LAGRANGE-D'ALEMBERT SPARK INTEGRATORS FOR NONHOLONOMIC LAGRANGIAN SYSTEMS

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Abstract. We consider Lagrangian systems with ideal nonholonomic constraints. These systems can be expressed as implicit index 2 differential-algebraic equations (DAEs) and can be derived from the Lagrange-d'Alembert principle. Methods based on a discrete Lagrange-d'Alembert principle are called Lagrange-d'Alembert integrators and they generalize variational integrators. We define a new nonholonomically constrained discrete Lagrange-d'Alembert principle based on a discrete Lagrange-d'Alembert principle for forced Lagrangian systems. The principle that we propose does not make explicit use of any Lagrange multiplier in its formulation. Nonholonomic constraints are considered as first integrals of the underlying forced Lagrangian system of ordinary differential equations. We show that a large class of specialized partitioned additive Runge-Kutta (SPARK) methods for index 2 DAEs satisfies the new discrete principle. Symmetric Lagrange-d'Alembert SPARK integrators of any order can be obtained based for example on Gauss and Lobatto coefficients as already proposed for more general index 2 DAEs. Our results are illustrated by several numerical experiments.

Key words. Differential-algebraic equations, discrete mechanics, forcing, Gauss coefficients, ideal constraints, index 2, Lagrange-d'Alembert principle, Lagrangian systems, Lobatto coefficients, nonholonomic constraints, SPARK methods.

AMS subject classifications. 65L05, 65L06, 65L80, 70F25, 70G45, 70H03, 70H45.

1. Introduction.

In this paper we consider the numerical solution of Lagrangian systems with ideal nonholonomic constraints. Nonholonomic systems in mechanics have a long and intriguing history [1, 5, 28]. Nonholonomic constraints involve velocities and are nonintegrable, i.e., they cannot be derived from holonomic constraints. The dynamics of nonholonomic systems has been the subject of a controversy between Lagrange-d'Alembert mechanics and vakonomic (variational nonholonomic) mechanics. It is nowadays accepted that vakonomic mechanics does not lead to the correct equations of motion of physical systems, but that Lagrange-d'Alembert mechanics generally does [5, 22, 28]. In this paper we consider methods which mimic faithfully at the discrete level the integral Lagrange-d'Alembert principle. Such methods are called *Lagrange-d'Alembert (LDA) integrators*. They fall under the framework of geometric integration methods and they generalize variational integrators [19, 24].

Geometric integration has attracted quite a lot of interest in recent years, see for example the book [13] and the survey paper [27]. Geometric integration methods can be classified as extrinsic or intrinsic. *Intrinsic* methods are coordinate-free methods, for example Lie group methods are defined intrinsically in terms of the exponential map or some approximation to it on the corresponding Lie algebra to advance the numerical solution in time. In this paper we will exclusively consider extrinsic methods. *Extrinsic* methods consider an embedding of the manifold in $\mathbb{R}^n$ and make use of coordinates. For unconstrained Hamiltonian and Lagrangian systems important classes of geometric integrators are symplectic/Poisson integrators [13, 14, 21, 31] and variational integrators which are based on a discrete version of Hamilton's principle [19, 24]. For unconstrained Lagrangian systems with forcing an important class of geometric integrators are Lagrange-d'Alembert (LDA) integrators which are based on a discrete version of the Lagrange-d'Alembert principle [19, 24].

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For ideal nonholonomic constraints the equations of motion do not derive from a standard variational principle, but for example from the Lagrange-d'Alembert principle [3, 4, 5, 20, 28] which is not a variational principle, but a differential principle. For Lagrangian systems and ideal scleronomic (i.e., time-independent) linear nonholonomic constraints in the velocities the Lagrange-d'Alembert principle is equivalent to a *skew critical problem* which is also not truly a variational principle [3, 7, 8, 25]. Methods based on a similar discrete skew critical problem in $Q \times Q$ where Q is the configuration space have been first introduced by Cortés in [6, 7] and have also been called Lagrange-d'Alembert (LDA) integrators. A few low order LDA integrators of this type have been developed in [11, 12, 25]. We believe that the discrete constrained Lagrange-d'Alembert principle of Cortés [6, 7] is not sufficiently general to include many methods of interest. Tentatives to extend this principle have been made by Cuell and Patrick. For Lagrangian systems with ideal scleronomic linear nonholonomic constraints these authors have shown the Lagrange-d'Alembert principle to be equivalent to a skew critical problem in the kinematic state space TQ [8, 9, 10]. This result has been extended to Lagrangian systems with ideal nonlinear scleronomic nonholonomic constraints [29]. For Lagrangian systems with ideal linear scleronomic nonholonomic constraints, they have proposed discrete skew critical methods defined directly in the kinematic state space TQ [8, 10]. We also mention the energy-preserving methods for Lagrangian systems with ideal linear scleronomic nonholonomic constraints considered by Betsch in [2].

In this paper we take a radically different and simpler approach. We quote from McLachlan and Perlmutter in [25]: *much work remains to be done to clarify the nature of discrete nonholonomic mechanics and to pinpoint the "correct" discrete analog of the Lagrange-d'Alembert principle.* The nonholonomically constrained discrete Lagrange-d'Alembert principle that we consider in this paper is certainly correct and sufficiently general to include many methods of interest. We define a general constrained discrete Lagrange-d'Alembert principle directly in $Q \times Q$ based on the discrete Lagrange-d'Alembert principle for forced Lagrangian systems proposed in [19], see [24, Section 3.2]. The principle that we propose does not make explicit use of any Lagrange multiplier in its formulation contrary to [6, 7, 8, 10, 11, 12, 25]. This is consistent with the fact that the Lagrange-d'Alembert principle for nonholonomic systems is not a variational principle. We remark that nonholonomic constraints can be mathematically realized with forcing as a forced Lagrangian system. The nonholonomically constrained discrete Lagrange-d'Alembert principle that we propose is therefore fully consistent with the unconstrained discrete Lagrange-d'Alembert principle for forced Lagrangian systems. It generalizes the one proposed by Cortés in [6, 7] which appears restrictive. It is an extension in a direction awaited by McLachlan and Perlmutter in [25, Section 8]. This extension was in fact partly suggested without details by Marsden and West in [24, Section 5.3.7]. A large class of specialized partitioned additive Runge-Kutta (SPARK) methods for index 2 DAEs is shown to satisfy the new discrete principle. Symmetric Lagrange-d'Alembert SPARK integrators of any order can be obtained based for example on Gauss and Lobatto coefficients as already proposed for more general index 2 DAEs in [15, 16, 17]. An extension of the results of this paper to submanifolds $Q \subset \mathbb{R}^n$ and holonomic constraints will be the subject of a forthcoming paper [18].

The paper is organized as follows. In section 2 the system of DAEs of Lagrangian systems with ideal nonholonomic constraints is given. The underlying forced Lagrangian system is also obtained. In section 3 the Lagrange-d'Alembert principle is

discussed. A forced discrete Lagrange-d'Alembert principle for Lagrangian systems with nonholonomic constraints is proposed in section 4. In section 5 the exact discrete forcing terms for Lagrangian systems with nonholonomic constraints are derived. In section 6 the main Theorem 6.1 gives sufficient conditions for SPARK methods to satisfy the forced discrete Lagrange-d'Alembert principle for Lagrangian systems with nonholonomic constraints. Several examples of Lagrange-d'Alembert SPARK integrators are given in section 7. In section 8 some numerical experiments are given to illustrate the favorable energy preservation property of Lagrange-d'Alembert SPARK integrators. Finally, a short conclusion is given in section 9.

2. Lagrangian systems with ideal nonholonomic constraints. For simplicity in this paper we suppose that the configuration space Q is the linear space $Q = \mathbb{R}^n$. The constrained Lagrangian system with Lagrangian $L : \mathbb{R} \times TQ \longrightarrow \mathbb{R}$ (where $TQ \cong \mathbb{R}^n \times \mathbb{R}^n$) and ideal nonholonomic constraints $k : \mathbb{R} \times TQ \longrightarrow \mathbb{R}^m$ ($m < n$) is given by the *Lagrange equations of the second kind*

$$\frac{d}{dt}q = v, \tag{2.1a}$$

$$\frac{d}{dt}\nabla_v L(t,q,v) = \nabla_q L(t,q,v) - K(t,q,v)^T\psi, \tag{2.1b}$$

$$0 = k(t,q,v), \tag{2.1c}$$

where

$$K(t,q,v) := k_v(t,q,v). \tag{2.1d}$$

In most applications the nonholonomic constraints (2.1c) are affine in the generalized velocities v, i.e.,

$$0 = k(t,q,v) = K(t,q)v + b(t,q). \tag{2.2}$$

Moreover, such ideal affine nonholonomic constraints (2.2) are oftentimes just linear in v, i.e., $b(t,q) \equiv 0$. The assumption (2.2) will actually not be needed in this paper.

