. The Lagrangian system with Lagrangian $L : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}$ and holonomic constraints $g : \mathbb{R}^n \longrightarrow \mathbb{R}^m$ $(m < n)$ is given by

$$q' = v, \tag{2.4a}$$

$$(L_v^T(q,v))' = L_q^T(q,v) - g_q^T(q)\lambda, \tag{2.4b}$$

$$0 = g(q). \tag{2.4c}$$

Differentiating (2.4c) once with respect to t, we obtain $g_q(q)q' = 0$, and from (2.4a) this leads to

$$0 = g_q(q)v. \tag{2.4d}$$

We assume that $g_q(q)$ is of full row rank m and that the Hessian matrix

$$L_{vv}^T(q,v) \text{ is invertible,} \tag{2.5}$$

for example, $L_{vv}^T(q,v)$ is generally assumed to be (strictly) positive definite. Equations (2.4a,b,c) are usually called *Euler–Lagrange equations* and are DAEs of index 3 [15]. The whole system (2.4) can be considered as a system of index 2 ODAEs. For consistent initial values, i.e., for $(q_0, v_0) \in W$, where

$$W := \{(q,v) \in \mathbb{R}^n \times \mathbb{R}^n \mid 0 = g(q),\ 0 = g_q(q)v\}, \tag{2.6}$$

we have existence and uniqueness of a solution. For Lagrangian systems with holonomic constraints (2.4), it is advantageous to consider directly the formulation (2.4b) instead of

$$L_{vv}^T(q,v)v' = -L_{vq}^T(q,v)v + L_q^T(q,v) - g_q^T(q)\lambda, \tag{2.7}$$

since this formulation (2.7) requires an extra term $L_{vq}^T(q,v)v$ which usually corresponds to Coriolis forces; see [14, 15]. Moreover, preserving the Lagrangian symplectic 2-form (2.10) for numerical methods is certainly more problematic with formulation (2.7) than with (2.4b); see also Corollary 4.2.

2.3. Relations and properties of Hamiltonian and Lagrangian systems with holonomic constraints. Lagrangian systems are closely related to Hamiltonian systems. The momenta p of a Lagrangian system are defined by

$$p := L_v^T(q,v). \tag{2.8}$$

From (2.5), the relation $p - L_v^T(q,v) = 0$ defines v as an implicit function $v(q,p)$. Under assumption (2.5) the Lagrangian system (2.4) is equivalent by the change of variables (2.8) to the Hamiltonian system (2.1) with Hamiltonian

$$H(q,p) := p^T v(q,p) - L(q, v(q,p)).$$

This is known as a Legendre transform. Assumption (2.5) is equivalent to (2.2). The velocities of a Hamiltonian system are defined by

$$v := H_p^T(q,p). \tag{2.9}$$

From (2.2), the relation $v - H_p^T(q,p) = 0$ defines p as an implicit function $p(q,v)$. Under assumption (2.2) Hamiltonian system (2.1) is equivalent by the change of variables (2.9) to Lagrangian system (2.4) with Lagrangian

$$L(q,v) := p^T(q,v)v - H(q,p(q,v)).$$

This is also a Legendre transform. Under the equivalent assumptions (2.2) and (2.5) we have the following symmetric relations between Lagrangian systems and their Hamiltonian counterparts:

$$p^T v = H(q,p) + L(q,v),$$

$$p = L_v^T(q,v),$$

$$v = H_p^T(q,p),$$

$$I_n = H_{pp}^T(q,p)L_{vv}^T(q,v).$$

Properties of Lagrangian systems can thus be transferred to Hamiltonian systems, and vice versa. Hence, here we state only five important properties of Lagrangian systems with holonomic constraints as follows:

1. Any solution to (2.4) must lie on the manifold of constraints W (2.6). In particular, any initial conditions (q_0, v_0) at t_0 must belong to W.

2. The energy function $E(q,v) := L_v(q,v)v - L(q,v)$ is invariant along a solution, i.e.,

$$E(q(t), v(t)) = \text{Const.}$$

3. The flow $\varphi_\tau : (q(t), v(t)) \mapsto (q(t+\tau), v(t+\tau))$ on the manifold of constraints W preserves the Lagrangian symplectic 2-form

$$\sum_{i=1}^{n} dq^i \wedge dL_{v^i}(q,v) = \sum_{i=1}^{n}\sum_{j=1}^{n}(L_{v^i q^j}(q,v)dq^i \wedge dq^j + L_{v^i v^j}(q,v)dq^i \wedge dv^j). \tag{2.10}$$

4. The *action* of the Lagrangian

$$\int_{t_a}^{t_b} L(q(t), v(t)) - g^T(q(t))\lambda(t)dt$$

is stationary. This is *Hamilton's variational principle*. The algebraic variables λ are Lagrange multipliers associated with the holonomic constraints (2.4c).

5. The flow may be γ-*reversible*, i.e., $\varphi_\tau = \gamma^{-1} \circ \varphi_\tau^{-1} \circ \gamma$ for some transformation γ of the variables (q,v). For example, for *conservative mechanical systems* in Lagrangian form, the Lagrangian is given by $L(q,v) = T(q,v) - U(q)$, where $T(q,v) = \frac{1}{2}v^T M(q)v$ is the *kinetic energy* with $M(q)$ being the (strictly) positive definite symmetric generalized mass matrix, and $U(q)$ is the *potential energy*. The flow is γ-reversible with respect to a reflection of the velocities $\gamma : (q,v) \mapsto (q,-v)$.

2.4. Unification and generalization of the formulation of Hamiltonian and Lagrangian systems with holonomic constraints. We present here a unified and generalized formulation of Hamiltonian and Lagrangian systems with holonomic constraints, consisting of a set of implicit ODAEs

$$y' = v(y,z), \tag{2.11a}$$

$$(p(y,z))' = f(y,z) + r(y,\lambda), \tag{2.11b}$$

$$0 = g(y), \tag{2.11c}$$

$$0 = g_y(y)v(y,z). \tag{2.11d}$$

These equations encompass the formulation of conservative mechanical systems with constraints of holonomic and scleronomic types [10, 22, 26, 27]. In mechanics the quantities y, v, p, f, r usually represent, respectively, generalized coordinates, generalized velocities, generalized momenta, generalized forces, and reaction forces due to the holonomic constraints (2.11c). These equations include Hamiltonian systems with holonomic constraints (2.1) and Lagrangian systems with holonomic constraints (2.4). For Hamiltonian systems (2.1) we have $q = y$, $p(y,z) = z$, $v(y,z) = H_z^T(y,z)$, $f(y,z) = -H_y^T(y,z)$, and $r(y,\lambda) = -g_y^T(y)\lambda$. For Lagrangian systems (2.4) we have $q = y$, $v(y,z) = z$, $p(y,z) = L_z^T(y,z)$, $f(y,z) = L_y^T(y,z)$, and $r(y,\lambda) = -g_y^T(y)\lambda$. Equation (2.11d) corresponds to $0 = (g(y))' = g_y(y)y'$. The variable $t \in \mathbb{R}$ is the independent variable and

$$\begin{aligned}
&y = (y^1, \ldots, y^{n_y})^T \in \mathbb{R}^{n_y},\\
&z = (z^1, \ldots, z^{n_z})^T \in \mathbb{R}^{n_z},\\
&\lambda = (\lambda^1, \ldots, \lambda^{n_\lambda})^T \in \mathbb{R}^{n_\lambda},\\
&p \,:\, \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \longrightarrow \mathbb{R}^{n_z},\\
&g \,:\, \mathbb{R} \times \mathbb{R}^{n_y} \longrightarrow \mathbb{R}^{n_\lambda},\\
&v \,:\, \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \longrightarrow \mathbb{R}^{n_y},\\
&f \,:\, \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} \longrightarrow \mathbb{R}^{n_z},\\
&r \,:\, \mathbb{R} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_\lambda} \longrightarrow \mathbb{R}^{n_z}.
\end{aligned}$$

The variables y, z are called the *differential* variables and the variables λ are called the *algebraic* variables. The latter correspond to Lagrange multipliers when the DAEs are derived from a constrained variational principle [10, 22]. The initial values y_0, z_0 at t_0 are assumed to be given and consistent, i.e., (2.11c) and (2.11d) must be satisfied. Some differentiability conditions on the above functions are also assumed to ensure existence and uniqueness of the solution. In a neighborhood of the solution the following conditions are assumed to be satisfied:

$$p_z \text{ is invertible,} \tag{2.12a}$$

$$\begin{pmatrix} p_z & -r_\lambda \\ g_y v_z & O \end{pmatrix} \text{ is invertible.} \tag{2.12b}$$

Differentiating the left-hand side of (2.11b), under the assumption (2.12a) we obtain the following expression:

$$z' = p_z(y,z)^{-1}\left(f(y,z) + r(y,\lambda) - p_y(y,z)v(y,z)\right). \tag{2.13}$$

Differentiating the constraints (2.11d) leads to

$$0 = g_{yy}(y)\left(v(y,z), v(y,z)\right) + g_y(y)(v_y(y,z)v(y,z) + v_z(y,z)z'). \tag{2.14}$$

Introducing the expression for z' from (2.13) into (2.14), we see that under assumption (2.12b) equations (2.14) form an implicit system of equations for λ whose solution exists and is locally unique by application of the implicit function theorem.

Introducing the new variables q, p and the relations

$$q = y, \qquad p = p(y,z), \tag{2.15}$$

under the assumption (2.12a) we can formally express the differential variables y and z as (implicit) functions of (q,p), i.e.,

$$y = q, \qquad z = z(q,p).$$

Defining

$$V(q,p) := v\left(q, z\left(q,p\right)\right),\ F(q,p) := f\left(q, z\left(q,p\right)\right),\ R(q,\lambda) := r\left(q,\lambda\right),\ G(q) := g\left(q\right),$$

the whole system (2.11) can be reformulated in an equivalent way as

$$q' = V(q,p), \tag{2.16a}$$

$$p' = F(q,p) + R(q,\lambda), \tag{2.16b}$$

$$0 = G(q), \tag{2.16c}$$

$$0 = G_q(q)V(q,p), \tag{2.16d}$$

and assumption (2.12b) is equivalent to

$$G_q V_p R_\lambda \text{ is invertible.} \tag{2.17}$$

There is no implicit derivative in (2.16b). Since the application of SPARK methods (3.2) below is invariant under the change of variables (2.15), for the analysis in section 5 we can simply consider $p(y,z) = z$ in (2.11b).

3. SPARK methods. After briefly considering the class of standard RK methods, we introduce the new class of SPARK methods for the ODAEs (2.11). Examples of SPARK methods are then given.

