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STRUCTURE PRESERVATION FOR CONSTRAINED DYNAMICS WITH SUPER PARTITIONED ADDITIVE RUNGE–KUTTA METHODS*

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Abstract. A broad class of partitioned differential equations with possible algebraic constraints is considered, including Hamiltonian and mechanical systems with holonomic constraints. For mechanical systems a formulation eliminating the Coriolis forces and closely related to the Euler–Lagrange equations is presented. A new class of integrators is defined: the super partitioned additive Runge–Kutta (SPARK) methods. This class is based on the partitioning of the system into different variables and on the splitting of the differential equations into different terms. A linear stability and convergence analysis of these methods is given. SPARK methods allowing the direct preservation of certain properties are characterized. Different structures and invariants are considered: the manifold of constraints, symplecticness, reversibility, contractivity, dilatation, energy, momentum, and quadratic invariants. With respect to linear stability and structure-preservation, the class of s-stage Lobatto IIIA-B-C-C* SPARK methods is of special interest. Controllable numerical damping can be introduced by the use of additional parameters. Some issues related to the implementation of a reversible variable stepsize strategy are discussed.

Key words. A-stability, algebraic stability, B-stability, conservative systems, contractivity, differential-algebraic equations, dilatation, explosivity, Hamiltonian systems, holonomic constraints, index, L-stability, Lobatto schemes, mechanical systems, numerical damping, P-stability, reversibility, Runge-Kutta methods, stiffness, structural dynamics, superconvergence, symplecticness

AMS subject classifications. 65L05, 65L06, 65L20, 58F05, 70H05

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1. Introduction.

Recently much interest has been devoted to numerical integration preserving certain structures and invariants for different classes of differential and differential-algebraic equations [11, 13, 25, 26, 30, 34, 42, 46, 50, 51, 53, 54, 58, 59, 60, 61, 62, 65, 67, 74, 76, 81]. This concerns mostly Hamiltonian systems, conservative mechanical systems, reversible systems, integrable systems, and systems with periodic solutions. Structure-preserving integrators do not only give numerical results which are usually qualitatively better, but they may also possess better long-time properties [11, 13, 25, 30, 34, 77]. On the other hand, a large effort has been spent during the past decades toward the numerical solution of stiff differential equations (see, e.g., [35] and the references therein). Methods used for stiff systems typically possess a numerical damping property. It is one of the goals of this article to present a class of integrators which can handle different kinds of systems in a unified way without introducing unnecessary numerical damping where it is not needed. Currently existing methods are useful for certain specific classes of problems, but they usually do not retain properties of other classes of problems. The class of partitioned Runge–Kutta

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(PRK) methods introduced in [44, 46] suffers from a lack of stability for a certain class of stiff oscillatory problems, which is another motivation to introduce a more general class of methods.

In this article we consider a broad class of partitioned differential equations with possible algebraic constraints and a splitting of the differential equations into different terms (see section 2). We are interested in numerical methods allowing the preservation of certain properties when present in the system, namely, the manifold of constraints, symplecticness, reversibility, contractivity, dilatation, energy, momentum, and quadratic invariants. In section 3 Hamiltonian systems and mechanical systems are analyzed. Hamiltonian systems arise in applications where dissipative forces can be neglected [3], such as in conservative mechanical systems [6], astronomy [80], electrodynamics, molecular dynamics [1, 2, 7, 8, 64, 78, 84], plasma physics, and fluid dynamics [83]. Mechanical systems arise in many applications, e.g., in multibody dynamics of rigid and/or flexible bodies [36, 69, 70, 71], in structural dynamics [14, 15, 17, 20, 37, 38, 39, 40, 55, 56], in real-time vehicle-systems simulation [57], in aerospace applications [9], in biomechanics [48], and in robotics [43]. For mechanical systems a formulation eliminating the Coriolis forces and closely related to the Euler–Lagrange equations is presented. In section 4 the new class of SPARK methods is defined taking advantage of the structure of the equations. Results about existence, uniqueness, and convergence of SPARK methods are stated. A motivation for this new class of integrators comes from the linear stability analysis of section 5. In section 6 conditions on the coefficients of SPARK methods are given to preserve the aforementioned properties. In section 7 we show how controllable numerical damping can be introduced by the use of additional parameters. Within the class of SPARK methods, the s-stage Lobatto IIIA-B-C-C* SPARK methods presented in section 8 are of special interest since they satisfy all requirements and desired properties. For these methods superconvergence of order $2s-2$ is stated. In section 9 comments are made related to the implementation of a reversible variable stepsize strategy. Finally, in section 10 some numerical experiments are given.