2.1. The underlying forced Lagrangian system. Expanding the left-hand side of (2.1b) we get

$$\nabla^2_{vv}L(t,q,v)\frac{d}{dt}v + K(t,q,v)^T\psi = -\nabla^2_{tv}L(t,q,v) - \nabla^2_{qv}L(t,q,v)v + \nabla_q L(t,q,v). \tag{2.3a}$$

From a computational point of view, see Section 6, it is in fact advantageous to consider directly the formulation (2.1b) instead of (2.3a) since (2.3a) requires the calculation of the extra terms $\nabla^2_{tv}L(t,q,v)$ and $\nabla^2_{qv}L(q,v)v$, the latter corresponding to Coriolis forces. Differentiating (2.1c) once with respect to t and using (2.1a) we obtain

$$K(t,q,v)\frac{d}{dt}v = -k_t(t,q,v) - k_q(t,q,v)v. \tag{2.3b}$$

In this paper we assume that the matrix

$$\begin{pmatrix} \nabla^2_{vv}L(t,q,v) & K(t,q,v)^T \\ K(t,q,v) & O \end{pmatrix} \quad \text{is nonsingular.} \tag{2.4}$$

For example, for ideal nonholonomic constraints one can assume that $K(t,q,v)$ is of full row rank m and that the Lagrangian L is regular, i.e., the Hessian matrix

$$\nabla^2_{vv} L(t,q,v) \quad \text{is nonsingular,} \tag{2.5}$$

$\nabla^2_{vv} L(t,q,v)$ is generally assumed to be positive definite. Under the assumption (2.4), from (2.3) we can express $\frac{d}{dt}v$ and ψ as explicit functions of (t,q,v). Hence, under the assumption (2.4) the equations (2.1) are implicit differential-algebraic equations (DAEs) of index 2 [16]. For consistent initial values (q_0, v_0) at t_0, i.e., such that

$$0 = k(t_0, q_0, v_0),$$

assuming (2.4) and sufficient smoothness of L and k, we have existence and uniqueness of a solution $(q(t), v(t), \psi(t))$ to (2.1). Expressing ψ as an implicit function of (t,q,v), i.e., $\psi = \Psi(t,q,v)$, we obtain from (2.1ab) the underlying forced Lagrangian system

$$\frac{d}{dt} q = v, \tag{2.6a}$$

$$\frac{d}{dt} \nabla_v L(t,q,v) = \nabla_q L(t,q,v) + f_L(t,q,v), \tag{2.6b}$$

where

$$f_L(t,q,v) := -K(t,q,v)^T \Psi(t,q,v) \tag{2.7}$$

can be interpreted as a *forcing term*. This corresponds to a mathematical realization of the nonholonomic constraints (2.1c). By construction the functions $k(t,q,v)$ of (2.1c) are first integrals of the forced Lagrangian system (2.6)-(2.7) since $\frac{d}{dt}k(t,q,v) \equiv 0$ by definition of $\Psi(t,q,v)$.

2.2. Energy. The energy of the system (2.1) is defined as

$$E(t,q,v) := L_v(t,q,v)v - L(t,q,v). \tag{2.8}$$

We have

$$\begin{aligned}
\frac{d}{dt}E(t,q,v) &= \left(\frac{d}{dt}L_v(t,q,v)\right) v + L_v(t,q,v)\dot{v} - L_t(t,q,v) - L_q(t,q,v)v - L_v(t,q,v)\dot{v} \\
&= L_q(t,q,v)v - \psi^T K(t,q,v)v - L_t(t,q,v) - L_q(t,q,v)v \\
&= -\psi^T K(t,q,v)v - L_t(t,q,v).
\end{aligned}$$

For ideal scleronomic (time-independent) nonholonomic constraints linear in v $0 = K(q)v$ and time-independent Lagrangians $L(t,q,v) = L(q,v)$ the energy is conserved since $K(q)v = 0$ and $L_t(q,v) \equiv 0$.

3. The Lagrange-d'Alembert principle. For ideal affine nonholonomic constraints (2.2) the equations (2.1) can be derived from the Lagrange-d'Alembert principle [3, 4, 5, 20, 28] which is a differential principle. The Lagrange-d'Alembert principle states that the virtual work vanishes

$$\delta^* W := \left(-\frac{d}{dt}L_v(t,q,\dot{q}) + L_q(t,q,\dot{q})\right)\delta^* q = 0 \tag{3.1a}$$

for all reversible (i.e., with q in the interior of the configuration space Q) *virtual displacements* $\delta^* q$ satisfying

$$K(t,q)\delta^* q = 0. \tag{3.1b}$$

Notice nevertheless that energy can still be created or dissipated along a trajectory of (2.1), see subsection 2.2 above. The definition of *ideal* nonholonomic constraints is equivalent to the Lagrange-d'Alembert principle (3.1ab) with (3.1b) for ideal nonlinear nonholonomic constraints simply replaced by

$$K(t,q,\dot{q})\delta^* q = 0. \tag{3.1c}$$

This is the *Maurer-Appell-Chetaev-Johnsen-Hamel rule*, see e.g. [28, p. 820], usually simply called *Chetaev's rule*. From (3.1c) we obtain the expression (2.1d) in (2.1b). For ideal nonholonomic constraints a different equivalent and finite-dimensional variational principle leading to (2.1) is *Gauss' principle of least constraint* [20, 28, 30], but it is based on the generalized accelerations $\ddot{q}$ and is thus generally seen as an inferior principle.

3.1. The Lagrange-d'Alembert principle as a skew critical problem. For ideal linear scleronomic nonholonomic constraints $0 = K(q)\dot{q}$, the Lagrange-d'Alembert principle is equivalent to a skew critical problem [3, 7, 8, 9, 10, 25, 29] described as follows. Given a Lagrangian $L(t,q,\dot{q}) \in \mathcal{C}^0([t_0,t_N],TQ)$ and ideal linear scleronomic nonholonomic constraints $0 = K(q)\dot{q}$ we form the *action* integral between q_0 at t_0 and q_N at t_N

$$A(q) := \int_{t_0}^{t_N} L(t,q(t),\dot{q}(t))dt$$

which is a functional for $q \in \mathcal{C}^1([t_0,t_N],Q)$ satisfying $q(t_0) = q_0$, $q(t_N) = q_N$, and $0 = K(q(t))\dot{q}(t)$. The Lagrange-d'Alembert principle is then equivalent to the skew critical problem

$$\delta A(q)(\delta q) = 0 \quad \forall \delta q \in \mathcal{C}^1_0([t_0,t_N],Q) \quad | \quad K(q)\delta q \equiv 0 \tag{3.2}$$

where $\delta A(q)$ is the first variation (i.e., the Gâteaux derivative) of the action. Hamilton's variational principle is not valid in the presence of ideal nonholonomic constraints contrary to ideal holonomic constraints. Observe that in (3.2) we do not have the seemingly more natural condition

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}K(q+\varepsilon\delta q)(\dot{q}+\varepsilon\dot{\delta q}) = K_q(q)(\dot{q},\delta q) + K(q)\dot{\delta q} \equiv 0.$$

Hamilton's principle applied to problems with ideal nonholonomic constraints leads to the generally different vakonomic equations [1, 5, 28] which do not agree with physical experiments [22]. It is worth mentioning that the practical realization of nonholonomic constraints is a problem in itself which may be quite difficult [23, 32].

3.2. The integral Lagrange-d'Alembert principle for forced Lagrangian systems and for Lagrangian systems with nonholonomic constraints. For forced Lagrangian systems (2.6) the (continuous) integral Lagrange-d'Alembert principle is

$$\delta A(q)(\delta q) + \int_{t_0}^{t_N} f_L(t,q(t),\dot{q}(t))^T \delta q(t)dt = 0 \quad \forall \delta q \in \mathcal{C}^1_0([t_0,t_N],Q).$$

For systems with nonholonomic constraints f_L is given by (2.7) and we can simply add the conditions

$$0 = k(t, q, \dot{q}).$$

This principle is simpler and more general than the skew critical problem of subsection 3.1.

3.3. Nonideal constraints. The constraints (2.1c) are called *nonideal* when the Lagrange-d'Alembert principle (3.1) does not hold. For example, Chetaev's rule (3.1c) may be unsuitable in certain situations, see, e.g., [23]. For Lagrangian systems with nonideal nonholonomic constraints (2.1b) is replaced by

$$\frac{d}{dt}\nabla_v L(t,q,v) = \nabla_q L(t,q,v) - K(t,q,v)^T\psi + N(t,q,v,\psi)$$

with $N_\psi \not\equiv 0$. For example dry sliding friction can lead to such formulations, see, e.g., [28, Example 3.2.6]. Even holonomic constraints can be nonideal, see, e.g., [33, 34]. Notice that the SPARK methods of Section 6 can deal with systems having nonideal constraints without any particular difficulty.

4. A forced discrete Lagrange-d'Alembert principle for Lagrangian systems with nonholonomic constraints. For Lagrangian systems with nonholonomic constraints we define in this section a general constrained discrete Lagrange-d'Alembert principle directly in $Q \times Q$ based on the discrete Lagrange-d'Alembert principle for forced Lagrangian systems.

4.1. The forced discrete Lagrange-d'Alembert principle and Euler-Lagrange equations. For forced Lagrangian systems (2.6) the corresponding forced discrete Lagrange-d'Alembert principle proposed in [19], see [24, Section 3.2], is

$$\begin{aligned}(4.1)\qquad &\delta\sum_{k=0}^{N-1} L_d(t_k,q_k,t_{k+1},q_{k+1})\\ &+\sum_{k=0}^{N-1}\left(f_d^-(t_k,q_k,t_{k+1},q_{k+1})^T\delta q_k + f_d^+(t_k,q_k,t_{k+1},q_{k+1})^T\delta q_{k+1}\right) = 0\end{aligned}$$

for all variations $\{\delta q_k\}_{k=0}^N$ with $\delta q_k \in \mathbb{R}^n$ satisfying $\delta q_0 = 0 = \delta q_N$. The *discrete Lagrangian* $L_d(t_k, q_k, t_{k+1}, q_{k+1})$ (or local discrete action) is an approximation to the exact discrete Lagrangian (the exact local action) between t_k and t_{k+1}

$$L_d(t_k,q_k,t_{k+1},q_{k+1}) \approx L_d^E(t_k,q_k,t_{k+1},q_{k+1}) := \int_{t_k}^{t_{k+1}} L(t,q(t),\dot{q}(t))dt$$

where $q(t) := q(t, t_k, q_k, t_{k+1}, q_{k+1})$. The *discrete forces* $f_d^-(t_k, q_k, t_{k+1}, q_{k+1})$ and $f_d^+(t_k, q_k, t_{k+1}, q_{k+1})$ above are approximation to the exact discrete forces between t_k and t_{k+1}

$$\begin{aligned}(4.2a)\qquad f_d^-(t_k,q_k,t_{k+1},q_{k+1})^T &\approx f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1})^T\\ &:= \int_{t_k}^{t_{k+1}} f_L(t,q(t),\dot{q}(t))^T\partial_{q_k}q(t)dt,\end{aligned}$$

$$\begin{aligned}(4.2b)\qquad f_d^+(t_k,q_k,t_{k+1},q_{k+1})^T &\approx f_d^{E+}(t_k,q_k,t_{k+1},q_{k+1})^T\\ &:= \int_{t_k}^{t_{k+1}} f_L(t,q(t),\dot{q}(t))^T\partial_{q_{k+1}}q(t)dt.\end{aligned}$$