3.1. Standard RK methods. The standard application of RK methods to the system of index 3 DAEs (2.11a,b,c) with $p(y,z) = z$ is as follows [6]:

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij} v(Y_j, Z_j) \quad \text{for } i = 1,\dots,s,$$

$$Z_i = z_0 + h\sum_{j=1}^{s} a_{ij}\left(f(Y_j, Z_j) + r(Y_j, \Lambda_j)\right) \quad \text{for } i = 1,\dots,s,$$

$$0 = g(Y_i) \quad \text{for } i = 1, \dots, s,$$

$$y_1 = y_0 + h \sum_{j=1}^{s} b_j v(Y_j, Z_j),$$

$$z_1 = z_0 + h \sum_{j=1}^{s} b_j \left(f(Y_j, Z_j) + r(Y_j, \Lambda_j) \right).$$

For example, the standard $s = 1$-stage Gauss RK method for Hamiltonian systems with holonomic constraints (2.1a,b,c), based on the implicit midpoint rule for ODEs, reads as

$$Q_1 = q_0 + h\frac{1}{2} H_p^T(Q_1, P_1) = \frac{1}{2}(q_1 + q_0),$$

$$P_1 = p_0 - h\frac{1}{2} H_q^T(Q_1, P_1) - h\frac{1}{2} g_q^T(q_1)\Lambda_1 = \frac{1}{2}(p_1 + p_0),$$

$$0 = g(Q_1),$$

$$q_1 = q_0 + h H_p^T(Q_1, P_1),$$

$$p_1 = p_0 - h H_q^T(Q_1, P_1) - h g_q^T(q_1)\Lambda_1.$$

Unfortunately, this method is in general divergent. More generally, the standard definition of RK methods does not take advantage of the additive structure of (2.11b) and of the presence of the two sets of constraints (2.11c,d). A different extension of the implicit midpoint rule, convergent even for the more general system of ODAEs (2.11), can be found within the class of SPARK methods (3.2) to be discussed hereafter. When $p(y, z) = z$, this extension is given by

$$Y_1 = y_0 + h\frac{1}{2} v(Y_1, Z_1) = \frac{1}{2}(y_1 + y_0), \tag{3.1a}$$

$$Z_1 = z_0 + h\frac{1}{2} f(Y_1, Z_1) + h\frac{1}{2} r(y_0, \Lambda_0), \tag{3.1b}$$

$$y_1 = y_0 + h v(Y_1, Z_1), \tag{3.1c}$$

$$0 = g(y_1), \tag{3.1d}$$

$$z_1 = z_0 + h f(Y_1, Z_1) + h\frac{1}{2} r(y_0, \Lambda_0) + h\frac{1}{2} r(y_1, \Lambda_1), \tag{3.1e}$$

$$0 = g_y(y_1) v(y_1, z_1) \tag{3.1f}$$

and is named a $(1, 1)$-Gauss–Lobatto SPARK method; see subsection 3.3. Note that the quantity Λ_0 is local to the current step and does not come from the previous step. For Hamiltonian systems with holonomic constraints (2.1), we obtain

$$Q_1 = q_0 + h\frac{1}{2} H_p^T(Q_1, P_1) = \frac{1}{2}(q_1 + q_0),$$

$$P_1 = p_0 - h\frac{1}{2} H_q^T(Q_1, P_1) - h\frac{1}{2} g_q^T(q_0)\Lambda_0,$$

$$q_1 = q_0 + hH_p^T(Q_1, P_1),$$

$$0 = g(q_1),$$

$$p_1 = p_0 - hH_q^T(Q_1, P_1) - h\frac{1}{2}g_q^T(q_0)\Lambda_0 - h\frac{1}{2}g_q^T(q_1)\Lambda_1,$$

$$0 = g_q(q_1)H_p^T(q_1, p_1).$$

For separable Hamiltonian systems of the form $H(q,p) = \frac{1}{2}p^T M^{-1}p + U(q)$, this method is equivalent to a method proposed by Reich in [24].

3.2. Definition of SPARK methods. We propose here a class of methods based on RK coefficients taking advantage of the structure of (2.11), in particular of the additive and partitioned structure of (2.11a,b) and of the presence of the two sets of constraints (2.11c,d). The definition of SPARK methods is given below. A similar application of SPARK methods has been proposed for the numerical solution of mechanical systems in [15]; see also [16].

DEFINITION 3.1. *One step of an* $(s, \widetilde{s})$-SPARK method *applied to the system of implicit overdetermined partitioned DAEs* (2.11) *with consistent initial values* (y_0, z_0) *at* t_0 *and stepsize* h *is given as follows:*

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij}v(Y_j, Z_j) \quad \text{for } i = 1, \dots, s, \tag{3.2a}$$

$$p(Y_i, Z_i) = p_0 + h\sum_{j=1}^{s} \widehat{a}_{ij}f(Y_j, Z_j) + h\sum_{j=0}^{\widetilde{s}} \widetilde{a}_{ij}r(\widetilde{Y}_j, \Lambda_j) \quad \text{for } i = 1, \dots, s, \tag{3.2b}$$

$$\widetilde{Y}_i = y_0 + h\sum_{j=1}^{s} \overline{a}_{ij}v(Y_j, Z_j) \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{3.2c}$$

$$0 = g(\widetilde{Y}_i) \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{3.2d}$$

$$y_1 = y_0 + h\sum_{j=1}^{s} b_j v(Y_j, Z_j), \tag{3.2e}$$

$$p(y_1, z_1) = p_0 + h\sum_{j=1}^{s} \widehat{b}_j f(Y_j, Z_j) + h\sum_{j=0}^{\widetilde{s}} \widetilde{b}_j r(\widetilde{Y}_j, \Lambda_j), \tag{3.2f}$$

$$0 = g(y_1), \tag{3.2g}$$

$$0 = g_y(y_1)v(y_1, z_1), \tag{3.2h}$$

where $p_0 := p(y_0, z_0)$. *We have four sets of coefficients* (b_j, a_{ij}, c_i), $(\widehat{b}_j, \widehat{a}_{ij})$, $(\widetilde{b}_j, \widetilde{a}_{ij})$, $(\overline{a}_{ij}, \widetilde{c}_i)$, *where we have defined*

$$c_i := \sum_{j=1}^{s} a_{ij} \quad \text{for } i = 1, \dots, s, \qquad \widetilde{c}_i := \sum_{j=1}^{s} \overline{a}_{ij} \quad \text{for } i = 0, 1, \dots, \widetilde{s}.$$

Notice that the coefficients $(b_j, c_j)_{j=1}^{s}$ *and* $(\widetilde{b}_j, \widetilde{c}_j)_{j=0}^{\widetilde{s}}$ *are generally two distinct quadrature formulas. The SPARK coefficients can be expressed concisely in four Butcher-style tableaux:*

$$\begin{array}{c|c} c_i & a_{ij} \\ \hline A & b_j \end{array} \qquad \begin{array}{c|c} & \widehat{a}_{ij} \\ \hline \widehat{A} & \widehat{b}_j \end{array} \qquad \begin{array}{c|c} & \widetilde{a}_{ij} \\ \hline \widetilde{A} & \widetilde{b}_j \end{array} \qquad \begin{array}{c|c} \widetilde{c}_i & \overline{a}_{ij} \\ \hline \overline{A} & \end{array}.$$

When the RK matrix $A = (a_{ij})_{i,j=1}^{s}$ is invertible we can express the values $\widetilde{Y}_i$ for $i = 0, 1, \ldots, \widetilde{s}$ and y_1 as linear combinations of y_0 and Y_j for $j = 1, \ldots, s$ as follows:

$$\widetilde{Y}_i = y_0 + \sum_{j=1}^{s} \eta_{ij}(Y_j - y_0), \qquad y_1 = y_0 + \sum_{j=1}^{s} \nu_j(Y_j - y_0),$$

where $\eta := \overline{A}A^{-1}$ and $\nu^T := b^T A^{-1}$. An $(s, \widetilde{s})$-SPARK method (3.2) can be seen as an extension of an s-stage standard (partitioned) RK method for partitioned ODEs

$$y' = v(y, z), \qquad z' = f(y, z).$$

To ensure existence and uniqueness of the SPARK solution (see Theorem 5.1), we assume the SPARK coefficients satisfy the following conditions:

(3.3a) $\overline{a}_{0j} = 0 \quad$ for $j = 1, \ldots, s$,

(3.3b) $\overline{a}_{\widetilde{s}j} = b_j \quad$ for $j = 1, \ldots, s$,

(3.3c) $$\sum_{j=1}^{s} \overline{a}_{ij} c_j = \sum_{j=1}^{s} \sum_{k=1}^{s} \overline{a}_{ij} \widehat{a}_{jk} = \sum_{j=1}^{s} \sum_{k=0}^{\widetilde{s}} \overline{a}_{ij} \widetilde{a}_{jk} = \frac{\widetilde{c}_i^2}{2} \quad \text{for } i = 0, 1, \ldots, \widetilde{s},$$

(3.3d) $$\overline{A}\widetilde{A} =: \begin{pmatrix} 0 & \cdots & 0 \\ & N & \end{pmatrix}, \qquad \begin{pmatrix} N \\ \widetilde{b}^T \end{pmatrix} \text{ is invertible.}$$

Condition (3.3a) implies that $\widetilde{c}_0 = 0$ and $\widetilde{Y}_0 = y_0$. Therefore $g(\widetilde{Y}_0) = 0$ is automatically satisfied since we assume $g(y_0) = 0$. Such SPARK methods generally do not require the evaluation of $v(y_0, z_0)$ and $f(y_0, z_0)$. However, $r(y_0, \Lambda_0)$ is required. Condition (3.3b) implies that $g(y_1) = 0$ is automatically satisfied since $g(\widetilde{Y}_{\widetilde{s}}) = 0$ from (3.2d) for $i = \widetilde{s}$ and $y_1 = \widetilde{Y}_{\widetilde{s}}$.

3.3. The (s, s)-Gauss–Lobatto SPARK methods. We are especially interested in extending Gauss RK methods for ODEs without constraints to corresponding (s, s)-SPARK methods (3.2) for the ODAEs (2.11) having an optimal order of convergence $2s$. The Gauss RK coefficients $\widehat{a}_{ij} = a_{ij}, \widehat{b}_j = b_j$ can be found, e.g., in [3, 7]. The Gauss RK coefficients satisfy

$$\sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, \ldots, 2s,$$

$$\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \qquad i = 1, \ldots, s, \quad k = 1, \ldots, s.$$

For the coefficients $\widetilde{b}_i$ and $\widetilde{c}_i$, we take the coefficients of the $(s+1)$-stage Lobatto quadrature formula ($\widetilde{c}_0 = 0, \widetilde{c}_s = 1$) of order $2s$ which satisfy

$$\sum_{i=0}^{s} \widetilde{b}_i \widetilde{c}_i^{k-1} = \frac{1}{k}, \qquad k = 1, \dots, 2s.$$

The coefficients $\overline{a}_{ij}$ can be taken according to

$$\sum_{j=1}^{s} \overline{a}_{ij} c_j^{k-1} = \frac{\widetilde{c}_i^k}{k}, \qquad i = 0, 1, \dots, s, \quad k = 1, \dots, s,$$

and the coefficients $\widetilde{a}_{ij}$ are then simply determined by

$$\widetilde{a}_{ij} = \widetilde{b}_j \left(1 - \frac{\overline{a}_{ji}}{b_i}\right), \qquad i = 1, \dots, s, \quad j = 0, 1, \dots, s.$$

These methods are called (s, s)-*Gauss–Lobatto SPARK methods*. They have order $2s$ of convergence; see Corollary 5.4. It can be shown that these methods satisfy conditions (3.3) and

$$\widetilde{a}_{i0} = \widetilde{b}_0, \quad \widetilde{a}_{is} = 0, \quad i = 1, \dots, s.$$

The algebraic variable Λ_s appears only in (3.2f) and is thus determined by (3.2h).

The $(1,1)$-Gauss–Lobatto SPARK method corresponds to the following Butcher-style tableaux of SPARK coefficients:

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline A & 1 \end{array} \qquad \begin{array}{c|c} & 1/2 \\ \hline \widehat{A} & 1 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0 \\ \hline \widetilde{A} & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|c} 0 & 0 \\ 1 & 1 \\ \hline \overline{A} & \end{array}.$$

We have $\widetilde{Y}_0 = y_0$ and $\widetilde{Y}_1 = y_1$. When $p(y, z) = z$ in (2.11b) the method simplifies to (3.1) for $Y_1, y_1, Z_1, z_1, \Lambda_0, \Lambda_1$.