The discrete principle (4.1) is equivalent to the *forced discrete Euler-Lagrange equations*

$$\begin{aligned}(4.3)\qquad &\nabla_4 L_d(t_{k-1},q_{k-1},t_k,q_k)+\nabla_2 L_d(t_k,q_k,t_{k+1},q_{k+1})\\ &+f_d^+(t_{k-1},q_{k-1},t_k,q_k)+f_d^-(t_k,q_k,t_{k+1},q_{k+1})=0\end{aligned}$$

for $k=1,\dots,N-1$. These equations (4.3) define a mapping

$$\Phi:\begin{cases}\mathbb{R}\times Q\times\mathbb{R}\times Q\longrightarrow\mathbb{R}\times Q\times\mathbb{R}\times Q,\\ (t_{k-1},q_{k-1},t_k,q_k)\mapsto(t_k,q_k,t_{k+1},q_{k+1}).\end{cases}$$

From $q(t,t_{k+1},q_{k+1},t_k,q_k)=q(t,t_k,q_k,t_{k+1},q_{k+1})$ we have the anti-symmetry properties

$$\begin{aligned}L_d^E(t_{k+1},q_{k+1},t_k,q_k)&=-L_d^E(t_k,q_k,t_{k+1},q_{k+1}),\\ f_d^{E+}(t_{k+1},q_{k+1},t_k,q_k))&=-f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1}),\\ f_d^{E-}(t_{k+1},q_{k+1},t_k,q_k))&=-f_d^{E+}(t_k,q_k,t_{k+1},q_{k+1}).\end{aligned}$$

Hence, from these properties we could require

$$\begin{aligned}L_d(t_{k+1},q_{k+1},t_k,q_k)&=-L_d(t_k,q_k,t_{k+1},q_{k+1}),\\ f_d^{+}(t_{k+1},q_{k+1},t_k,q_k))&=-f_d^{-}(t_k,q_k,t_{k+1},q_{k+1}),\\ f_d^{-}(t_{k+1},q_{k+1},t_k,q_k))&=-f_d^{+}(t_k,q_k,t_{k+1},q_{k+1}),\end{aligned}$$

as part of the conditions of the forced discrete Lagrange-d'Alembert principle (4.1). This makes sense from a boundary value problem point of view, but this is not fully justified from an initial value problem point of view. For an initial value problem, we are only interested in integrating in a specific time t direction and nonsymmetric methods may also be appropriate when the forced Lagrangian system (2.6) has no symmetry or reversibility properties.

4.2. The nonholonomically constrained discrete Lagrange-d'Alembert principle and Euler-Lagrange equations. For Lagrangian systems with nonholonomic constraints, the integral Lagrange-d'Alembert principle for Lagrangian systems with nonholonomic constraints stated in subsection 3.2 and the forced discrete Lagrange-d'Alembert principle (4.1) motivate the following definition:

DEFINITION 4.1. *For Lagrangian systems with ideal nonholonomic constraints (2.1) we define the* nonholonomically constrained discrete Lagrange-d'Alembert principle *as*

$$\begin{aligned}(4.4a)\quad &\delta\sum_{k=0}^{N-1}L_d(t_k,q_k,t_{k+1},q_{k+1})\\ &+\sum_{k=0}^{N-1}\left(f_d^-(t_k,q_k,t_{k+1},q_{k+1})^T\delta q_k+f_d^+(t_k,q_k,t_{k+1},q_{k+1})^T\delta q_{k+1}\right)=0,\\ (4.4b)\quad &0=c(t_k,q_k,t_{k+1},q_{k+1})\qquad \textit{for}\ \ k=0,\dots,N-1,\end{aligned}$$

for all variations $\{\delta q_k\}_{k=0}^N$ *satisfying* $\delta q_0=0=\delta q_N$, *with* f_d^- *and* f_d^+ *as in (4.2),* f_L *as in (2.7), and*

$$c(t_k,q_k,t_{k+1},q_{k+1}):=k(t_{k+1},q_{k+1},u(t_{k+1},t_k,q_k,t_{k+1},q_{k+1}))$$

with

$$u(t,t_k,q_k,t_{k+1},q_{k+1}) \approx \frac{d}{dt}q(t,t_k,q_k,t_{k+1},q_{k+1}).$$

We assume that $c(t,q,t,q)=0\ \forall t\in\mathbb{R}\ \forall q\in Q$.

The nonholonomically constrained discrete Lagrange-d'Alembert principle of Definition 4.1 is equivalent to the *nonholonomically constrained discrete Euler-Lagrange equations*

$$\begin{aligned}(4.5a)\qquad &\nabla_4 L_d(t_{k-1},q_{k-1},t_k,q_k)+\nabla_2 L_d(t_k,q_k,t_{k+1},q_{k+1})\\ &\quad +f_d^+(t_{k-1},q_{k-1},t_k,q_k)+f_d^-(t_k,q_k,t_{k+1},q_{k+1})=0,\\ (4.5b)\qquad &c(t_{k-1},q_{k-1},t_k,q_k)=c(t_k,q_k,t_{k+1},q_{k+1})\end{aligned}$$

for $k=1,\dots,N-1$ where we assume that $c(t_0,q_0,t_1,q_1)=0$ or $c(t_{N-1},q_{N-1},t_N,q_N)=0$. Notice that (4.5b) implies (4.4b). Assuming $c(t_0,q_0,t_1,q_1)=0$ the equations (4.5) define a mapping

$$\Phi:\begin{cases} C_d\longrightarrow C_d,\\ (t_{k-1},q_{k-1},t_k,q_k)\mapsto(t_k,q_k,t_{k+1},q_{k+1}).\end{cases}$$

on the constraint submanifold

$$C_d:=\{(s,q,t,r)\in\mathbb{R}\times Q\times\mathbb{R}\times Q\mid c(s,q,t,r)=0\}.$$

We remark that ideal nonholonomic constraints can be mathematically realized with forcing (2.7) as a forced Lagrangian system (2.6). The nonholonomically constrained discrete Lagrange-d'Alembert principle that we propose here is fully consistent with the unconstrained forced discrete Lagrange-d'Alembert principle (4.1) for forced Lagrangian systems as briefly suggested by Mardsen and West in [24, Section 5.3.7]. It also generalizes the one proposed by Cortés in [6, 7] which appears restrictive. It is an extension in a direction awaited by McLachlan and Perlmutter in [25, Section 8].

5. The exact discrete forcing terms for Lagrangian systems with nonholonomic constraints. Consider a solution to (2.1)

$$q(t)=q(t,t_0,q_0,t_1,q_1)$$

passing through q_0 at t_0 and q_1 at t_1 and let

$$v(t)=v(t,t_0,q_0,t_1,q_1):=\frac{d}{dt}q(t,t_0,q_0,t_1,q_1)=\partial_t q(t,t_0,q_0,t_1,q_1).$$

Consider the exact discrete Lagrangian (the exact local action) as a function of (t_0,q_0,t_1,q_1)

$$L_d^E(t_0,q_0,t_1,q_1):=\int_{t_0}^{t_1}L(t,q(t),v(t))dt.$$

Notice that for unconstrained systems $S_1(q_0,q_1):=L_d^E(t_0,q_0,t_1,q_1)$ can play the role of a generating function of type I. We denote

$$v_0:=v(t_0),\quad v_1:=v(t_1),\quad p_0:=\nabla_v L(t_0,q_0,v_0),\quad p_1:=\nabla_v L(t_1,q_1,v_1).$$

We have

$$\begin{aligned}\partial_{q_0} L_d^E(t_0,q_0,t_1,q_1) &= \int_{t_0}^{t_1} L_q(t,q(t),v(t))\partial_{q_0}q(t) + L_v(t,q(t),v(t))\partial_{q_0}v(t)dt \\ &= \int_{t_0}^{t_1} L_q(t,q(t),v(t))\partial_{q_0}q(t) - \frac{d}{dt}L_v(t,q(t),v(t))\partial_{q_0}q(t)dt \\ &\quad + L_v(t,q(t),v(t))\partial_{q_0}q(t)|_{t_0}^{t_1} \\ &= \int_{t_0}^{t_1} \left(L_q(t,q(t),v(t)) - \frac{d}{dt}L_v(t,q(t),v(t))\right)\partial_{q_0}q(t)dt \\ &\quad + L_q(t_1,q_1,v_1)\partial_{q_0}q_1 - L_v(t_0,q_0,v_0)\partial_{q_0}q_0 \\ &= \int_{t_0}^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))\partial_{q_0}q(t)dt - p_0^T.\end{aligned}$$

Defining

$$f_d^{E-}(t_0,q_0,t_1,q_1) := -p_0 - \nabla_{q_0} L_d^E(t_0,q_0,t_1,q_1),$$

we have obtained

$$\partial_{q_0} L_d^E(t_0,q_0,t_1,q_1) = -p_0^T - f_d^{E-}(t_0,q_0,t_1,q_1)^T \tag{5.1}$$

where

$$f_d^{E-}(t_0,q_0,t_1,q_1)^T = -\int_{t_0}^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))\partial_{q_0}q(t)dt.$$

From the Fundamental Theorem of Calculus we have

$$q(t) = q_1 + \int_{t_1}^{t} \frac{d}{ds}q(s)ds = q_1 - \int_t^{t_1} v(s)ds$$

leading to

$$\partial_{q_0}q(t) = -\int_t^{t_1} \partial_{q_0}v(s)ds.$$

Hence,

$$\begin{aligned}f_d^{E-}(t_0,q_0,t_1,q_1)^T &= \int_{t_0}^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t)) \left(\int_t^{t_1} \partial_{q_0}v(s)ds\right) dt \\ &= \int_{t_0}^{t_1} \left(\int_t^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))\partial_{q_0}v(s)ds\right) dt \\ &= \int_{t_0}^{t_1} \left(\int_{t_0}^{s} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))\partial_{q_0}v(s)dt\right) ds \\ &= \int_{t_0}^{t_1} \left(\int_{t_0}^{s} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))dt\right) \partial_{q_0}v(s)ds. \qquad (5.2)\end{aligned}$$

Similarly, we obtain

$$\partial_{q_1} L_d^E(t_0,q_0,t_1,q_1) = p_1^T + \int_{t_0}^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))\partial_{q_1}q(t)dt.$$

Defining

$$f_d^{E+}(t_0,q_0,t_1,q_1) := p_1 - \nabla_{q_1} L_d^E(t_0,q_0,t_1,q_1),$$

we have

$$\partial_{q_1} L_d^E(t_0,q_0,t_1,q_1) = p_1^T - f_d^{E+}(t_0,q_0,t_1,q_1)^T. \tag{5.3}$$

We obtain

$$f_d^{E+}(t_0,q_0,t_1,q_1)^T = -\int_{t_0}^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t)) \partial_{q_1} q(t) dt$$

and

$$\partial_{q_1} q(t) = \int_{t_0}^{t} \partial_{q_1} v(s) ds$$

leading to

$$f_d^{E+}(t_0,q_0,t_1,q_1)^T = -\int_{t_0}^{t_1} \left(\int_s^{t_1} \Psi(t,q(t),v(t))^T K(t,q(t),v(t)) dt \right) \partial_{q_1} v(s) ds. \tag{5.4}$$

We assume that the values t_k are independent of the values q_j. For example one considers a constant stepsize h and the values

$$t_k := t_0 + kh \quad \text{for} \quad k = 0, \ldots, N.$$

We calculate for $k = 1, \ldots, N-1$

$$\begin{aligned}
\nabla_{q_k} \sum_{j=0}^{N-1} L_d^E(t_j,q_j,t_{j+1},q_{j+1}) &= \nabla_{q_k} \left(L_d^E(t_{k-1},q_{k-1},t_k,q_k) + L_d^E(t_k,q_k,t_{k+1},q_{k+1}) \right) \\
&= \nabla_4 L_d^E(t_{k-1},q_{k-1},t_k,q_k) + \nabla_2 L_d^E(t_k,q_k,t_{k+1},q_{k+1}) \\
&= p_k - f_d^{E+}(t_{k-1},q_{k-1},t_k,q_k) \\
&\quad -p_k - f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1}) \\
&= -f_d^{E+}(t_{k-1},q_{k-1},t_k,q_k) - f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1}).
\end{aligned}$$

This leads to

$$\begin{aligned}
&\nabla_4 L_d^E(t_{k-1},q_{k-1},t_k,q_k) + \nabla_2 L_d^E(t_k,q_k,t_{k+1},q_{k+1}) \\
&\quad + f_d^{E+}(t_{k-1},q_{k-1},t_k,q_k) + f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1}) = 0
\end{aligned}$$

where

$$\begin{aligned}
f_d^{E+}(t_{k-1},q_{k-1},t_k,q_k)^T &= -\int_{t_{k-1}}^{t_k} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))^T \partial_{q_k} q(t) dt \\
&= -\int_{t_{k-1}}^{t_k} \left(\int_s^{t_k} \Psi(t,q(t),v(t))^T K(t,q(t),v(t)) dt \right) \partial_{q_k} v(s) ds, \qquad \text{(5.5a)} \\
f_d^{E-}(t_k,q_k,t_{k+1},q_{k+1})^T &= -\int_{t_k}^{t_{k+1}} \Psi(t,q(t),v(t))^T K(t,q(t),v(t))^T \partial_{q_k} q(t) dt \\
&= \int_{t_k}^{t_{k+1}} \left(\int_{t_k}^{s} \Psi(t,q(t),v(t))^T K(t,q(t),v(t)) dt \right) \partial_{q_k} v(s) ds. \qquad \text{(5.5b)}
\end{aligned}$$

5.1. Ideal holonomic constraints. When the constraints (2.1c) are holonomic, we have

$$0 = g(t,q)$$

for a certain function $g : \mathbb{R} \times \mathbb{R}^n \longrightarrow \mathbb{R}^m$. Therefore, we get

$$0 = \partial_{q_0} g(t, q(t)) = g_q(t, q(t)) \partial_{q_0} q(t).$$

In this situation, since

$$0 = g_t(t,q) + g_q(t,q)v =: k(t,q,v),$$

we have $k_v(t,q,v) = g_q(t,q)$, hence we must have

$$0 = k_v(t, q(t), v(t)) \partial_{q_0} q(t), \quad 0 = k_v(t, q(t), v(t)) \partial_{q_1} q(t).$$

For ideal holonomic constraints we have $K(t,q,v) = k_v(t,q,v)$, and since $k_v(t,q,v) = g_q(t,q)$ we obtain

$$\nabla_{q_0} L_d^E(t_0, q_0, t_1, q_1) = -p_0, \quad \nabla_{q_1} L_d^E(t_0, q_0, t_1, q_1) = p_1,$$

and thus

$$f_d^{E+} \equiv 0, \quad f_d^{E-} \equiv 0.$$

6. Lagrange-d'Alembert SPARK integrators. Following [15, 16, 17] the application of an s-stage SPARK method to Lagrangian systems (2.1) with nonholonomic constraints, stepsize h, and consistent initial values (t_0, q_0, v_0) at t_0, i.e., $0 = k(t_0, q_0, v_0)$, can be expressed as

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} V_j \quad \text{for } i = 1, \ldots, s, \tag{6.1a}$$

$$P_i = p_0 + h \sum_{j=1}^{s} \widehat{a}_{ij} F_j + h \sum_{j=1}^{s} \widetilde{a}_{ij} R_j \quad \text{for } i = 1, \ldots, s, \tag{6.1b}$$

$$q_1 = q_0 + h \sum_{j=1}^{s} b_j V_j, \tag{6.1c}$$

$$p_1 = p_0 + h \sum_{j=1}^{s} \widehat{b}_j F_j + h \sum_{j=1}^{s} \widetilde{b}_j R_j, \tag{6.1d}$$

$$0 = \sum_{j=1}^{s} \omega_{ij} K_j \quad \text{for } i = 1, \ldots, s-1, \tag{6.1e}$$

$$0 = k(t_1, q_1, v_1), \tag{6.1f}$$

where $t_1 := t_0 + h$ and

$$\begin{aligned} &T_i := t_0 + c_i h, \quad P_i := \nabla_v L(T_i, Q_i, V_i), \quad F_i := \nabla_q L(T_i, Q_i, V_i), \\ &R_i := -K(T_i, Q_i, V_i)^T \Psi_i, \quad K_i := k(T_i, Q_i, V_i) \quad \text{for } i = 1, \ldots, s, \\ &p_0 := \nabla_v L(t_0, q_0, v_0), \quad p_1 := \nabla_v L(t_1, q_1, v_1). \end{aligned}$$

The coefficients ω_{ij} in (6.1e) can be taken for example as $\omega_{ij} := b_j c_j^{i-1}$ for $i = 1, \ldots, s-1$, $j = 1, \ldots, s$. Under certain assumptions on the coefficients of the SPARK method we obtain a mapping $(t_1, q_1, v_1) = \Phi_h(t_0, q_0, v_0)$ for $|h|$ sufficiently small [15, 16, 17]. Instead of considering the unknown quantities in equations (6.1) as implicit functions of (t_0, q_0, v_0, h) for $h = t_1 - t_0$, we consider them as implicit functions of (t_0, q_0, t_1, q_1). More precisely, we implicitly define by (6.1) as functions of (t_0, q_0, t_1, q_1) the quantities $v_0, v_1, p_0, p_1, Q_i, V_i, \Psi_i, P_i, F_i, R_i, K_i$ for $i = 1, \ldots, s$. The main result of this paper is as follows:

THEOREM 6.1. *For Lagrangian systems with nonholonomic constraints (2.1) and a corresponding s-stage SPARK method (6.1), suppose t_0, q_0 and t_1, q_1 to be given. If the SPARK coefficients satisfy*

$$\widehat{b}_i = b_i \qquad \text{for } i = 1, \ldots, s, \tag{6.2a}$$

$$\widehat{b}_i a_{ij} + b_j \widehat{a}_{ji} - \widehat{b}_i b_j = 0 \qquad \text{for } i, j = 1, \ldots, s, \tag{6.2b}$$

then we have a nonholonomically constrained discrete Lagrange-d'Alembert integrator in the sense of Definition 4.1 with

$$\begin{aligned}
L_d(t_0, q_0, t_1, q_1) &= h \sum_{i=1}^{s} b_i L(T_i, Q_i, V_i), \\
f_d^+(t_0, q_0, t_1, q_1)^T &= -h \sum_{i=1}^{s} b_i \left(h \sum_{j=1}^{s} (\widetilde{b}_j - \widetilde{a}_{ij}) \Psi_j^T K(T_j, Q_j, V_j) \right) \partial_{q_1} V_i, \\
f_d^-(t_0, q_0, t_1, q_1)^T &= h \sum_{i=1}^{s} b_i \left(h \sum_{j=1}^{s} \widetilde{a}_{ij} \Psi_j^T K(T_j, Q_j, V_j) \right) \partial_{q_0} V_i.
\end{aligned}$$

Suppose in addition that the SPARK coefficients satisfy the symmetry conditions

$$c_{s+1-i} + c_i = 1 \qquad \text{for } i = 1, \ldots, s, \tag{6.3a}$$

$$a_{s+1-i,s+1-j} + a_{ij} = b_{s+1-j} = b_j \qquad \text{for } i, j = 1, \ldots, s, \tag{6.3b}$$

$$\widehat{a}_{s+1-i,s+1-j} + \widehat{a}_{ij} = \widehat{b}_{s+1-j} = \widehat{b}_j \qquad \text{for } i, j = 1, \ldots, s, \tag{6.3c}$$

$$\widetilde{a}_{s+1-i,s+1-j} + \widetilde{a}_{ij} = \widetilde{b}_{s+1-j} = \widetilde{b}_j \qquad \text{for } i, j = 1, \ldots, s \tag{6.3d}$$

then the SPARK method (6.1) is symmetric and we have

$$\begin{aligned}
L_d(t_1, q_1, t_0, q_0) &= -L_d(t_0, q_0, t_1, q_1), \\
f_d^+(t_1, q_1, t_0, q_0) &= -f_d^-(t_0, q_0, t_1, q_1), \\
f_d^-(t_1, q_1, t_0, q_0) &= -f_d^+(t_0, q_0, t_1, q_1).
\end{aligned}$$