The $(2,2)$-Gauss–Lobatto SPARK method corresponds to the following Butcher-style tableaux of SPARK coefficients:

$$\begin{array}{c|ccc} 1/2 - \sqrt{3}/6 & 1/4 & 1/4 - \sqrt{3}/6 \\ 1/2 + \sqrt{3}/6 & 1/4 + \sqrt{3}/6 & 1/4 \\ \hline A & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} & 1/4 & 1/4 - \sqrt{3}/6 \\ & 1/4 + \sqrt{3}/6 & 1/4 \\ \hline \widehat{A} & 1/2 & 1/2 \end{array}$$

$$\begin{array}{c|ccc} & 1/6 & 1/3 - \sqrt{3}/6 & 0 \\ & 1/6 & 1/3 + \sqrt{3}/6 & 0 \\ \hline \widetilde{A} & 1/6 & 2/3 & 1/6 \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/4 + \sqrt{3}/8 & 1/4 - \sqrt{3}/8 \\ 1 & 1/2 & 1/2 \\ \hline \overline{A} & & \end{array}.$$

We have $\widetilde{Y}_0 = y_0$ and $\widetilde{Y}_2 = y_1$.

3.4. The Lobatto IIIA-B partitioned RK (PRK) methods. SPARK methods (3.2) include the Lobatto IIIA-B PRK methods of [12, 13]. For example, the

$(2,1)$-Lobatto IIIA-B SPARK method of order 2 (an extension of the Störmer/leap-frog/Verlet/RATTLE/ SHAKE methods) corresponds to the following Butcher-style tableaux of SPARK coefficients:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline A & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0 \\ & 1/2 & 0 \\ \hline \widehat{A} & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0 \\ & 1/2 & 0 \\ \hline \widetilde{A} & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline \overline{A} & & \end{array}.$$

For this method we have $Y_1 = \widetilde{Y}_0 = y_0$ and $Y_2 = \widetilde{Y}_1 = y_1$. When $p(y,z) = z$ in (2.11b) the method simplifies to the following equations for $y_1, Z_1 = Z_2, z_1, \Lambda_0, \Lambda_1$:

$$\begin{aligned} y_1 &= y_0 + h\frac{1}{2}v(y_0, Z_1) + h\frac{1}{2}v(y_1, Z_2), \\ Z_1 &= z_0 + h\frac{1}{2}f(y_0, Z_1) + h\frac{1}{2}r(y_0, \Lambda_0), \\ 0 &= g(y_1), \\ z_1 &= z_0 + h\frac{1}{2}f(y_0, Z_1) + h\frac{1}{2}f(y_1, Z_2) + h\frac{1}{2}r(y_0, \Lambda_0) + h\frac{1}{2}r(y_1, \Lambda_1) \\ &= Z_1 + h\frac{1}{2}f(y_1, Z_2) + h\frac{1}{2}r(y_1, \Lambda_1), \\ 0 &= g_y(y_1)v(y_1, z_1). \end{aligned}$$

3.5. The symplectic Euler method. For Hamiltonian systems with holonomic constraints (2.1), the symplectic Euler method [7, 9, 23] is defined as follows:

$$P_1 = p_0 - hH_q^T(q_0, P_1) - hg_q^T(q_0)\Psi_0, \tag{3.4a}$$

$$q_1 = q_0 + hH_p^T(q_0, P_1), \tag{3.4b}$$

$$0 = g(q_1), \tag{3.4c}$$

$$p_1 = p_0 - hH_q^T(q_0, P_1) - hg_q^T(q_0)\Psi_0 - hg_q^T(q_1)\Psi_1 = P_1 - hg_q^T(q_1)\Psi_1, \tag{3.4d}$$

$$0 = g_q(q_1)H_p^T(q_1, p_1). \tag{3.4e}$$

It is a method of order 1 and the two quantities Ψ_0, Ψ_1 are locally determined by these equations. The symplectic Euler method can be interpreted as a SPARK method (3.2) with coefficients

$$\begin{array}{c|c} 0 & 0 \\ \hline A & 1 \end{array} \qquad \begin{array}{c|c} & 1 \\ \hline \widehat{A} & 1 \end{array} \qquad \begin{array}{c|cc} & \alpha & 0 \\ \hline \widetilde{A} & \alpha & 1-\alpha \end{array} \qquad \begin{array}{c|c} 0 & 0 \\ 1 & 1 \\ \hline \overline{A} & \end{array},$$

which we call the *"natural" symplectic Euler method*. The quantities Ψ_0 and Ψ_1 correspond to $\Psi_0 = \alpha\Lambda_0$ and $\Psi_1 = (1-\alpha)\Lambda_1$. Unfortunately, this method does not satisfy (3.3c), and when applied to the more general problem (2.11) this SPARK method is generally not convergent [17] when $r(y,\lambda)$ is nonlinear in λ. A convergent

extension of the symplectic Euler method to (2.11) (here given when $p(y,z)=z$ in (2.11b)) is as follows:

$$\begin{aligned}
Z_1 &= z_0 + hf(y_0, Z_1) + h\alpha r(y_0, \Lambda_0),\\
y_1 &= y_0 + hv(y_0, Z_1),\\
0 &= g(y_1),\\
z_1 &= z_0 + hf(y_0, Z_1) + h\alpha(r(y_0,\Lambda_0) - r(y_1,\Lambda_0)) + hr(y_1, \widetilde{\Lambda}_1)\\
&= Z_1 - h\alpha r(y_1,\Lambda_0) + hr(y_1,\widetilde{\Lambda}_1),\\
0 &= g_y(y_1)v(y_1, z_1),
\end{aligned}$$

with $\alpha \neq 0$. We call this method the *"true" symplectic Euler method*. It is convergent of order 1 [17]. It cannot be expressed in the format of a SPARK method (3.2) when $r(y,\lambda)$ is nonlinear in λ. When $r(y,\lambda)$ is affine in λ it is equivalent to the natural symplectic Euler method, which is symplectic for Hamiltonian systems with holonomic constraints (2.1) and for Lagrangian systems with holonomic constraints (2.4); see Theorems 4.1 and 4.2.

4. Symplecticness and variational properties of SPARK methods. The preservation of the symplecticness of the flow of Hamiltonian and Lagrangian systems with holonomic constraints by SPARK methods is considered in this section. The variational properties of the discrete trajectories of symplectic SPARK methods are also examined.

4.1. Symplectic SPARK methods. For Hamiltonian systems with holonomic constraints (2.1), SPARK methods whose numerical flow preserves (locally) the symplecticness property are characterized as follows.

THEOREM 4.1. *We consider Hamiltonian systems with holonomic constraints* (2.1) *satisfying the assumptions given in section* 2.1. *If the SPARK method* (3.2) *applied to* (2.1) *satisfies*

$$\widehat{b}_i = b_i \qquad \text{for } i = 1,\dots,s, \tag{4.1a}$$

$$\widehat{b}_i a_{ij} + b_j \widehat{a}_{ji} - \widehat{b}_i b_j = 0 \qquad \text{for } i,j = 1,\dots,s, \tag{4.1b}$$

$$\widetilde{b}_i \overline{a}_{ij} + b_j \widetilde{a}_{ji} - \widetilde{b}_i b_j = 0 \qquad \text{for } i = 0,1,\dots,\widetilde{s},\quad j = 1,\dots,s, \tag{4.1c}$$

then the numerical flow $(q_0,p_0)\mapsto(q_1,p_1)$ *preserves on* V (2.3) *the symplectic* 2*-form* $\sum_{i=1}^n dq^i \wedge dp^i$.

Proof. We denote

$$V_j := H_p^T(Q_j,P_j), \quad F_j := -H_q^T(Q_j,P_j), \quad R_j := -g_q^T(\widetilde{Q}_j)\Lambda_j.$$

We have

$$\begin{aligned}
dq_1^J \wedge dp_1^J - dq_0^J \wedge dp_0^J = h\sum_{i=1}^{s} \widehat{b}_i dq_0^J \wedge dF_i^J + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i dq_0^J \wedge dR_i^J + h\sum_{j=1}^{s} b_j dV_j^J \wedge dp_0^J\\
+h^2 \sum_{j=1}^{s} b_j dV_j^J \wedge \sum_{i=1}^{s} \widehat{b}_i dF_i^J + h^2 \sum_{j=1}^{s} b_j dV_j^J \wedge \sum_{i=0}^{\widetilde{s}} \widetilde{b}_i dR_i^J.
\end{aligned}$$

Introducing in the first three terms the following three relations for q_0 and p_0, respectively:

$$q_0 = Q_i - h\sum_{j=1}^{s} a_{ij}V_j, \quad q_0 = \widetilde{Q}_i - h\sum_{j=1}^{s} \overline{a}_{ij}V_j, \quad p_0 = P_j - h\sum_{i=1}^{s} \widehat{a}_{ji}F_i - h\sum_{i=0}^{\widetilde{s}} \widetilde{a}_{ji}R_i,$$

we obtain

$$\begin{aligned}\sum_{J=1}^{n} dq_1^J \wedge dp_1^J - \sum_{J=1}^{n} dq_0^J \wedge dp_0^J = {} & h\sum_{i=1}^{s}\left(\widehat{b}_i \sum_{J=1}^{n} dQ_i^J \wedge dF_i^J + b_i \sum_{J=1}^{n} dV_i^J \wedge dP_i^J\right) \\ & + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i \left(\sum_{J=1}^{n} d\widetilde{Q}_i^J \wedge dR_i^J\right) \\ & + h^2 \sum_{J=1}^{n}\sum_{j=1}^{s}\sum_{i=1}^{s}\left(b_j\widehat{b}_i - b_j\widehat{a}_{ji} - \widehat{b}_i a_{ij}\right) dV_j^J \wedge dF_i^J \\ & + h^2 \sum_{J=1}^{n}\sum_{j=1}^{s}\sum_{i=0}^{\widetilde{s}}\left(b_j\widetilde{b}_i - b_j\widetilde{a}_{ji} - \widetilde{b}_i\overline{a}_{ij}\right) dV_j^J \wedge dR_i^J.\end{aligned}$$

The first term vanishes by assumption (4.1a) and

$$\sum_{J=1}^{n}(dQ_i^J \wedge dF_i^J + dV_i^J \wedge dP_i^J) = 0;$$

see [8, Formula (II.16.18)]. The last two terms also vanish by assumptions (4.1b,c). It remains to show that the second term also vanishes. We have

$$dR_i^J = -\sum_{L=1}^{m}\sum_{K=1}^{n} \frac{\partial^2 g^L}{\partial q^K \partial q^J}(\widetilde{Q}_i)\Lambda_i^L d\widetilde{Q}_i^K - \sum_{L=1}^{m} \frac{\partial g^L}{\partial q^J}(\widetilde{Q}_i) d\Lambda_i^L.$$

We thus get

$$\begin{aligned}\sum_{J=1}^{n} d\widetilde{Q}_i^J \wedge dR_i^J = {} & -\sum_{L=1}^{m} \Lambda_i^L \left(\sum_{J=1}^{n}\sum_{K=1}^{n} \frac{\partial^2 g^L}{\partial q^K \partial q^J}(\widetilde{Q}_i) d\widetilde{Q}_i^J \wedge d\widetilde{Q}_i^K\right) \\ & - \sum_{L=1}^{m}\left(\sum_{J=1}^{n} \frac{\partial g^L}{\partial q^J}(\widetilde{Q}_i) d\widetilde{Q}_i^J\right) \wedge d\Lambda_i^L.\end{aligned}$$

Since the second derivative of g^L is symmetric the expression in brackets in the first term vanishes. Moreover, since $g^L(\widetilde{Q}_i) = 0$ the expression in brackets in the second term also vanishes. This concludes the proof. ∎

Notice that by adding the terms $\overline{a}_{i0}v(y_0, z_0)$ in (3.2c) and $b_0 v(y_0, z_0)$ in (3.2e), we obtain in Theorem 4.1 the additional condition (4.1c) for $j = 0$. For $b_0 = 0$ this implies $\overline{a}_{i0} = 0$ if $\widetilde{b}_i \neq 0$ $(i = 0, 1, \ldots, \widetilde{s})$.