Proof. We calculate

$$\begin{aligned}
\partial_{q_0} L_d(t_0, q_0, t_1, q_1) &= h \sum_{i=1}^{s} b_i L_q(Q_i, V_i) \partial_{q_0} Q_i + h \sum_{i=1}^{s} b_i L_v(Q_i, V_i) \partial_{q_0} V_i \\
&= h \sum_{i=1}^{s} b_i F_i^T \left(I + h \sum_{j=1}^{s} a_{ij} \partial_{q_0} V_j \right) + h \sum_{i=1}^{s} b_i P_i^T \partial_{q_0} V_i
\end{aligned}$$

$$
\begin{aligned}
&= h\sum_{i=1}^{s} b_i F_i^T I + h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} b_i a_{ij} F_i^T \partial_{q_0} V_j \\
&\quad + h\sum_{i=1}^{s} b_i \left(p_0^T + h\sum_{j=1}^{s} \widehat{a}_{ij} F_j^T + h\sum_{j=1}^{s} \widetilde{a}_{ij} R_j^T \right) \partial_{q_0} V_i \\
&= h\sum_{j=1}^{s} b_j F_j^T I + h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_j a_{ji} + b_i \widehat{a}_{ij}) F_j^T \partial_{q_0} V_i \\
&\quad + p_0^T h\sum_{i=1}^{s} b_i \partial_{q_0} V_i + h^2 \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{s} \widetilde{a}_{ij} R_j^T \right) \partial_{q_0} V_i.
\end{aligned}
$$

From (6.1c) we have

$$
0 = I + h\sum_{i=1}^{s} b_i \partial_{q_0} V_i,
$$

hence

$$
\begin{aligned}
\partial_{q_0} L_d(t_0, q_0, t_1, q_1) &= h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_j a_{ji} + b_i \widehat{a}_{ij} - b_j b_i) F_j^T \partial_{q_0} V_i - p_0^T \\
&\quad + h^2 \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{s} \widetilde{a}_{ij} R_j^T \right) \partial_{q_0} V_i.
\end{aligned}
$$

Under the assumptions (6.2) we obtain

$$
\partial_{q_0} L_d(t_0, q_0, t_1, q_1) = -p_0^T - h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} \widetilde{a}_{ij} \Psi_j^T K(T_j, Q_j, V_j) \right) \partial_{q_0} V_i
$$

which is the discrete analogue of (5.1)-(5.2). Similarly, we get

$$
\begin{aligned}
\partial_{q_1} L_d(t_0, q_0, t_1, q_1) &= h^2 \sum_{i=1}^{s}\sum_{j=1}^{s} (b_j a_{ji} + b_i \widehat{a}_{ij} - \widehat{b}_j b_i) F_j^T \partial_{q_1} V_i + p_1^T \\
&\quad + h^2 \sum_{i=1}^{s} b_i \left(\sum_{j=1}^{s} (\widetilde{a}_{ij} - \widetilde{b}_j) R_j^T \right) \partial_{q_1} V_i.
\end{aligned}
$$

Under the assumptions (6.2) we obtain

$$
\partial_{q_1} L_d(t_0, q_0, t_1, q_1) = p_1^T + h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} (\widetilde{b}_j - \widetilde{a}_{ij}) \Psi_j^T K(T_j, Q_j, V_j) \right) \partial_{q_1} V_i
$$

which is the discrete analogue of (5.3)-(5.4). Under the additional symmetry conditions (6.3) the SPARK method (6.1) is symmetric, and the internal values of the adjoint method satisfy $\overline{T}_i = T_{s+1-i}, \overline{Q}_i = Q_{s+1-i}, \overline{V}_i = V_{s+1-i}, \overline{\Psi}_i = \Psi_{s+1-i}$, see

[16, 17]. We have

$$\begin{aligned}
L_d(t_1,q_1,t_0,q_0) &= -h\sum_{i=1}^{s} b_i L(\overline{T}_i,\overline{Q}_i,\overline{V}_i)\\
&= -h\sum_{i=1}^{s} b_i L(T_{s+1-i},Q_{s+1-i},V_{s+1-i})\\
&= -h\sum_{i=1}^{s} b_{s+1-i} L(T_i,Q_i,V_i)\\
&= -h\sum_{i=1}^{s} b_i L(T_i,Q_i,V_i) = -L_d(t_0,q_0,t_1,q_1).
\end{aligned}$$

We have

$$\begin{aligned}
&f_d^-(t_1,q_1,t_0,q_0)^T\\
&\quad = (-h)\sum_{i=1}^{s} b_i \left((-h)\sum_{j=1}^{s} \widetilde{a}_{ij} \overline{\Psi}_j{}^T K(\overline{T}_j,\overline{Q}_j,\overline{V}_j) \right) \partial_{q_1}\overline{V}_i\\
&\quad = h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} \widetilde{a}_{ij} \Psi_{s+1-j}^T K(T_{s+1-j},Q_{s+1-j},V_{s+1-j}) \right) \partial_{q_1} V_{s+1-i}\\
&\quad = h\sum_{i=1}^{s} b_{s+1-i} \left(h\sum_{j=1}^{s} \widetilde{a}_{s+1-i,s+1-j} \Psi_j^T K(T_j,Q_j,V_j) \right) \partial_{q_1} V_i\\
&\quad = h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} (\widetilde{b}_j - \widetilde{a}_{ij}) \Psi_j^T K(T_j,Q_j,V_j) \right) \partial_{q_1} V_i = -f_d^+(t_0,q_0,t_1,q_1)^T.
\end{aligned}$$

Similarly, we get

$$\begin{aligned}
&f_d^+(t_1,q_1,t_0,q_0)^T\\
&\quad = -(-h)\sum_{i=1}^{s} b_i \left((-h)\sum_{j=1}^{s} (\widetilde{b}_j - \widetilde{a}_{ij}) \overline{\Psi}_j{}^T K(\overline{T}_j,\overline{Q}_j,\overline{V}_j) \right) \partial_{q_0}\overline{V}_i\\
&\quad = -h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} (\widetilde{b}_j - \widetilde{a}_{ij}) \Psi_{s+1-j}^T K(T_{s+1-j},Q_{s+1-j},V_{s+1-j}) \right) \partial_{q_0} V_{s+1-i}\\
&\quad = -h\sum_{i=1}^{s} b_{s+1-i} \left(h\sum_{j=1}^{s} (\widetilde{b}_{s+1-j} - \widetilde{a}_{s+1-i,s+1-j}) \Psi_j^T K(T_j,Q_j,V_j) \right) \partial_{q_0} V_i\\
&\quad = -h\sum_{i=1}^{s} b_i \left(h\sum_{j=1}^{s} \widetilde{a}_{ij} \Psi_j^T K(T_j,Q_j,V_j) \right) \partial_{q_0} V_i = -f_d^-(t_0,q_0,t_1,q_1)^T.
\end{aligned}$$

□

Results about global convergence of SPARK methods can be found in [16, 17].

7. Examples of Lagrange-d'Alembert SPARK integrators. Examples of SPARK methods satisfying the conditions of Theorem 6.1 are given by the family of Lobatto SPARK methods described in [16] and the family of Gauss SPARK (also called SRK-DAE2) methods given in [17]. The s-stage Gauss SPARK methods have optimal global order of convergence $2s$, while the s-stage Lobatto SPARK methods have global order of convergence $2s-2$ as shown in [16, 17]. We present a few specific examples of such methods below. In particular we consider their application to time-independent Lagrangians of the form $L(t,q,v) = \frac{1}{2}v^T M v - U(q)$ with M symmetric and nonsingular, and scleronomic nonholonomic constraints affine in v, i.e., $k(t,q,v) = K(q)v + b(q)$.

7.1. The "symplectic" Euler SPARK method I. For $s=1$ the Butcher-tableaux of coefficients of the "symplectic" Euler SPARK method I of order 1 are given by

$$\begin{array}{c|c} 0 & 0 \\ \hline A & 1 \end{array} \qquad \begin{array}{c|c} & 1 \\ \hline \widehat{A} & \end{array} \qquad \begin{array}{c|c} & 1 \\ \hline \widetilde{A} & \end{array} \qquad \widehat{b} = \widetilde{b} = b.$$

The method reads as follows

$$q_1 = q_0 + hV_1, \qquad P_1 = p_0 + h(F_1 + R_1), \qquad p_1 = P_1, \qquad 0 = k(t_1, q_1, v_1),$$

where

$$\begin{aligned} &t_1 := t_0 + h, \qquad p_0 := \nabla_v L(t_0, q_0, v_0), \qquad p_1 := \nabla_v L(t_1, q_1, v_1), \\ &P_1 := \nabla_v L(t_0, q_0, V_1), \qquad F_1 := \nabla_q L(t_0, q_0, V_1), \qquad R_1 := -K(t_0, q_0, V_1)^T \Psi_1. \end{aligned}$$

This method does not satisfy the symmetry conditions (6.3). For $L(t,q,v) = \frac{1}{2}v^T M v - U(q)$ with M symmetric and nonsingular, $k(t,q,v) = K(q)v + b(q)$, we have $V_1 = v_1$ and we obtain a system of nonlinear equations for q_1, v_1, and Ψ_1

$$q_1 = q_0 + hv_1, \qquad Mv_1 = Mv_0 - h(\nabla U(q_0) + K(q_0)^T \Psi_1), \qquad 0 = K(q_1)v_1 + b(q_1).$$

When $K(q) = K = Const$ and $b(q) = b = const$, the method is linearly implicit, i.e., only a linear system needs to be solved. This is a method given in [25, Formula (4.17)] (with a typo, there should be $\nabla V(q_i)$) when $M = I$ and $b(q) \equiv 0$.