A consequence of Theorem 4.1 is the following.

COROLLARY 4.2. *We consider Lagrangian systems with holonomic constraints* (2.4) *satisfying the assumptions given in section* 2.2. *If the SPARK method* (3.2)

applied to (2.4) *satisfies* (4.1)*, then the numerical flow* $(q_0, v_0) \mapsto (q_1, v_1)$ *preserves on* W (2.6) *the Lagrangian symplectic* 2*-form* (2.10).

Proof. For systems without constraints this result was stated in [14]. The result follows from the equivalence between Hamiltonian and Lagrangian systems as described in section 2.3. Under assumption (2.5), Lagrangian system (2.4) with variables (q, v) can be reformulated in terms of an equivalent Hamiltonian system (2.1) with variables (q, p). A SPARK method (3.1) can be formally applied to this Hamiltonian system (2.1) and then rewritten in terms of the variables (q, v) of the Lagrangian form. This is in fact equivalent to applying a SPARK method (3.1) with the same coefficients directly to Lagrangian system (2.4). ∎

Assuming coefficients (b_i, a_{ij}) and $(\widehat{b}_i)$ are given, to satisfy the symplecticness conditions (4.1b) we must have

$$\widehat{a}_{ij} = \widehat{b}_j \left(1 - \frac{a_{ji}}{b_i}\right) \quad \text{for } i, j = 1, \dots, s, \quad \text{when } b_i \neq 0.$$

Assuming coefficients $(\widetilde{b}_i, \overline{a}_{ij})$ and (b_i) are given, to satisfy the symplecticness conditions (4.1c) we must have

$$\widetilde{a}_{ij} = \widetilde{b}_j \left(1 - \frac{\overline{a}_{ji}}{b_i}\right) \quad \text{for } i = 1, \dots, s, \quad j = 0, 1, \dots, \widetilde{s}, \quad \text{when } b_i \neq 0.$$

From the symplecticness condition (4.1c), the assumption $\overline{a}_{0j} = 0$ (3.3a) implies $b_j = 0$ or $\widetilde{a}_{j0} = \widetilde{b}_0$. We are thus particularly interested in SPARK methods satisfying

$$\widetilde{a}_{i0} = \widetilde{b}_0 \quad \text{for } i = 1, \dots, s. \tag{4.2}$$

From the symplecticness condition (4.1c), the assumption $\overline{a}_{\widetilde{s}j} = b_j$ implies $b_j = 0$ or $\widetilde{a}_{j\widetilde{s}} = 0$. We are thus particularly interested in SPARK methods satisfying

$$\widetilde{a}_{i\widetilde{s}} = 0 \quad \text{for } i = 1, \dots, s. \tag{4.3}$$

From this condition the algebraic variable $\Lambda_{\widetilde{s}}$ appears only in (3.2f) and is determined by (3.2h).

4.2. Symplectic SPARK methods are variational integrators. The application of a SPARK method to Lagrangian systems (2.4) with holonomic constraints and consistent initial values q_0, v_0 at t_0, i.e., $g(q_0) = 0$ and $g_q(q_0)v_0 = 0$, reads as

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} V_j \quad \text{for } i = 1, \dots, s, \tag{4.4a}$$

$$P_i = p_0 + h \sum_{j=1}^{s} \widehat{a}_{ij} F_j + h \sum_{j=0}^{\widetilde{s}} \widetilde{a}_{ij} R_j \quad \text{for } i = 1, \dots, s, \tag{4.4b}$$

$$\widetilde{Q}_i = q_0 + h \sum_{j=1}^{s} \overline{a}_{ij} V_j \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{4.4c}$$

$$0 = g(\widetilde{Q}_i) \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{4.4d}$$

$$q_1 = q_0 + h\sum_{j=1}^{s} b_j V_j, \tag{4.4e}$$

$$p_1 = p_0 + h\sum_{j=1}^{s} \widehat{b}_j F_j + h\sum_{j=0}^{\widetilde{s}} \widetilde{b}_j R_j, \tag{4.4f}$$

$$0 = g(q_1), \tag{4.4g}$$

$$0 = g_q(q_1)v_1, \tag{4.4h}$$

where

$$p_0 := L_v^T(q_0, v_0), \quad p_1 := L_v^T(q_1, v_1), \quad P_i := L_v^T(Q_i, V_i) \quad \text{for } i = 1, \dots, s,$$

$$F_i := L_q^T(Q_i, V_i) \quad \text{for } i = 1, \dots, s, \qquad R_i := -g_q^T(\widetilde{Q}_i)\Lambda_i \quad \text{for } i = 0, 1, \dots, \widetilde{s}.$$

When the SPARK coefficients satisfy symplecticness conditions (4.1), SPARK method (4.4) can also be derived from a variational point of view following the ideas introduced by Marsden and West [21]. Notice that the variational property in a backward analysis sense of symplectic PRK integrators was derived in [14]. The nonequivalent derivation of [7] would consider $V_1, \dots, V_s$ as independent variables and would remove the constraints (4.4b). This derivation would be difficult to apply in our context due to the presence of holonomic constraints.

Following Marsden and West [21], instead of considering the unknown quantities in (3.2) as implicit functions of q_0, v_0, and h, we consider them as implicit functions of q_0, q_1, and h. More precisely, assuming $g(q_0) = 0$ and $g(q_1) = 0$ we implicitly define as functions of q_0, q_1, and h the quantities $p_0, p_1, v_0, v_1, Q_i, P_i, V_i, F_i$ for $i = 1, \dots, s$ and $\widetilde{Q}_i, R_i, \Lambda_i$ for $i = 0, 1, \dots, \widetilde{s}$ by (4.4), except that we replace (4.4g) $g(q_1) = 0$ by $0 = g_q(q_0)v_0$. Formally speaking, we should make a distinction between the solution of (4.4) and the solution of (4.4) with the equation $g(q_1) = 0$ replaced by $0 = g_q(q_0)v_0$. In any case, the solution to one system is also the solution to the other under the assumptions $g(q_0) = 0$ and $g_q(q_0)v_0 = 0$ for the first system of equations and $g(q_0) = 0$ and $g(q_1) = 0$ for the second system of equations.

Considering the discrete action

$$A_d(q_0, q_1, h) := h\sum_{i=1}^{s} b_i L(Q_i, V_i) - h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i \Lambda_i g(\widetilde{Q}_i),$$

we can show after some lengthy calculations (see the proof of Theorem 4.3) that when the SPARK coefficients satisfy the symplecticness assumptions (4.1), we have the relations

$$p_0 = -\nabla_1 A_d(q_0, q_1, h), \qquad p_1 = \nabla_2 A_d(q_0, q_1, h).$$

Therefore, the discrete Euler–Lagrange equations

$$\nabla_2 A_d(q_{n-1}, q_n, h) + \nabla_1 A_d(q_n, q_{n+1}, h) = 0$$

are satisfied for $n = 1, \dots, N-1$. This implies stationarity of the total discrete action

$$\sum_{n=1}^{N} A_d(q_{n-1}, q_n, h) \tag{4.5}$$

with respect to q_n for $n = 1, \dots, N-1$. This is nothing else but a discrete version of Hamilton's principle applied to this sum (4.5). Therefore a SPARK symplectic integrator is also a variational integrator in this sense; more precisely, we have the following.

THEOREM 4.3. *For Lagrangian systems with holonomic constraints* (2.4) *and a corresponding SPARK method* (4.4)*, assume q_0 and q_N are fixed and consistent. Replace $0 = g(q_{n+1})$ for $n = 0, 1, \dots, N-1$ by $0 = g_q(q_n)v_n$. If the SPARK coefficients satisfy symplecticness assumptions* (4.1)*, then we have a variational integrator in the sense of Marsden and West* [21]*; i.e., we have stationarity of the total discrete action* (4.5) *with respect to q_n for $n = 1, \dots, N-1$.*

Proof. We show now the relation $-\nabla_1 A_d(q_0, q_1, h) = p_0$. We have

$$
\begin{aligned}
-\frac{\partial A_d}{\partial q_0}(q_0,q_1,h) &= -h\sum_{i=1}^{s} b_i L_q(Q_i,V_i)\frac{\partial Q_i}{\partial q_0} - h\sum_{i=1}^{s} b_i L_v(Q_i,V_i)\frac{\partial V_i}{\partial q_0} \\
&\quad + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i \Lambda_i^T \left(g_q(\widetilde{Q}_i)\frac{\partial \widetilde{Q}_i}{\partial q_0}\right) + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i g^T(\widetilde{Q}_i)\frac{\partial \Lambda_i}{\partial q_0} \\
&= -h\sum_{i=1}^{s} b_i F_i^T \left(I + h\sum_{j=1}^{s} a_{ij}\frac{\partial V_j}{\partial q_0}\right) - h\sum_{i=1}^{s} b_i P_i^T \frac{\partial V_i}{\partial q_0} \\
&\quad + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i \Lambda_i^T g_q(\widetilde{Q}_i) \left(I + h\sum_{j=1}^{s} \overline{a}_{ij}\frac{\partial V_j}{\partial q_0}\right) + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i g^T(\widetilde{Q}_i)\frac{\partial \Lambda_i}{\partial q_0} \\
&= -h\sum_{i=1}^{s} b_i F_i^T I - h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i a_{ij} F_i^T \frac{\partial V_j}{\partial q_0} \\
&\quad - h\sum_{i=1}^{s} b_i \left(p_0^T + h\sum_{j=1}^{s} \widehat{a}_{ij} F_j^T + h\sum_{j=0}^{\widetilde{s}} \widetilde{a}_{ij} R_j^T \right) \frac{\partial V_i}{\partial q_0} - h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i R_i^T I \\
&\quad - h^2 \sum_{i=0}^{\widetilde{s}}\sum_{j=1}^{s} \widetilde{b}_i \overline{a}_{ij} R_i^T \frac{\partial V_j}{\partial q_0} + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i g^T(\widetilde{Q}_i)\frac{\partial \Lambda_i}{\partial q_0} \\
&= -h\sum_{j=1}^{s} b_j F_j^T I - h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_j a_{ji} + b_i \widehat{a}_{ij}) F_j^T \frac{\partial V_i}{\partial q_0} \\
&\quad - p_0^T h\sum_{i=1}^{s} b_i \frac{\partial V_i}{\partial q_0} - h^2 \sum_{i=1}^{s}\sum_{j=0}^{\widetilde{s}} b_i \widetilde{a}_{ij} R_j^T \frac{\partial V_i}{\partial q_0} - h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i R_i^T I \\
&\quad - h^2 \sum_{i=0}^{\widetilde{s}}\sum_{j=1}^{s} \widetilde{b}_i \overline{a}_{ij} R_i^T \frac{\partial V_j}{\partial q_0} + h\sum_{i=0}^{\widetilde{s}} \widetilde{b}_i g^T(\widetilde{Q}_i)\frac{\partial \Lambda_i}{\partial q_0}.
\end{aligned}
$$

From (4.4e) we have

$$0 = I + h\sum_{i=1}^{s} b_i \frac{\partial V_i}{\partial q_0};$$

hence

$$-\frac{\partial A_d}{\partial q_0}(q_0,q_1,h) = -h^2\sum_{i=1}^{s}\sum_{j=1}^{s}(b_j a_{ji} + b_i\widehat{a}_{ij} - b_j b_i)F_j^T\frac{\partial V_i}{\partial q_0} + p_0^T$$

$$-h^2\sum_{i=0}^{\widetilde{s}}\sum_{j=1}^{s}(b_j\widetilde{a}_{ji} + \widetilde{b}_i\overline{a}_{ij} - \widetilde{b}_i b_j)R_i^T\frac{\partial V_j}{\partial q_0} + h\sum_{i=0}^{\widetilde{s}}\widetilde{b}_i g^T(\widetilde{Q}_i)\frac{\partial \Lambda_i}{\partial q_0}.$$

From (4.4d) and symplecticness assumptions (4.1) we obtain the desired result of

$$-\frac{\partial A_d}{\partial q_0}(q_0,q_1,h) = p_0^T.$$

The relation $\nabla_2 A_d(q_0,q_1,h) = p_1$ can be shown in a similar way; thus we skip its proof. ∎

A consequence of Theorem 4.3 is the following.

COROLLARY 4.4. *For Hamiltonian systems with holonomic constraints* (2.1)*, assume q_0 and q_N are fixed and consistent. Replace the equations $0 = g(q_{n+1})$ for $n = 0, 1, \ldots, N-1$ by $0 = g_q(q_n)H_p(q_n,p_n)$. If the SPARK coefficients satisfy symplecticness assumptions* (4.1)*, then we have a variational integrator in the sense of Marsden and West* [21]*; i.e., we have stationarity of the total discrete action*

$$\sum_{n=1}^{N} A_d(q_{n-1},q_n,h)$$

with respect to q_n for $n = 1, \ldots, N-1$, where

$$A_d(q_0,q_1,h) := h\sum_{i=1}^{s} b_i\ell(Q_i,P_i) - h\sum_{i=0}^{\widetilde{s}}\widetilde{b}_i\Lambda_i^T g(\widetilde{Q}_i)$$

and where $\ell(q,p) := p^T H_p^T(q,p) - H(q,p)$.

Proof. The result follows from the equivalence between Hamiltonian and Lagrangian systems described in section 2.3. Under assumption (2.2), Hamiltonian system (2.1) with variables (q,p) can be reformulated in terms of an equivalent Lagrangian system (2.4) with variables (q,v). A SPARK method (3.1) can be formally applied to this Lagrangian system (2.1) and then rewritten in terms of the variables (q,p) of the Hamiltonian form. This is in fact equivalent to applying a SPARK method (3.1) with the same coefficients directly to Hamiltonian system (2.1). ∎

5. Analysis of SPARK methods. In this section we give results about existence, uniqueness, local error, and global convergence of SPARK methods. Since SPARK methods are invariant under the change of variables (2.15) (see (2.16) and (2.17)), for the analysis we can simply consider $p(y,z) = z$ in (2.11b), under the assumption

$$g_y v_z r_\lambda \text{ is invertible.}$$

5.1. Existence and uniqueness. Generally there does not exist a solution to the nonlinear system of Definition 3.1 without any assumption on the coefficients of the SPARK method. For consistent SPARK methods satisfying (3.3), existence and

uniqueness for the nonlinear system can be shown under some additional assumptions (see Theorem 5.1). A very accurate value for λ_1 may be unnecessary. For a consistent SPARK method, by (3.3b) we have $\widetilde{c}_{\widetilde{s}} = 1$. Hence, a fairly good choice for λ_1 is given by $\lambda_1 := \Lambda_{\widetilde{s}}$ if one is not interested in enforcing constraints (2.14). The accuracy of the numerical λ-component does not influence the convergence of the (y, z)-components and the properties of the SPARK method. Existence and uniqueness for the system of nonlinear equations of SPARK methods (3.1) are shown in the following theorem.

THEOREM 5.1. *Suppose that* $y_0 = y_0(h), z_0 = z_0(h), \lambda_0 = \lambda_0(h)$ *satisfy*

$$0 = g(y_0), \tag{5.1a}$$

$$O(h^2) = g_y(y_0)v(y_0, z_0), \tag{5.1b}$$

$$\begin{aligned} O(h) = {} & g_{yy}(y_0)(v(y_0, z_0), v(y_0, z_0)) + g_y(y_0)v_y(y_0, z_0)v(y_0, z_0) \\ & + g_y(y_0)v_z(y_0, z_0)(f(y_0, z_0) + r(y_0, \lambda_0)), \end{aligned} \tag{5.1c}$$

where (2.12) *is satisfied in a neighborhood of* (y_0, z_0, λ_0). *Then for SPARK methods satisfying* (3.3) *and* $|h| \le h_0$ *there exists a locally unique SPARK solution of*

$$0 = Y_i - y_0 - h\sum_{j=1}^{s} a_{ij}v(Y_j, Z_j) \quad \text{for } i = 1, \dots, s, \tag{5.2a}$$

$$0 = Z_i - z_0 - h\sum_{j=1}^{s} \widehat{a}_{ij}f(Y_j, Z_j) - h\sum_{j=0}^{\widetilde{s}} \widetilde{a}_{ij}r(\widetilde{Y}_j, \Lambda_j) \quad \text{for } i = 1, \dots, s, \tag{5.2b}$$

$$0 = \widetilde{Y}_i - y_0 - h\sum_{j=1}^{s} \overline{a}_{ij}v(Y_j, Z_j) \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{5.2c}$$

$$0 = g(\widetilde{Y}_i) \quad \text{for } i = 0, 1, \dots, \widetilde{s}, \tag{5.2d}$$

$$0 = y_1 - y_0 - h\sum_{j=1}^{s} b_j v(Y_j, Z_j), \tag{5.2e}$$

$$0 = z_1 - z_0 - h\sum_{j=1}^{s} \widehat{b}_j f(Y_j, Z_j) - h\sum_{j=0}^{\widetilde{s}} \widetilde{b}_j r(\widetilde{Y}_j, \Lambda_j), \tag{5.2f}$$

$$0 = g(y_1), \tag{5.2g}$$

$$0 = g_y(y_1)v(y_1, z_1), \tag{5.2h}$$

which satisfies

$$\begin{aligned} & & Y_i - y_0 = O(h) \quad & \text{for } i = 1, \dots, s, & & \\ \widetilde{Y}_0 = y_0, \quad & \widetilde{Y}_i - y_0 = O(h) \quad & \text{for } i = 1, \dots, \widetilde{s}, \quad & y_1 = \widetilde{Y}_{\widetilde{s}}, \\ & Z_i - z_0 = O(h) \quad & \text{for } i = 1, \dots, s, \quad & z_1 - z_0 = O(h), \\ & \Lambda_i - \lambda_0 = O(h) \quad & \text{for } i = 0, 1, \dots, \widetilde{s}. & \end{aligned}$$

Proof. The proof of this theorem can be done by application of the implicit function theorem, as in the proof of [12, Theorem V.4.1]. We have $\widetilde{Y}_0 = y_0$; hence $g(\widetilde{Y}_0) = 0$ is automatically satisfied by assumption. We have $\widetilde{Y}_{\widetilde{s}} = y_1$; hence (5.2g) can be removed since it is equivalent to (5.2d) for $i = \widetilde{s}$. We expand $g(\widetilde{Y}_i)$ for $i = 1, \dots, \widetilde{s}$ and $v(Y_i, Z_i)$ for $i = 1, \dots, s$ into Taylor series around y_0

$$
\begin{aligned}
g(\widetilde{Y}_i) &= g(y_0) + g_y(y_0)(\widetilde{Y}_i - y_0) \\
&\quad + \int_0^1 (1-\tau) g_{yy}(y_0 + \tau(\widetilde{Y}_i - y_0)) d\tau (\widetilde{Y}_i - y_0, \widetilde{Y}_i - y_0), \\
v(Y_i, Z_i) &= v(y_0, z_0) + \int_0^1 v_y(y_0 + \tau(Y_i - y_0), z_0 + \tau(Z_i - z_0)) d\tau (Y_i - y_0) \\
&\quad + \int_0^1 v_z(y_0 + \tau(Y_i - y_0), z_0 + \tau(Z_i - z_0)) d\tau (Z_i - z_0) \\
&= v(y_0, z_0) + h \int_0^1 v_y(y_0 + \tau(Y_i - y_0), z_0 + \tau(Z_i - z_0)) d\tau \sum_{j=1}^{s} a_{ij} v(Y_j, Z_j) \\
&\quad + h \int_0^1 v_z(y_0 + \tau(Y_i - y_0), z_0 + \tau(Z_i - z_0)) d\tau \left(\sum_{j=1}^{s} \widehat{a}_{ij} f(Y_j, Z_j) + \sum_{j=0}^{\widetilde{s}} \widetilde{a}_{ij} r(\widetilde{Y}_j, \Lambda_j) \right).
\end{aligned}
$$

Dividing $g(\widetilde{Y}_i)$ by h^2 and replacing the terms $\widetilde{Y}_i - y_0$, $Y_i - y_0$, and $Z_i - z_0$ by using (5.2a,b,c), we obtain

$$
\begin{aligned}
\frac{1}{h^2} g(\widetilde{Y}_i) &= \frac{1}{h^2} g(y_0) + \frac{1}{h} \sum_{j=1}^{s} \overline{a}_{ij} g_y(y_0) v(Y_j, Z_j) \\
&\quad + \sum_{j=1}^{s} \sum_{k=1}^{s} \overline{a}_{ij} \overline{a}_{ik} \int_0^1 (1-\tau) g_{yy}(y_0 + \tau(\widetilde{Y}_i - y_0)) d\tau (v(Y_j, Z_j), v(Y_k, Z_k)) \\
&= \frac{1}{h^2} g(y_0) + \frac{1}{h} \sum_{j=1}^{s} \overline{a}_{ij} g_y(y_0) v(y_0, z_0) \\
&\quad + \sum_{j=1}^{s} \sum_{k=1}^{s} \overline{a}_{ij} a_{jk} g_y(y_0) \int_0^1 v_y(y_0 + \tau(Y_j - y_0), z_0 + \tau(Z_j - z_0)) d\tau v(Y_k, Z_k) \\
&\quad + \sum_{j=1}^{s} \sum_{k=1}^{s} \overline{a}_{ij} \widehat{a}_{jk} g_y(y_0) \int_0^1 v_z(y_0 + \tau(Y_j - y_0), z_0 + \tau(Z_j - z_0)) d\tau f(Y_k, Z_k) \\
&\quad + \sum_{j=1}^{s} \sum_{k=0}^{\widetilde{s}} \overline{a}_{ij} \widetilde{a}_{jk} g_y(y_0) \int_0^1 v_z(y_0 + \tau(Y_j - y_0), z_0 + \tau(Z_j - z_0)) d\tau r(\widetilde{Y}_k, \Lambda_k) \\
&\quad + \sum_{j=1}^{s} \sum_{k=1}^{s} \overline{a}_{ij} \overline{a}_{ik} \int_0^1 (1-\tau) g_{yy}(y_0 + \tau(\widetilde{Y}_i - y_0)) d\tau (v(Y_j, Z_j), v(Y_k, Z_k)).
\end{aligned}
$$

By (3.3c), for the values $Y_i := y_0$, $\widetilde{Y}_i := y_0$, $Z_i := z_0$, and $\Lambda_i = \lambda_0$ we obtain

$$\frac{1}{h^2}g(\widetilde{Y}_i) = \frac{\widetilde{c}_i^2}{2}\big(g_y(y_0)v_y(y_0,z_0)v(y_0,z_0) + g_y(y_0)v_z(y_0,z_0)f(y_0,z_0) + g_y(y_0)v_z(y_0,z_0)r(y_0,\lambda_0) + g_{yy}(y_0)(v(y_0,z_0),v(y_0,z_0))\big) = O(h).$$