7.2. The "symplectic" Euler SPARK method II. For $s=1$ the Butcher-tableaux of coefficients of the "symplectic" Euler SPARK method II of order 1 are given by

$$\begin{array}{c|c} 1 & 1 \\ \hline A & 1 \end{array} \qquad \begin{array}{c|c} & 0 \\ \hline \widehat{A} & \end{array} \qquad \begin{array}{c|c} & 0 \\ \hline \widetilde{A} & \end{array} \qquad \widehat{b} = \widetilde{b} = b.$$

The method reads as follows

$$q_1 = q_0 + hV_1, \qquad P_1 = p_0, \qquad p_1 = p_0 + h(F_1 + R_1), \qquad 0 = k(t_1, q_1, v_1),$$

where

$$\begin{aligned} &t_1 := t_0 + h, \qquad p_0 := \nabla_v L(t_0, q_0, v_0), \qquad p_1 := \nabla_v L(t_1, q_1, v_1), \\ &P_1 := \nabla_v L(t_1, q_1, V_1), \qquad F_1 := \nabla_q L(t_1, q_1, V_1), \qquad R_1 := -K(t_1, q_1, V_1)^T \Psi_1. \end{aligned}$$

This method does not satisfy the symmetry conditions (6.3). For $L(t,q,v) = \frac{1}{2}v^T M v - U(q)$ with M symmetric and nonsingular, $k(t,q,v) = K(q)v + b(q)$, we have $V_1 = v_0$ and we obtain a system of linear equations for q_1, v_1, and Ψ_1

$$q_1 = q_0 + hv_0, \qquad Mv_1 = Mv_0 - h(\nabla U(q_1) + K(q_1)^T \Psi_1), \qquad 0 = K(q_1)v_1 + b(q_1).$$

The method is thus linearly implicit. This is a method given in [25, Formula (4.12)] when $M = I$ and $b(q) \equiv 0$.

7.3. The 1-stage Gauss SPARK method, the SPARK midpoint rule. For $s = 1$ the Butcher-tableaux of coefficients of the 1-stage Gauss SPARK method of order 2, the SPARK midpoint rule, are given by

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline A & 1 \end{array}, \qquad \widehat{A} = \widetilde{A} = A, \qquad \widehat{b} = \widetilde{b} = b.$$

The method reads as follows

$$\begin{aligned} &Q_1 = q_0 + h\frac{1}{2}V_1, \qquad P_1 = p_0 + h\frac{1}{2}(F_1 + R_1), \\ &q_1 = q_0 + hV_1, \qquad p_1 = p_0 + h(F_1 + R_1), \qquad 0 = k(t_1, q_1, v_1), \end{aligned}$$

where

$$\begin{aligned} &T_1 := t_0 + \frac{h}{2}, \qquad t_1 := t_0 + h, \qquad p_0 := \nabla_v L(t_0, q_0, v_0), \qquad p_1 := \nabla_v L(t_1, q_1, v_1), \\ &P_1 := \nabla_v L(T_1, Q_1, V_1), \qquad F_1 := \nabla_q L(T_1, Q_1, V_1), \qquad R_1 := -K(T_1, Q_1, V_1)^T \Psi_1. \end{aligned}$$

This method satisfies the symmetry conditions (6.3). With $0 = k(T_1, Q_1, V_1)$ instead of $0 = k(t_1, q_1, v_1)$ to treat the nonholonomic constraint (2.1c), the "standard" 1-stage Gauss IRK method does not satisfy the nonholonomic constraints (2.1c) and it has only order 1. For $L(t,q,v) = \frac{1}{2}v^T M v - U(q)$ with M symmetric and nonsingular, $k(t,q,v) = K(q)v + b(q)$, we obtain a system of nonlinear equations for q_1, v_1, and Ψ_1

$$\begin{aligned} q_1 &= q_0 + \frac{h}{2}(v_0 + v_1), \\ Mv_1 &= Mv_0 - h\nabla U\left(\frac{q_0 + q_1}{2}\right) - hK\left(\frac{q_0 + q_1}{2}\right)^T \Psi_1, \\ 0 &= K(q_1)v_1 + b(q_1). \end{aligned}$$

7.4. The 2-stage Gauss SPARK method. For $s = 2$ the Butcher-tableaux of coefficients of the 2-stage Gauss SPARK method of order 4 are given by

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

The method reads as follows

$$Q_1 = q_0 + h\left(\frac{1}{4}V_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)V_2\right),$$

$$
\begin{aligned}
P_1 &= p_0 + h\left(\frac{1}{4}(F_1+R_1) + \left(\frac{1}{4}-\frac{\sqrt{3}}{6}\right)(F_2+R_2)\right),\\
Q_2 &= q_0 + h\left(\left(\frac{1}{4}+\frac{\sqrt{3}}{6}\right)V_1 + \frac{1}{4}V_2\right),\\
P_2 &= p_0 + h\left(\left(\frac{1}{4}+\frac{\sqrt{3}}{6}\right)(F_1+R_1) + \frac{1}{4}(F_2+R_2)\right),\\
q_1 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right),\\
p_1 &= p_0 + h\left(\frac{1}{2}(F_1+R_1) + \frac{1}{2}(F_2+R_2)\right),\\
0 &= \frac{1}{2}K_1 + \frac{1}{2}K_2,\\
0 &= k(t_1,q_1,v_1).
\end{aligned}
$$

where

$$
\begin{aligned}
&T_1 := t_0 + \left(\frac{1}{2}-\frac{\sqrt{3}}{6}\right)h, \qquad T_2 := t_0 + \left(\frac{1}{2}+\frac{\sqrt{3}}{6}\right)h, \qquad t_1 := t_0 + h,\\
&p_0 := \nabla_v L(t_0,q_0,v_0), \qquad p_1 := \nabla_v L(t_1,q_1,v_1), \qquad P_1 := \nabla_v L(T_1,Q_1,V_1),\\
&P_2 := \nabla_v L(T_2,Q_2,V_2), \qquad F_1 := \nabla_q L(T_1,Q_1,V_1), \qquad F_2 := \nabla_q L(T_2,Q_2,V_2),\\
&R_1 := -K(T_1,Q_1,V_1)^T\Psi_1, \qquad R_2 := -K(T_2,Q_2,V_2)^T\Psi_2,\\
&K_1 := k(T_1,Q_1,V_1), \qquad K_2 := k(T_2,Q_2,V_2).
\end{aligned}
$$

This method satisfies the symmetry conditions (6.3). With $0 = K_1$ and $0 = K_2$ instead of $0 = \frac{1}{2}K_1 + \frac{1}{2}K_2$ and $0 = k(t_1,q_1,v_1)$ to treat the nonholonomic constraint (2.1c), the "standard" 2-stage Gauss IRK method does not satisfy the nonholonomic constraints (2.1c) and it has only order 2.

7.5. The 2-stage Lobatto IIIA-B SPARK method. For $s = 2$ the Butcher-tableaux of coefficients of the 2-stage Lobatto IIIA-B SPARK method of order 2 are given by

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

The method reads as follows

$$
\begin{aligned}
Q_1 &= q_0,\\
P_1 &= p_0 + h\frac{1}{2}(F_1+R_1),\\
Q_2 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right),\\
P_2 &= p_0 + h\frac{1}{2}(F_1+R_1),\\
q_1 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right),
\end{aligned}
$$

$$
\begin{aligned}
p_1 &= p_0 + h\left(\frac{1}{2}(F_1+R_1)+\frac{1}{2}(F_2+R_2)\right),\\
0 &= \frac{1}{2}K_1+\frac{1}{2}K_2,\\
0 &= k(t_1,q_1,v_1),
\end{aligned}
$$

where

$$
\begin{aligned}
&T_1 := t_0, \qquad T_2 := t_0+h, \qquad t_1 := t_0+h, \qquad (7.1)\\
&p_0 := \nabla_v L(t_0,q_0,v_0), \qquad p_1 := \nabla_v L(t_1,q_1,v_1), \qquad P_1 := \nabla_v L(T_1,Q_1,V_1),\\
&P_2 := \nabla_v L(T_2,Q_2,V_2), \qquad F_1 := \nabla_q L(T_1,Q_1,V_1), \qquad F_2 := \nabla_q L(T_2,Q_2,V_2),\\
&R_1 := -K(T_1,Q_1,V_1)^T\Psi_1, \qquad R_2 := -K(T_2,Q_2,V_2)^T\Psi_2,\\
&K_1 := k(T_1,Q_1,V_1), \qquad K_2 := k(T_2,Q_2,V_2).
\end{aligned}
$$

This method satisfies the symmetry conditions (6.3). It is interesting to notice that this method is not equal to the composition with stepsize $h/2$ of the "symplectic" Euler SPARK method I with the "symplectic" Euler SPARK method II or vice versa. For $L(t,q,v)=\frac{1}{2}v^TMv-U(q)$ with M symmetric and nonsingular, $k(t,q,v)=K(q)v+b(q)$, we obtain first a system of nonlinear equations for q_1, V_1, Ψ_1

$$
\begin{aligned}
MV_1 &= Mv_0 - h\frac{1}{2}(\nabla U(q_0)+K(q_0)^T\Psi_1),\\
q_1 &= q_0 + hV_1,\\
0 &= \frac{1}{2}(K(q_0)V_1+b(q_0))+\frac{1}{2}(K(q_1)V_1+b(q_1)),
\end{aligned}
\qquad (7.2)
$$

which is a linear system when $K(q)=K=Const$ and $b(q)=b=const$, and then a system of linear equations for $v_1, (h/2)\Psi_2$

$$
\begin{aligned}
Mv_1 + K(q_1)^T\left(\frac{h}{2}\Psi_2\right) &= MV_1 - h\frac{1}{2}\nabla U(q_1),\\
K(q_1)v_1 &= -b(q_1).
\end{aligned}
$$

This is the analog for systems with nonholonomic constraints of the Störmer/leap-frog/Verlet/RATTLE/SHAKE/2-stage Lobatto IIIA-B SPARK methods for systems with or without holonomic constraints. For constant stepsizes $h_k=h$ the step-by-step integration of the above method can be simply expressed as follows

$$
\begin{aligned}
Mv_{k+\frac{1}{2}} &= Mv_{k-\frac{1}{2}} - h(\nabla U(q_k)+K(q_k)^T\widetilde{\Psi}_k),\\
q_{k+1} &= q_k + hv_{k+\frac{1}{2}},\\
0 &= \frac{1}{2}(K(q_k)v_{k+\frac{1}{2}}+b(q_k))+\frac{1}{2}(K(q_{k+1})v_{k+\frac{1}{2}}+b(q_{k+1})).
\end{aligned}
$$

In this situation the values of $v_k, \Psi_{2,k}$ and the equations

$$
\begin{aligned}
Mv_k + K(q_k)^T\left(\frac{h}{2}\Psi_{2,k}\right) &= Mv_{k+\frac{1}{2}} - h\frac{1}{2}\nabla U(q_k),\\
K(q_k)v_k &= -b(q_k).
\end{aligned}
$$

are not needed in a step-by-step integration. The method above is not equivalent to [12, Formula (11)] which does not make use of the additional constraint (7.2). It is also

not equivalent to the McLachlan-Perlmutter's 2-stage Lobatto IIIB-A LDA method, see [25, Formula (4.18)] and [26], which does not make use of the additional constraint (7.2), but which can be interpreted as a 2-stage Lobatto IIIB-A method where the 2-stage Lobatto IIIB coefficients are applied to $\dot{q} = v$ and the 2-stage Lobatto IIIA coefficients are applied to $M\dot{v} = -\nabla U(q) - K(q)^T\psi$. The McLachlan-Perlmutter's 2-stage Lobatto IIIB-A LDA method can be expressed as

$$Q_1 = q_0 + h\frac{1}{2}v_0, \tag{7.3a}$$

$$Mv_1 = Mv_0 - h(\nabla U(Q_1) + K(Q_1)^T\Psi_1), \tag{7.3b}$$

$$q_1 = q_0 + h\left(\frac{1}{2}v_0 + \frac{1}{2}v_1\right), \tag{7.3c}$$

$$0 = K(q_1)v_1 + b(q_1). \tag{7.3d}$$

All those methods are semi-implicit and ∇U must be evaluated only once per time step.