Hence the values $Y_i(0) := y_0(0)$, $\widetilde{Y}_i(0) := y_0(0)$, $Z_i(0) := z_0(0)$, and $\Lambda_i(0) = \lambda_0(0)$ satisfy (5.2a,b,c) and

$$0 = \frac{1}{h^2}g(\widetilde{Y}_i) \tag{5.3}$$

$$= \sum_{j=1}^{s}\sum_{k=1}^{s}\overline{a}_{ij}a_{jk}g_y(y_0)\int_0^1 v_y(y_0+\tau(Y_j-y_0),z_0+\tau(Z_j-z_0))d\tau v(Y_k,Z_k) + \cdots.$$

Similarly we have

$$g_y(y_1) = g_y(y_0) + \int_0^1 g_{yy}(y_0+\tau(y_1-y_0))d\tau(y_1-y_0,\cdot)$$

$$= g_y(y_0) + h\sum_{j=1}^{s} b_j\int_0^1 g_{yy}(y_0+\tau(y_1-y_0))d\tau(v(Y_j,Z_j),\cdot),$$

$$v(y_1,z_1) = v(y_0,z_0) + \int_0^1 v_y(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau(y_1-y_0) + \int_0^1 v_z(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau(z_1-z_0)$$

$$= v(y_0,z_0) + h\int_0^1 v_y(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau\sum_{j=1}^{s} b_j v(Y_j,Z_j)$$

$$+ h\int_0^1 v_z(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau\left(\sum_{j=1}^{s}\widehat{b}_j f(Y_j,Z_j) + \sum_{j=0}^{\widetilde{s}}\widetilde{b}_j r(\widetilde{Y}_j,\Lambda_j)\right).$$

Hence, dividing $g_y(y_1)v(y_1,z_1)$ by h, we obtain

$$\frac{1}{h}g_y(y_1)v(y_1,z_1) = \frac{1}{h}g_y(y_0)v(y_0,z_0) + \sum_{j=1}^{s} b_j g_y(y_0)\int_0^1 v_y(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau v(Y_j,Z_j)$$

$$+ \sum_{j=1}^{s}\widehat{b}_j\int_0^1 v_z(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau f(Y_j,Z_j)$$

$$+ \sum_{j=0}^{\widetilde{s}}\widetilde{b}_j\int_0^1 v_z(y_0+\tau(y_1-y_0),z_0+\tau(z_1-z_0))d\tau r(\widetilde{Y}_j,\Lambda_j)$$

$$+ \sum_{j=1}^{s} b_j\int_0^1 g_{yy}(y_0+\tau(y_1-y_0))d\tau(v(Y_j,Z_j),v(y_1,z_1)).$$

By consistency $\sum_{j=1}^{s} b_j = 1$, $\sum_{j=1}^{s} \widehat{b}_j = 1$, $\sum_{j=0}^{\widetilde{s}} \widetilde{b}_j = 1$, for the values $Y_i := y_0$, $\widetilde{Y}_i := y_0$, $y_1 := y_0$, $Z_i := z_0$, $z_1 := z_0$, and $\Lambda_i = \lambda_0$, we obtain

$$\frac{1}{h} g_y(y_1) v(y_1, z_1) = g_y(y_0) v_y(y_0, z_0) v(y_0, z_0) + g_y(y_0) v_z(y_0, z_0) f(y_0, z_0) + g_y(y_0) v_z(y_0, z_0) r(y_0, \lambda_0) + g_{yy}(y_0)(v(y_0, z_0), v(y_0, z_0)) = O(h).$$

Hence the values $Y_i(0) := y_0(0)$, $\widetilde{Y}_i(0) := y_0(0)$, $y_1(0) := y_0(0)$, $Z_i(0) := z_0(0)$, $z_1(0) := z_0(0)$, and $\Lambda_i(0) = \lambda_0(0)$ satisfy

$$0 = \frac{1}{h} g_y(y_1) v(y_1, z_1) = \sum_{j=1}^{s} b_j g_y(y_0) \int_0^1 v_y(y_0 + \tau(y_1 - y_0), z_0 + \tau(z_1 - z_0)) d\tau v(Y_j, Z_j) + \cdots . \tag{5.4}$$

Replacing y_1 and z_1 in (5.3)–(5.4) by using (5.2e,f), and using tensor matrix product notations, we see that the Jacobian of (5.2a,b,c), (5.3), and (5.4) with respect to Y_i $(i = 1, \ldots, s)$, Z_i $(i = 1, \ldots, s)$, $\widetilde{Y}_i$ $(i = 1, \ldots, \widetilde{s})$, and Λ_i $(i = 0, 1, \ldots, \widetilde{s})$ is of the form

$$\begin{pmatrix} I_{sn_y} + O(h) & O & O(h) & O \\ O(h) & I_{sn_z} + O(h) & O(h) & O(h) \\ O(h) & O(h) & I_{\widetilde{s}n_y} & O \\ O(1) & O(1) & O(1) & \begin{pmatrix} N \\ \widetilde{b}^T \end{pmatrix} \otimes g_y(y_0) v_z(y_0, z_o) r_\lambda(y_0, \lambda_0) + O(h) \end{pmatrix}$$

with N as defined in (3.3d). This Jacobian matrix is invertible for $|h| \le h_0$ sufficiently small. Therefore, the implicit function theorem yields the existence of a locally unique solution to (5.2a,b,c), (5.3), and (5.4), and hence to the corresponding SPARK method (5.2). ∎

5.2. Local error of the (s, s)-Gauss–Lobatto SPARK methods. A thorough local error analysis of the whole class of SPARK methods (3.2) based on using simplifying assumptions is beyond the scope of this paper. SPARK methods include a class of PRK methods whose local error analysis based on trees is long and technical [12, 13]. For Lobatto IIIA-B methods, an alternative proof using the idea of discontinuous collocation can be found in [7, section VII.1]. Here we will analyze only the local error of the (s, s)-Gauss–Lobatto SPARK methods as defined in subsection 3.3.

THEOREM 5.2. *Consider the system of ODAEs* (2.11), *consistent initial values* y_0, z_0 *at* t_0, *where* (2.12) *is satisfied in a neighborhood of* (y_0, z_0, λ_0). *Then for* $|h| \le h_0$ *the local error of the* (s, s)*-Gauss–Lobatto SPARK methods satisfies*

$$y_1 - y(t_0 + h) = O(h^{2s+1}), \quad z_1 - z(t_0 + h) = O(h^{2s+1}). \tag{5.5}$$

Proof. For the proof we can consider $p(y, z) = z$ in (2.11b). To prove this theorem we use the same techniques of proof as used in [11] for collocation methods. We define the polynomials $Y(t)$, $\widetilde{Y}(t)$, $Z(t)$, and $\Lambda(t)$ of degree s by

$$Y(t) = \sum_{i=0}^{s} \ell_i \left(\frac{t - t_0}{h} \right) Y_i, \qquad \widetilde{Y}(t) = \sum_{i=0}^{s} \widetilde{\ell}_i \left(\frac{t - t_0}{h} \right) \widetilde{Y}_i,$$

$$Z(t)=\sum_{i=0}^{s}\ell_i\left(\frac{t-t_0}{h}\right)Z_i,\qquad \Lambda(t)=\sum_{i=0}^{s}\widetilde{\ell}_i\left(\frac{t-t_0}{h}\right)\Lambda_i,$$

where

$$\ell_i(\tau):=\prod_{\substack{j=0\\ j\neq i}}^{s}\left(\frac{\tau-c_j}{c_i-c_j}\right),\qquad \widetilde{\ell}_i(\tau):=\prod_{\substack{j=0\\ j\neq i}}^{s}\left(\frac{\tau-\widetilde{c}_j}{\widetilde{c}_i-\widetilde{c}_j}\right),$$

$c_0:=0$, $Y_0:=y_0$, and $Z_0:=z_0$. We have $Y(t_0)=\widetilde{Y}(t_0)=y_0$, $Z(t_0)=z_0$, $Y(t_0+h)=\widetilde{Y}(t_0+h)=y_1$, $Z(t_0+h)=z_1$, and

$$Y'(t)=v(Y(t),Z(t))+\delta(t), \tag{5.6a}$$

$$\widetilde{Y}'(t)=v(Y(t),Z(t))+\widetilde{\delta}(t), \tag{5.6b}$$

$$Z'(t)=f(Y(t),Z(t))+r(\widetilde{Y}(t),\Lambda(t))+\mu(t), \tag{5.6c}$$

$$0=g(\widetilde{Y}(t))+\widetilde{\theta}(t), \tag{5.6d}$$

$$0=g_y(\widetilde{Y}(t))(v(Y(t),Z(t))+\widetilde{\delta}(t))+\widetilde{\theta}'(t), \tag{5.6e}$$

with defects $\delta(t)$, $\widetilde{\delta}(t)$, $\mu(t)$, $\widetilde{\theta}(t)$ satisfying

$$\delta(t_0+c_ih)=0\quad \text{for } i=1,\dots,s,$$

$$\widetilde{\delta}(t_0+\widetilde{c}_ih)=0\quad \text{for } i=0,1,\dots,s,$$

$$\mu(t_0+c_ih)=0\quad \text{for } i=1,\dots,s,$$

$$\widetilde{\theta}(t_0+\widetilde{c}_ih)=0\quad \text{for } i=0,1,\dots,s,$$

$$\widetilde{\theta}'(t_0)=-g_y(\widetilde{Y}(t_0))\widetilde{\delta}(t_0)=0,$$

$$\widetilde{\theta}'(t_0+h)=-g_y(\widetilde{Y}(t_0+h))\widetilde{\delta}(t_0+h)=0.$$

The exact solution $(y(t),y(t),z(t),\lambda(t))$ satisfies the same above relations (5.6) with $\delta(t)\equiv 0$, $\widetilde{\delta}(t)\equiv 0$, $\mu(t)\equiv 0$, and $\widetilde{\theta}(t)\equiv 0$. One more differentiation of (5.6e) yields

$$\begin{aligned}0=&\,g_{yy}(\widetilde{Y}(t))(v(Y(t),Z(t))+\widetilde{\delta}(t),v(Y(t),Z(t))+\widetilde{\delta}(t))\\&+g_y(\widetilde{Y}(t))v_y(Y(t),Z(t))(v(Y(t),Z(t))+\delta(t))\\&+g_y(\widetilde{Y}(t))v_z(Y(t),Z(t))(f(Y(t),Z(t))+r(\widetilde{Y}(t),\Lambda(t))+\mu(t))\\&+g_y(\widetilde{Y}(t))\widetilde{\delta}'(t)+\widetilde{\theta}''(t).\end{aligned}$$

We can express $\Lambda(t)$ from this equation as an implicit function

$$\Lambda(t)=\Upsilon(Y(t),\widetilde{Y}(t),Z(t),\delta(t),\widetilde{\delta}(t),\widetilde{\delta}'(t),\mu(t),\widetilde{\theta}''(t)).$$

Inserting this relation into (5.6c), we obtain the system of ODEs

$$Y'(t) = v(Y(t), Z(t)) + \delta(t),$$

$$\widetilde{Y}'(t) = v(Y(t), Z(t)) + \widetilde{\delta}(t),$$

$$Z'(t) = f(Y(t), Z(t)) + r(\widetilde{Y}(t), \Upsilon(Y(t), \widetilde{Y}(t), Z(t), \delta(t), \widetilde{\delta}(t), \widetilde{\delta}'(t), \mu(t), \widetilde{\theta}''(t))) + \mu(t).$$

To apply the Gröbner–Alekseev formula [8, Theorem I.14.5] we need the defect $d(t) := (d_1(t), d_2(t), d_3(t))^T$:

$$d_1(t) := Y'(t) - v(Y(t), Z(t)) = \delta(t),$$

$$d_2(t) := \widetilde{Y}'(t) - v(Y(t), Z(t)) = \widetilde{\delta}(t),$$

$$d_3(t) := Z'(t) - f(Y(t), Z(t)) - r(\widetilde{Y}(t), \Upsilon(Y(t), \widetilde{Y}(t), Z(t), 0, 0, 0, 0, 0)).$$

We have

$$d_3(t) = \Phi_3(t, 1) - \Phi_3(t, 0) = \int_0^1 \frac{\partial \Phi_3}{\partial \tau}(t, \tau) d\tau,$$

where

$$\Phi_3(t, \tau) := r(\widetilde{Y}(t), \Upsilon(Y(t), \widetilde{Y}(t), Z(t), \tau\delta(t), \tau\widetilde{\delta}(t), \tau\widetilde{\delta}'(t), \tau\mu(t), \tau\widetilde{\theta}''(t))) + \tau\mu(t).$$

Hence, we get

$$d_3(t) = Q_1(t)\delta(t) + Q_2(t)\widetilde{\delta}(t) + Q_3(t)\widetilde{\delta}'(t) + (I + Q_4(t))\mu(t) + Q_5(t)\widetilde{\theta}''(t),$$

where we give only the expressions of $Q_3(t)$ and $Q_5(t)$:

$$Q_3(t) = -\int_0^1 (r_\lambda (g_y v_z r_\lambda)^{-1} g_y)(Y(t), \widetilde{Y}(t), Z(t), \Upsilon(Y(t), \widetilde{Y}(t), Z(t), \tau\delta(t), \tau\widetilde{\delta}(t), \tau\widetilde{\delta}'(t), \tau\mu(t), \tau\widetilde{\theta}''(t)) d\tau,$$

$$Q_5(t) = -\int_0^1 (r_\lambda (g_y v_z r_\lambda)^{-1}(Y(t), \widetilde{Y}(t), Z(t), \Upsilon(Y(t), \widetilde{Y}(t), Z(t), \tau\delta(t), \tau\widetilde{\delta}(t), \tau\widetilde{\delta}'(t), \tau\mu(t), \tau\widetilde{\theta}''(t)) d\tau.$$

We denote the resolvent of the exact solution

$$R(t, s) := R(t, s, y_s, \widetilde{Y}_s, z_s) = \frac{\partial(y, \widetilde{Y}, z)}{\partial(y_s, \widetilde{Y}_s, z_s)}(t, s, y_s, \widetilde{Y}_s, z_s).$$

From the Gröbner–Alekseev formula we have

$$\begin{pmatrix} Y(t) - y(t) \\ \widetilde{Y}(t) - y(t) \\ Z(t) - z(t) \end{pmatrix} = \int_{t_0}^t R(t, s) d(s) ds$$

$$= \int_{t_0}^t S_1(t, s)\delta(s) + S_2(t, s)\widetilde{\delta}(s) + S_3(t, s)\widetilde{\delta}'(s) + S_4(t, s)\mu(s) + S_5(t, s)\widetilde{\theta}''(s) ds,$$

where

$$S_1(t,s)=R(t,s)\begin{pmatrix} I \\ O \\ Q_1(s) \end{pmatrix}, \qquad S_2(t,s)=R(t,s)\begin{pmatrix} O \\ I \\ Q_2(s) \end{pmatrix},$$

$$S_3(t,s)=R(t,s)\begin{pmatrix} O \\ O \\ Q_3(s) \end{pmatrix}, \qquad S_4(t,s)=R(t,s)\begin{pmatrix} O \\ O \\ I+Q_4(s) \end{pmatrix},$$

$$S_5(t,s)=R(t,s)\begin{pmatrix} O \\ O \\ Q_5(s) \end{pmatrix}.$$

Hence, by integration by parts, we obtain

$$\begin{pmatrix} Y(t)-y(t) \\ \widetilde{Y}(t)-y(t) \\ Z(t)-z(t) \end{pmatrix} = S_3(t,s)\widetilde{\delta}(s) - \frac{\partial S_5}{\partial s}(t,s)\widetilde{\theta}(s) + S_5(t,s)\widetilde{\theta}'(s)\Big|_{s=t_0}^{t}$$

$$+\int_{t_0}^{t}\sigma(t,s)ds+\int_{t_0}^{t}\widetilde{\sigma}(t,s)ds,$$

where

$$\sigma(t,s):=S_1(t,s)\delta(s)+S_4(t,s)\mu(s),$$

$$\widetilde{\sigma}(t,s):=\left(S_2(t,s)-\frac{\partial S_3}{\partial s}(t,s)\right)\widetilde{\delta}(s)+\frac{\partial^2 S_5}{\partial s^2}(t,s)\widetilde{\theta}(s).$$

We have $\widetilde{\delta}(t_0)=0=\widetilde{\delta}(t_0+h)$, $\widetilde{\theta}(t_0)=0=\widetilde{\theta}(t_0+h)$, $\widetilde{\theta}'(t_0)=0=\widetilde{\theta}'(t_0+h)$; hence at $t=t_0+h$ we are left with

$$\begin{pmatrix} y_1-y(t_0+h) \\ y_1-y(t_0+h) \\ z_1-z(t_0+h) \end{pmatrix} = \int_{t_0}^{t_0+h}\sigma(t_0+h,s)ds+\int_{t_0}^{t_0+h}\widetilde{\sigma}(t_0+h,s)ds.$$

Applying the Gauss quadrature formula with s nodes of order $2s$ for the first integral, and the Lobatto quadrature formula with $s+1$ nodes of order $2s$ for the second integral, we obtain

$$\int_{t_0}^{t_0+h}\sigma(t_0+h,s)ds=h\sum_{i=1}^{s}\sigma(t_0+h,t_0+c_ih)+O(h^{2s+1}),$$

$$\int_{t_0}^{t_0+h}\widetilde{\sigma}(t_0+h,s)ds=h\sum_{i=0}^{s}\widetilde{\sigma}(t_0+h,t_0+\widetilde{c}_ih)+O(h^{2s+1}),$$

and since $\sigma(t,t_0+c_ih)=0$ for $i=1,\dots,s$ and $\widetilde{\sigma}(t,t_0+\widetilde{c}_ih)=0$ for $i=0,1,\dots,s$, this leads to the desired result (5.5). ∎

5.3. Global convergence of SPARK methods. Once local error estimates of SPARK methods are known, global convergence results can be obtained without too much difficulty.

THEOREM 5.3. *Consider the system of ODAEs* (2.11) *under assumptions* (2.12) *and a SPARK method* (3.2) *of local order p satisfying assumptions* (3.3). *Then it is globally convergent of order p, i.e.,*

$$y_n - y(t_n) = O(h^p), \quad z_n - z(t_n) = O(h^p)$$

for $t_n - t_0 = nh \leq \text{Const}$.

Proof. For the proof we can consider $p(y,z) = z$ in (2.11b). Replacing (5.2d,g,h), respectively, by

$$\begin{aligned} g(\widetilde{Y}_i) &= g(y_0) + h\widetilde{c}_i g_y(y_0)v(y_0,z_0) \quad \text{for } i = 0,1,\dots,\widetilde{s}, \\ g(y_1) &= g(y_0) + h g_y(y_0)v(y_0,z_0), \\ g_y(y_1)v(y_1,z_1) &= g_y(y_0)v(y_0,z_0) \end{aligned}$$

extends the definition of SPARK methods to a neighborhood of (y_0,z_0) in $\mathbb{R}^{n_y} \times \mathbb{R}^{n_z}$; i.e., SPARK methods are not restricted to just the manifold of constraints $\{(y,z) \in \mathbb{R}^{n_y} \times \mathbb{R}^{n_z} | 0 = g(y), 0 = g_y(y)v(y,z)\}$. Hence, SPARK methods can be locally expressed as a mapping

$$\begin{pmatrix} y_{n+1} \\ z_{n+1} \end{pmatrix} = \begin{pmatrix} y_n \\ z_n \end{pmatrix} + h_n \Phi(h_n, y_n, z_n)$$

from $\mathbb{R}^{n_y} \times \mathbb{R}^{n_z}$ to $\mathbb{R}^{n_y} \times \mathbb{R}^{n_z}$. Hence, classical convergence results, like those for RK methods applied to ODEs, can then be applied [8]. ∎

For the (s,s)-Gauss–Lobatto SPARK methods, as a consequence of Theorem 4.1, Corollary 4.2, Theorem 4.3, Corollary 4.4, and Theorems 5.2 and 5.3, we can now state a major result of this paper.

COROLLARY 5.4. *Consider the system of ODAEs* (2.11) *under assumptions* (2.12). *The* (s,s)*-Gauss–Lobatto SPARK method* (3.2) *is constraint-preserving, symmetric, and of maximal order* $2s$, *i.e.,*

$$y_n - y(t_n) = O(h^{2s}), \quad z_n - z(t_n) = O(h^{2s})$$

for $|t_n - t_0| \leq \text{Const}$ *and* $h := \max(|h_1|,\dots,|h_n|)$. *For holonomically constrained Hamiltonian systems* (2.1) *and Lagrangian systems* (2.4) *these methods are also symplectic and variational.*

6. Numerical experiments. Figure 6.3

To illustrate Corollary 5.4, we have applied (s,s)-Gauss–Lobatto SPARK methods with constant stepsize h to the following system of ODAEs:

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} 2z_1 \\ -z_2 \end{pmatrix}, \tag{6.1a}$$

$$\begin{pmatrix} z_1' \\ z_2' \end{pmatrix} = \begin{pmatrix} 2y_1y_2z_1z_2 - y_1z_1z_2 \\ z_1 - y_1z_2^3 \end{pmatrix} + \begin{pmatrix} y_1y_2\lambda_1^2 \\ -\sqrt{y_1}\lambda_1 \end{pmatrix}, \tag{6.1b}$$

$$0 = y_1y_2^2 - 1, \tag{6.1c}$$

$$0 = 2y_2(z_1y_2 - y_1z_2). \tag{6.1d}$$

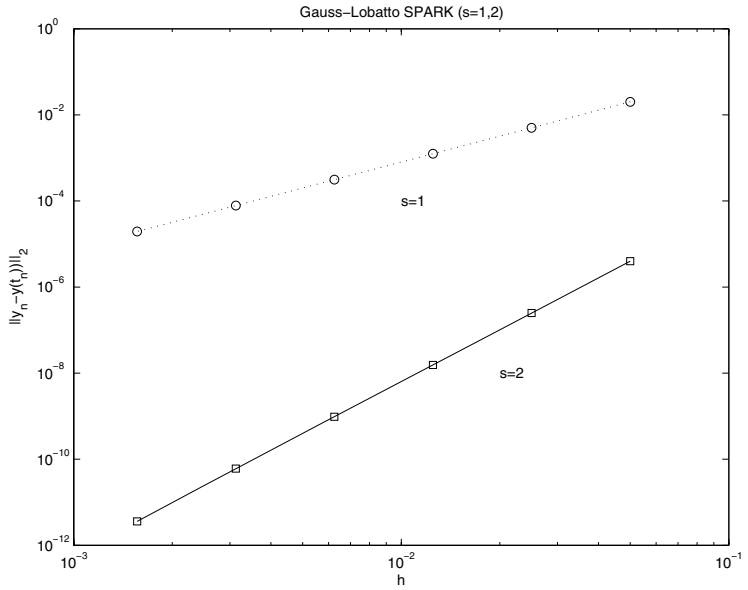

FIG. 6.1. *Global error in y at $t_n = 1$ of (s,s)-Gauss–Lobatto SPARK methods ($s = 1, 2$) applied with various constant stepsizes h to the test problem* (6.1).