7.6. The 2-stage Lobatto IIIA-B-D SPARK method. For $s = 2$ the Butcher-tableaux of coefficients of the 2-stage Lobatto IIIA-B-D SPARK method of order 2 are given by

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline A & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} & 1/2 & 0 \\ & 1/2 & 0 \\ \hline \widehat{A} & & \end{array} \qquad \begin{array}{c|cc} & 1/4 & -1/4 \\ & 3/4 & 1/4 \\ \hline \widetilde{A} & & \end{array} \qquad \widehat{b} = \widetilde{b} = b.$$

For $s = 2$ the Lobatto IIIA-B-D SPARK method of order 2 reads as follows

$$\begin{aligned} Q_1 &= q_0, \\ P_1 &= p_0 + h\left(\frac{1}{2}F_1 + \frac{1}{4}R_1 - \frac{1}{4}R_2\right), \\ Q_2 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right), \\ P_2 &= p_0 + h\left(\frac{1}{2}F_1 + \frac{3}{4}R_1 + \frac{1}{4}R_2\right), \\ q_1 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right), \\ p_1 &= p_0 + h\left(\frac{1}{2}(F_1 + R_1) + \frac{1}{2}(F_2 + R_2)\right), \\ 0 &= \frac{1}{2}K_1 + \frac{1}{2}K_2, \\ 0 &= k(t_1, q_1, v_1), \end{aligned}$$

with $T_1, T_2, t_1, p_0, p_1, P_1, P_2, F_1, F_2, R_1, R_2, K_1, K_2$ as in (7.1). This method satisfies the symmetry conditions (6.3). We could also have considered the Lobatto IIIA-D SPARK method of order 2, the pure Lobatto IIID SPARK method of order 2, etc.

8. Numerical experiments.

8.1. The nonholonomic particle. This problem can be found in [6, 7, 12]. We consider the time-independent Lagrangian

$$L(q, v) = T(v) - U(q), \quad T(v) := \frac{1}{2}(v_1^2 + v_2^2 + v_3^2), \quad U(q) := q_1^2 + q_2^2,$$

with ideal scleronomic nonholonomic constraint

$$v_3 - q_2 v_1 = 0$$

which is linear in v. From subsection 2.2 the energy

$$E(q,v) = T(v) + U(q)$$

is conserved. The system is reversible under the transformation $R : (q,v) \mapsto (q,-v)$. We consider the following initial conditions at $t_0 = 0$

$$q_0 = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}^T, \qquad v_0 = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}^T.$$

We have applied the s-stage Gauss SPARK methods for $s = 1,2,3$ with stepsize $h = 0.2$ on the interval $t \in [0,250]$. The energy errors are plotted in Fig. 8.1 and clearly remain bounded.

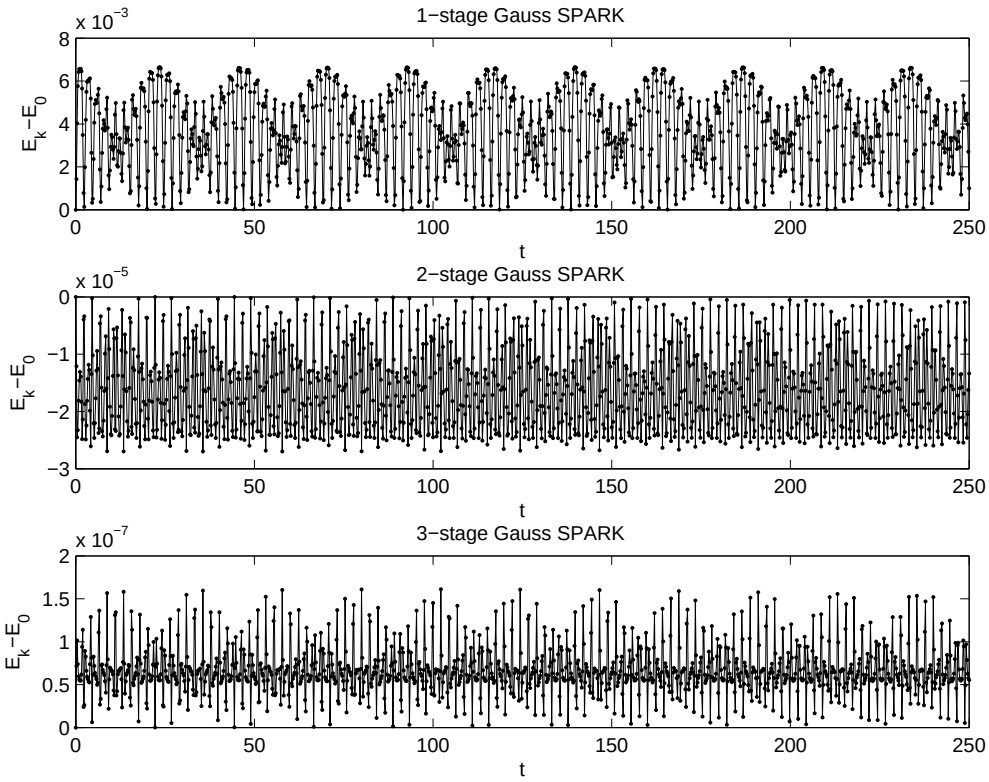

FIG. 8.1. *Energy error of the s-stage Gauss SPARK methods for $s = 1,2,3$ applied with constant stepsize $h = 0.2$ on the interval $[0,250]$ to the nonholonomic particle.*

8.2. The skate on an inclined plane. This problem can be found in [3, 30]. We consider the time-independent Lagrangian

$$L(q,v) = T(v) - U(q), \quad T(v) := \frac{1}{2}m(v_1^2 + v_2^2) + \frac{1}{2}Iv_3^2, \quad U(q) := -mgq_1\sin(\beta),$$

with ideal scleronomic nonholonomic constraint

$$\cos(q_3)v_2 - \sin(q_3)v_1 = 0$$

which is linear in $v = (v_1, v_2, v_3)^T$. From subsection 2.2 the energy

$$E(q, v) = T(v) + U(q)$$

is conserved. The system is reversible under the transformation $R : (q, v) \mapsto (q, -v)$. As in [30] we consider the parameters $m = 1$, $I = 1$, $g = 1$, $\beta = \pi/2$, and the following initial conditions at $t_0 = 0$

$$q_0 = \begin{pmatrix} 0 & 0 & 0 \end{pmatrix}^T, \qquad v_0 = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}^T.$$

We have applied the s-stage Lobatto IIIA-B SPARK methods for $s = 2, 3, 4$ with stepsize $h = 0.1$ on the interval $t \in [0, 100]$. The energy errors are plotted in Fig. 8.2 and clearly remain bounded.

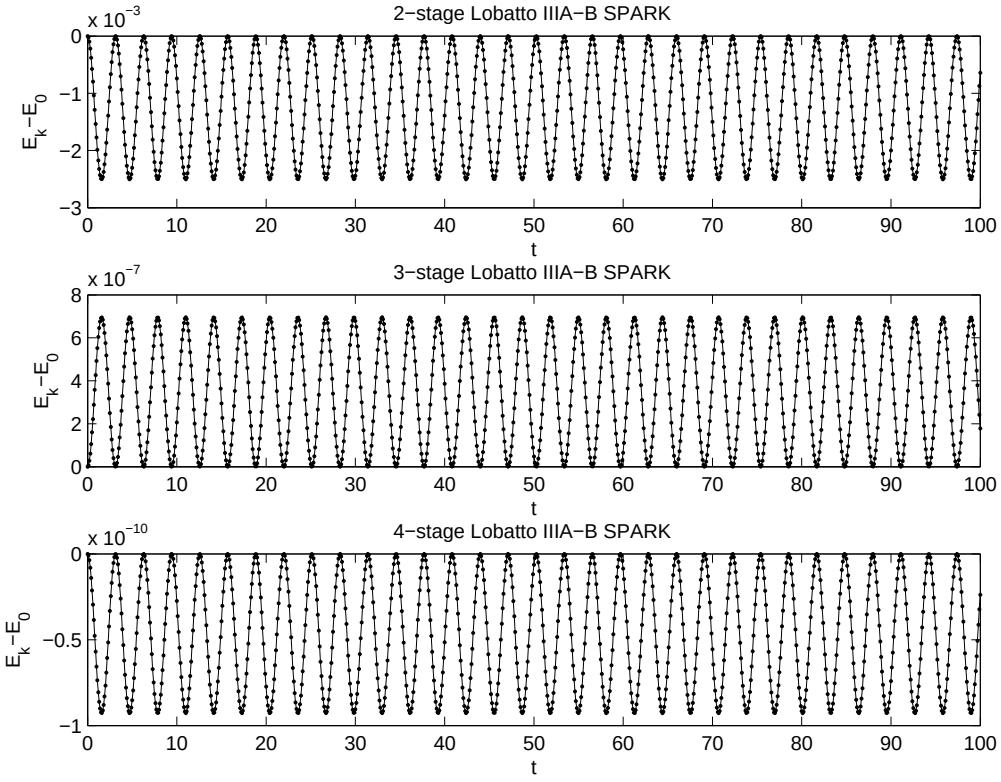

FIG. 8.2. *Energy error of the s-stage Lobatto IIIA-B SPARK methods for $s = 2, 3, 4$ applied with constant stepsize $h = 0.1$ on the interval $[0, 100]$ to the skate on an inclined plane.*