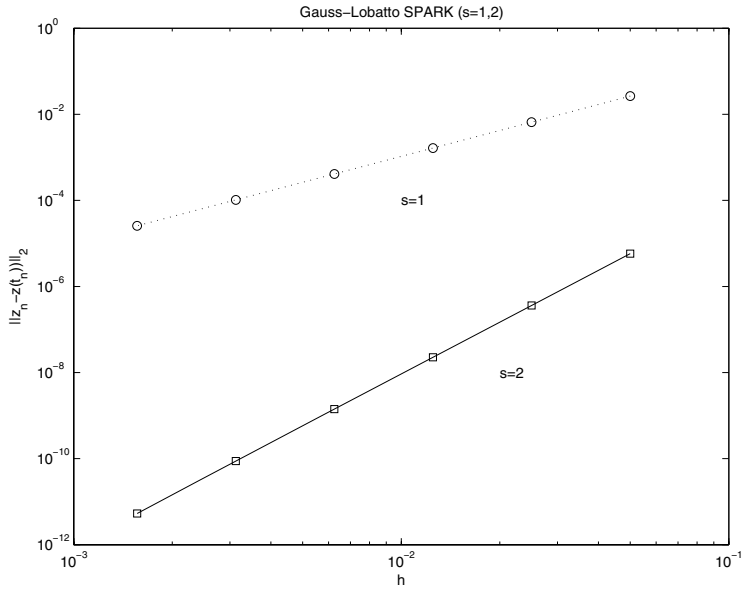

FIG. 6.2. *Global error in z at $t_n = 1$ of (s,s)-Gauss–Lobatto SPARK methods ($s = 1, 2$) applied with various constant stepsizes h to the test problem* (6.1).

For the initial conditions $y_1(0) = y_2(0) = z_1(0) = z_2(0) = 1$ at $t_0 = 0$, the exact solution to this test problem is given by $y_1(t) = z_1(t) = e^{2t}$, $y_2(t) = z_2(t) = e^{-t}$, $\lambda_1(t) = e^t$. We have plotted in Figures 6.1 and 6.2 the global errors for the y- and z-components at $t_n = 1$ with respect to various constant stepsizes h. Logarithmic scales have been used so that a curve appears as a straight line of slope k whenever

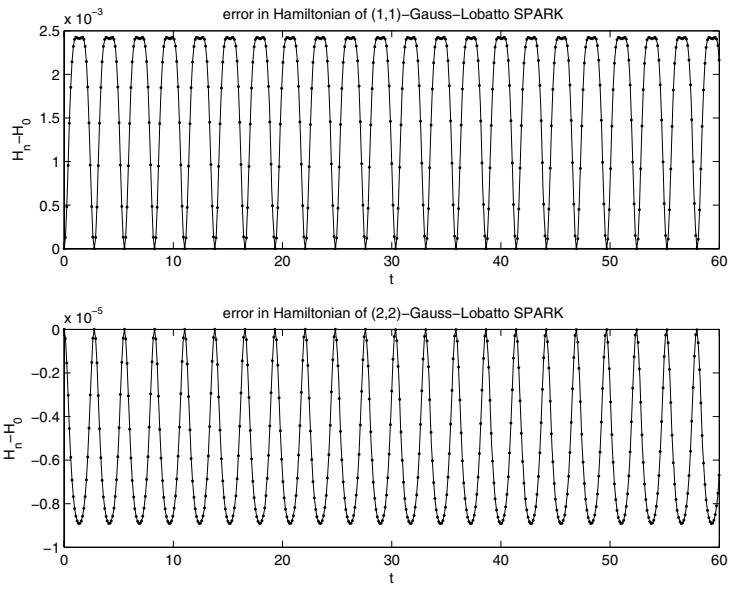

FIG. 6.3. *Error in Hamiltonian of* (s,s)*-Gauss–Lobatto SPARK methods* $(s=1,2)$ *applied with constant stepsize* $h=0.12$ *to the test problem* (6.2).

the leading term of the global error is of order k, i.e., when $\|y_n - y(t_n)\| = O(h^k)$. For the (s,s)-Gauss–Lobatto SPARK methods with $s=1,2$ of order $2s=2,4$ we observe straight lines of slope $2s=2,4$, thus confirming the orders of convergence predicted by Corollary 5.4.

As a second test problem, we consider the motion of a particle of mass m and electric charge e under the influence of an electric field $(0,0,E)^T$ and a magnetic field $(0,0,B)^T$ and restricted to a sphere of radius R [4, Problem 7.16]. This system can be described in term of Cartesian coordinates $(q_1,q_2,q_3)^T$ and generalized momenta $(p_1,p_2,p_3)^T$ with a nonseparable Hamiltonian

$$H = \frac{1}{2m}((p_1+m\omega q_2)^2 + (p_2 - m\omega q_1)^2 + p_3^2) - eEq_3 \tag{6.2a}$$

with $\omega := eB/(2mc)$ and holonomic constraint

$$\sqrt{q_1^2+q_2^2+q_3^2} - R = 0. \tag{6.2b}$$

We choose the parameters

$$m=1, \quad \omega=1, \quad R=1, \quad eE=1$$

and initial conditions

$$q_1(0)=0.2,\ q_2(0)=0.2,\ q_3(0)=\sqrt{0.92},\ p_1(0)=1,\ p_2(0)=-1,\ p_3(0)=0.$$

In Figure 6.3 we plot the Hamiltonian error of (s,s)-Gauss–Lobatto SPARK methods $(s=1,2)$ applied with constant stepsize $h=0.12$ to this system. As expected for a symplectic integrator, we observe that the Hamiltonian error remains bounded and small over long-time intervals.

7. Conclusion. We have considered a general class of ODAEs, and, more particularly, a unified formulation of Hamiltonian and Lagrangian systems with holonomic constraints. We have defined the application of SPARK methods for these systems, including in particular the new (s, s)-Gauss–Lobatto SPARK methods and also well-known schemes such as the Lobatto IIIA-B PRK methods. SPARK methods preserve the constraints. The (s, s)-Gauss–Lobatto SPARK methods have been proved to be of optimal order of convergence $2s$. For Hamiltonian and Lagrangian systems with holonomic constraints, these methods have also been shown to be symplectic and to preserve the variational nature of trajectories.

REFERENCES

[1] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, 2nd ed., Grad. Texts in Math. 60, Springer-Verlag, New York, 1989.

[2] K. E. Brenan, S. L. Campbell, and L. R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, Classics in Appl. Math., SIAM, Philadelphia, 1996.

[3] J. C. Butcher, *Numerical Methods for Ordinary Differential Equations*, 2nd ed., John Wiley & Sons, Chichester, 2003.

[4] P. Choquard, *Mécanique Analytique*, Vol. 1, of Cahiers Math. Ecole Polytech. Fédérale de Lausanne, Presses Polytechniques et Universitaires Romandes, Lausanne, Switzerland, 1992.

[5] E. Hairer and L. O. Jay, *Implicit Runge–Kutta Methods for Higher Index Differential-Algebraic Systems*, in Contributions in Numerical Mathematics, World Sci. Ser. Appl. Anal. 2, World Sci. Publ., River Edge, NJ, 1993, pp. 213–224.

[6] E. Hairer, Ch. Lubich, and M. Roche, *The Numerical Solution of Differential-Algebraic Systems by Runge–Kutta Methods*, Lecture Notes in Math. 1409, Springer, Berlin, 1989.

[7] E. Hairer, Ch. Lubich, and G. Wanner, *Geometric Numerical Integration*, 2nd ed., Comput. Math. 31, Springer, Berlin, 2006.

[8] E. Hairer, S. P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations* I. *Nonstiff Problems*, 2nd revised ed., Comput. Math. 18, Springer, Berlin, 1993.

[9] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations* II. *Stiff and Differential-Algebraic Problems*, 2nd revised ed., Comput. Math. 14, Springer, Berlin, 1996.

[10] E. J. Haug, *Computer Aided Kinematics and Dynamics of Mechanical Systems. Volume* I: *Basic Methods*, Allyn and Bacon, Boston, MA, 1989.

[11] L. O. Jay, *Collocation methods for differential-algebraic equations of index* 3, Numer. Math., 65 (1993), pp. 407–421.

[12] L. O. Jay, *Runge–Kutta Type Methods for Index Three Differential-Algebraic Equations with Applications to Hamiltonian Systems*, Ph.D. thesis, Department of Mathematics, University of Geneva, Geneva, Switzerland, 1994.

[13] L. Jay, *Symplectic partitioned Runge–Kutta methods for constrained Hamiltonian systems*, SIAM J. Numer. Anal., 33 (1996), pp. 368–387.

[14] L. O. Jay, *Lagrangian Integration with Symplectic Methods*, Tech. report 97-009, Army High Performance Computing Research Center, University of Minnesota, Minneapolis, MN, 1997.

[15] L. O. Jay, *Structure preservation for constrained dynamics with super partitioned additive Runge–Kutta methods*, SIAM J. Sci. Comput., 20 (1998), pp. 416–446.

[16] L. O. Jay, *Iterative solution of nonlinear equations for SPARK methods applied to DAEs*, Numer. Algorithms, 31 (2002), pp. 171–191.

[17] L. O. Jay, *A Note on the Symplectic Euler Method for DAEs with Holonomic Constraints*, Tech. report 165, Department of Mathematics, University of Iowa, Iowa City, IA, 2006.

[18] L. O. Jay, *Specialized Runge–Kutta methods for index* 2 *differential algebraic equations*, Math. Comput., 75 (2006), pp. 641–654.

[19] B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge Monogr. Appl. Comput. Math. 14, Cambridge University Press, Cambridge, UK, 2004.

[20] J. E. Marsden and T. S. Ratiu, *Introduction to Mechanics and Symmetry*, Texts Applied Math. 17, Springer, New York, 1994.

[21] J. E. Marsden and M. West, *Discrete mechanics and variational integrators*, Acta Numer., 10 (2001), pp. 357–514.

[22] P. J. Rabier and W. C. Rheinboldt, *Nonholonomic Motion of Rigid Mechanical Systems from a DAE Viewpoint*, SIAM, Philadelphia, 2000.
[23] S. Reich, *Symplectic Integration of Constrained Hamiltonian Systems by Runge–Kutta Methods*, Tech. report 93-13, Department of Computer Science, University of British Columbia, Vancouver, BC, Canada, 1993.
[24] S. Reich, *Symplectic integration of constrained Hamiltonian systems by composition methods*, SIAM J. Numer. Anal., 33 (1996), pp. 475–491.
[25] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems*, Appl. Math. Math. Comput. 7, Chapman & Hall, London, 1994.
[26] W. O. Schiehlen, ed., *Multibody Systems Handbook*, Springer-Verlag, Berlin, 1990.
[27] W. O. Schiehlen, ed., *Advanced Multibody System Dynamics, Simulation and Software Tools*, Kluwer Academic Publishers, London, 1993.
[28] A. M. Stuart and A. R. Humphries, *Dynamical Systems and Numerical Analysis*, Cambridge Monogr. Appl. Comput. Math. 2, Cambridge University Press, Cambridge, UK, 1998.