8.3. A mobile robot with fixed orientation and a potential. This problem can be found in [6, 7]. We consider the time-independent Lagrangian

$$L(q, v) = T(v) - U(q), \quad T(v) := \frac{1}{2}m(v_1^2 + v_2^2) + \frac{1}{2}Iv_3^2 + \frac{3}{2}I_\omega v_4^2, \quad U(q) := 10\sin(q_4),$$

with ideal scleronomic nonholonomic constraints

$$v_1 - \ell\cos(q_3)v_4 = 0, \quad v_2 - \ell\sin(q_3)v_4 = 0,$$

which are linear in $v = (v_1, v_2, v_3, v_4)^T$. From subsection 2.2 the energy

$$E(q, v) = T(v) + U(q)$$

is conserved. The system is reversible under the transformation $R : (q, v) \mapsto (q, -v)$. We consider the parameters $m = 1$, $I = 1$, $I_\omega = 1$, $\ell = 1$, and the following initial conditions at $t_0 = 0$

$$q_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \end{pmatrix}^T, \qquad v_0 = \begin{pmatrix} 1 & 0 & 0 & 1 \end{pmatrix}^T.$$

We have applied the s-stage Lobatto IIIA-B-D SPARK methods for $s = 2, 3, 4$ with stepsize $h = 0.2$ on the interval $t \in [0, 150]$. The energy errors are plotted in Fig. 8.3 and clearly remain bounded.

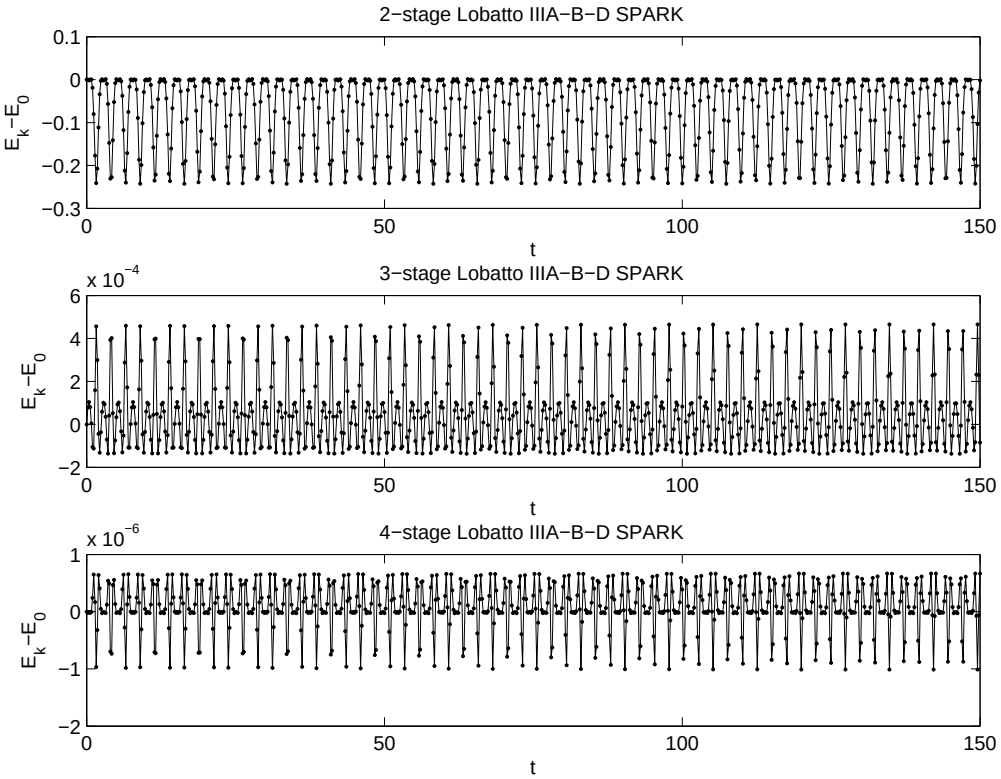

FIG. 8.3. *Energy error of the s-stage Lobatto IIIA-B-D SPARK methods for $s = 2, 3, 4$ applied with constant stepsize $h = 0.2$ on the interval $[0, 150]$ to the mobile robot with fixed orientation and a potential.*

8.4. The McLachlan and Perlmutter's particles. This chaotic problem can be found in [25, 26]. We consider the time-independent Lagrangian

$$L(q, v) = T(v) - U(q)$$

where $q, v \in \mathbb{R}^n$ with $n = 2m + 1$, $m \geq 2$,

$$T(v) := \frac{1}{2}\|v\|_2^2, \qquad U(q) := \frac{1}{2}\left(\|q\|_2^2 + q_{m+2}^2 q_{m+3}^2 + \sum_{i=1}^{m} q_{1+i}^2 q_{m+1+i}^2\right),$$

with ideal scleronomic nonholonomic constraint

$$v_1 + \sum_{i=m+2}^{n} q_i v_i = 0,$$

which is linear in v. From subsection 2.2 the energy

$$E(q, v) = T(v) + U(q)$$

is conserved. The system is reversible under the transformation $R : (q, v) \mapsto (q, -v)$. As in [25, 26], for $m = 3$ ($n = 7$) we consider the $J + 1$ following initial conditions at $t_0 = 0$

$$q_{j0} = \begin{pmatrix} \alpha_j & 0.6 & 0.4 & 0.2 & 1 & 1 & 1 \end{pmatrix}^T, \qquad v_{j0} = \begin{pmatrix} 0 & \beta_j & 0 & 0 & 0 & 0 & 0 \end{pmatrix}^T.$$

where $\alpha_j := \cos(j\pi/(2J)), \beta_j := \sin(j\pi/(2J))$ for $j = 0, \ldots, J$. For those initial conditions the energy is independent of j and we have $E(q_{j0}, v_{j0}) = E_0 = 3.06$. As a first method we consider the 2-stage Lobatto IIIA-B SPARK method. As a second method we consider a modified 2-stage Lobatto IIIA-B SPARK method where the condition $0 = \frac{1}{2}K_1 + \frac{1}{2}K_2$ is replaced by

$$0 = k\left(t_0 + \frac{h}{2}, q_0 + \frac{h}{2}V_1, V_1\right).$$

As a third method we consider McLachlan-Perlmutter's 2-stage Lobatto IIIB-A LDA method (7.3). For these 3 methods we consider a constant stepsize $h = 0.05$ and the interval $t \in [0, 50000]$ for $J + 1 = 10$ different initial conditions on the same energy surface $E_0 = 3.06$. In Fig. 8.4 the quantities at $t_k := t_0 + 100kh$ for $k = 0, 1, 2, \ldots, 10000$

$$\frac{1}{h^4}\mu((E_{\cdot k} - E_0)^2) \quad \text{where} \quad \mu((E_{\cdot k} - E_0)^2) := \frac{1}{(J+1)}\sum_{j=0}^{J}(E_{jk} - E_0)^2$$

are plotted for the 3 methods where $E_{jk} := E(q_{jk}, v_{jk})$. These 3 methods clearly behave very similarly and one can say that they are all equally good for this problem. The energy error for these 3 methods seems to follow a random walk, after time t_k we observe that we have approximately

$$\frac{1}{h^4}\mu((E_{\cdot k} - E_0)^2) \approx O(t_k) \quad \text{or equivalently} \quad \sqrt{\mu((E_{\cdot k} - E_0)^2)} \approx O(h^2\sqrt{t_k}).$$

9. Conclusion. For systems in mechanics with ideal nonholonomic constraints we have defined a new discrete Lagrange-d'Alembert principle based on a discrete Lagrange-d'Alembert principle for forced Lagrangian systems. A large class of specialized partitioned additive Runge-Kutta (SPARK) methods has been shown to satisfy this principle. In particular symmetric Lagrange-d'Alembert SPARK integrators of any order have been obtained based on Gauss and Lobatto coefficients.

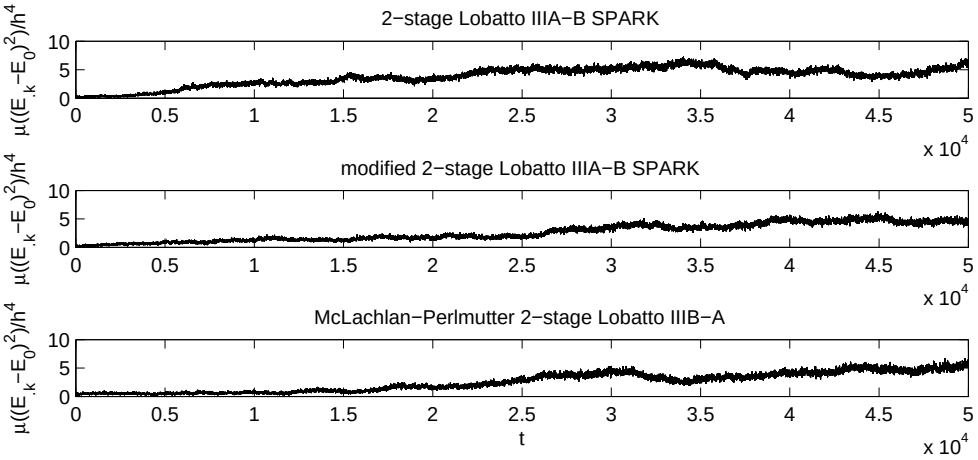

FIG. 8.4. *A measure of energy error for the* 2*-stage Lobatto IIIA-B SPARK method, the modified* 2*-stage Lobatto IIIA-B SPARK method, and the McLachlan-Perlmutter* 2*-stage Lobatto IIIB-A LDA method, applied with constant stepsize* $h = 0.05$ *on the interval* $[0, 50000]$ *to the McLachlan and Perlmutter's particles.*

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