To give an example of the application of a Lobatto IIIA-B-C-C* SPARK method, we consider the following class of mechanical systems with constraints arising in structural dynamics:

$$q' = v \ , \tag{1a}$$

$$Mv' = F(t) - Cv - Kq - G^T\lambda \ , \tag{1b}$$

$$0 = Gq - c \ , \tag{1c}$$

$$0 = Gv \tag{1d}$$

where M, C, K, and G are the constant *mass*, *damping*, *stiffness*, and *constraint* matrices, respectively; $F(t)$ is the vector of *applied forces*; q is the vector of *displacements*; v is the vector of *velocities*; and λ is the vector of *Lagrange multipliers*. One step $(q_0, v_0) \mapsto (q_1, v_1)$ of the second-order Lobatto IIIA-B-C-C* SPARK method with stepsize h can be applied to this system as follows:

$$Q_1 = q_0 + h\left(\frac{1}{2}V_1 - \frac{1}{2}V_2\right) \ ,$$

$$Q_2 = q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right) \ ,$$

$$MV_1 = Mv_0 - h\left(\frac{1}{2}CV_1 - \frac{1}{2}CV_2\right) - h\left(\frac{1}{2}KQ_1 - \frac{1}{2}KQ_2\right) - \frac{h}{2}G^T\Lambda_1 \ ,$$

$$
\begin{aligned}
MV_2 &= Mv_0 + hF(t_0) - h\left(\frac{1}{2}CV_1 + \frac{1}{2}CV_2\right) - h\left(\frac{1}{2}KQ_1 + \frac{1}{2}KQ_2\right) - \frac{h}{2}G^T\Lambda_1 \ , \\
q_1 &= q_0 + h\left(\frac{1}{2}V_1 + \frac{1}{2}V_2\right) \ , \\
0 &= Gq_1 - c \ , \\
Mv_1 &= Mv_0 + h\Big(\frac{1}{2}(F(t_0) - CV_1 - KQ_1 - G^T\Lambda_1) \\
&\qquad + \frac{1}{2}(F(t_0+h) - CV_2 - KQ_2 - G^T\Lambda_2)\Big) \ , \\
0 &= Gv_1
\end{aligned}
$$

The Lobatto IIIA coefficients are used for the constraints (1c). The velocities in (1a) are treated with the Lobatto IIIC coefficients. The forces terms in (1b) are treated differently: $F(t)$ is treated with the Lobatto IIIC* coefficients, $-Cv$ and $-Kq$ with the Lobatto IIIC coefficients, and $-G^T\lambda$ with the Lobatto IIIB coefficients. Different alternatives are possible, however.

2. The system of equations. We consider more generally the following class of partitioned differential-algebraic equations:

$$y' = f(y,z) \ , \tag{2a}$$

$$M(y)z' = k(y,z,u) \ , \tag{2b}$$

$$0 = g(y) \tag{2c}$$

where $y = (y^1,\dots,y^n)^T \in \mathbf{R}^n, z = (z^1,\dots,z^p)^T \in \mathbf{R}^p, u = (u^1,\dots,u^m)^T \in \mathbf{R}^m$ ($m < n$ and $2m < n+p$), $f : \mathbf{R}^n \times \mathbf{R}^p \to \mathbf{R}^n, M : \mathbf{R}^n \to \mathbf{R}^{p\times p}, k : \mathbf{R}^n \times \mathbf{R}^p \times \mathbf{R}^m \to \mathbf{R}^p, g : \mathbf{R}^n \to \mathbf{R}^m$. For the ease of presentation we will consider only autonomous systems, although results can be easily extended to time-dependent systems. The *mass matrix* $M(y)$ is assumed to be invertible in a neighborhood of the solution (for mechanical systems this assumption can be relaxed; see subsection 3.2). The variables (y,z) are called the *differential variables*, and the variables u are called the *algebraic variables*. Differentiating twice the *holonomic constraints* (2c) we obtain the following additional constraints:

$$0 = g_y(y)f(y,z) \ , \tag{2d}$$

$$
\begin{aligned}
0 = {} & g_{yy}(y)(f(y,z),f(y,z)) + g_y(y)f_y(y,z)f(y,z) \\
& + g_y(y)f_z(y,z)M^{-1}(y)k(y,z,u) \ .
\end{aligned} \tag{2e}
$$

In the presence of constraints we suppose that the matrix

$$g_y(y)f_z(y,z)M^{-1}(y)k_u(y,z,u) \text{ is invertible} \tag{3}$$

in a neighborhood of the exact solution. This implies that the above *overdetermined differential-algebraic system* (2) is of *differential* and *perturbation index one* [44, p. 28] since only one more differentiation of the constraints (2e) is required to express u' as a function of the differential variables (y,z). Such problems are well-posed, contrary to higher index problems, e.g., index three problems such as (2a), (2b), (2c).

An alternative formulation to (2b) is given by

$$(M(y)z)' = M_y(y)(f(y,z),z) + k(y,z,u) =: \widehat{k}(y,z,u) \ . \tag{4}$$

This may seem more costly because of the need to compute the term $M_y(y)(f(y,z),z)$, but for mechanical systems this is even less costly since the corresponding term (the Coriolis forces) cancels out (see subsection 3.2). With the equations of mechanical systems in mind, where different types of forces are present (see subsection 3.2), we will consider in (2a) and (4) the decompositions

$$f(y,z) = \sum_{m=1}^{4} f^{(m)}(y,z) \ , \tag{5a}$$

$$\widehat{k}(y,z,u) = k^{(1)}(y,z) + \sum_{m=2}^{4} k^{(m)}(y,z,u) \tag{5b}$$

where the functions $f^{(m)}$ and $k^{(m)}$ are supposed to have distinct properties and can therefore be numerically treated in a different way. We stress the point that any ordinary differential system of the form $y' = f(y)$ or $y' = f(y,z)$, $z' = k(y,z)$ can be seen as a particular case of (2). Hence, most of the ideas and of the results developed in this paper remain valid in this situation, e.g., for the pure differential equations of unconstrained Hamiltonian and mechanical systems.

3. Hamiltonian and mechanical systems. Two important classes of differential-algebraic systems enter into the class of (2): Hamiltonian and mechanical systems with holonomic constraints. They are the subject of the forthcoming subsections.

3.1. Hamiltonian systems. The first class of equations are those of *Hamiltonian systems* with *holonomic constraints*

$$q' = H_p^T(q,p) \ , \tag{6a}$$

$$p' = -H_q^T(q,p) - G^T(q)\lambda \ , \tag{6b}$$

$$0 = g(q) \ , \tag{6c}$$

$$0 = G(q)H_p^T(q,p) \ , \tag{6d}$$

$$\begin{aligned} 0 = {} & G_q(q)(H_p^T(q,p), H_p^T(q,p)) + G(q)H_{pq}^T(q,p)H_p^T(q,p) \\ & -G(q)H_{pp}^T(q,p)H_q^T(q,p) - G(q)H_{pp}^T(q,p)G^T(q)\lambda, \end{aligned} \tag{6e}$$

where $G(q) := g_q(q)$. The variables (q,p,λ) play the role of (y,z,u) in (2): $q = (q^1,\dots,q^n)^T \in \mathbf{R}^n$ are the *generalized coordinates*, $p = (p^1,\dots,p^n)^T \in \mathbf{R}^n$ are the *generalized momenta*, and $\lambda = (\lambda^1,\dots,\lambda^m)^T \in \mathbf{R}^m$ are the *Lagrange multipliers*. The scalar function $H(q,p)$ is called the *Hamiltonian*. Assumption (3) is read here as

$$G(q)H_{pp}^T(q,p)G^T(q) \text{ is invertible} \ . \tag{7}$$

Four properties of Hamiltonian systems with holonomic constraints are the following:

1. Any solution must lie on the *manifold of constraints*

$$V = \left\{(q,p) \in \mathbf{R}^n \times \mathbf{R}^n \mid 0 = g(q),\ 0 = G(q)H_p^T(q,p)\right\} \ .$$

2. The Hamiltonian is invariant along a solution, i.e., $H(q(t),p(t)) = \text{Const}$.

3. The flow $\phi_\tau : (q(t),p(t)) \mapsto (q(t+\tau),p(t+\tau))$ is *symplectic* on the manifold of constraints V, i.e., on V the 2-form $dq \wedge dp = \sum_{i=1}^{n} dq_i \wedge dp_i$ is preserved by the flow.

4. The flow may be *ρ-reversible*, i.e., $\phi_\tau = \rho^{-1} \circ \phi_\tau^{-1} \circ \rho$ for some linear transformation ρ of the variables (q,p). For example for *conservative mechanical systems* in Hamiltonian form (see subsection 3.2), the Hamiltonian is given by $H(q,p) = T(q,p) + U(q)$, where $T(q,p) = \frac{1}{2} p^T M^{-1}(q) p$ is the *kinetic energy* and $U(q)$ is the *potential energy*. The flow is ρ-reversible with respect to a reflection of the generalized momenta $\rho : (q,p) \mapsto (q,-p)$.

3.2. Mechanical systems. The second class of equations are those of *mechanical systems* with *holonomic constraints*

$$q' = v \ , \tag{8a}$$

$$M(q)v' = f(q,v,\lambda) - G^T(q)\lambda \ , \tag{8b}$$

$$0 = g(q) \ , \tag{8c}$$

$$0 = G(q)v \ , \tag{8d}$$

$$0 = G_q(q)(v,v) + G(q)v' \tag{8e}$$

where $G(q) := g_q(q)$, $M(q)$ is the symmetric *generalized mass matrix*, and $f(q,v,\lambda)$ is the vector of *generalized forces*. The variables (q,v,λ) play the role of (y,z,u) in (2): $q = (q^1,\dots,q^n)^T \in \mathbf{R}^n$ are the *generalized coordinates*, $v = (v^1,\dots,v^n)^T \in \mathbf{R}^n$ are the *generalized velocities*, and $\lambda = (\lambda^1,\dots,\lambda^m)^T \in \mathbf{R}^m$ are the *Lagrange multipliers*. The above formulation is called the *descriptor form* and is referred in classical mechanics as the *Lagrange equations of the first kind*. The importance of this formulation lies in the fact that it is independent of the choice of the coordinates. The generalized forces $f(q,v,\lambda)$ contain the term

$$-M_q(q)(v,v),$$

which is referred to as the *Coriolis forces*. In (4) the term $M_y(y)(f(y,z),z)$ corresponds here exactly to the term $M_q(q)(v,v)$; hence the computational work is reduced by using, instead of (8b), the formulation

$$(M(q)v)' = M_q(q)(v,v) + f(q,v,\lambda) - G^T(q)\lambda \ , \tag{8f}$$

since the term corresponding to the Coriolis forces cancels out. If the generalized mass matrix $M(q)$ is invertible, then (8e) can be rewritten

$$0 = G_q(q)(v,v) + G(q)M(q)^{-1}\left(f(q,v,\lambda) - G^T(q)\lambda\right),$$

and assumption (3) reads

$$G(q)M(q)^{-1}(G^T(q) - f_\lambda(q,v,\lambda)) \text{ is invertible} \ . \tag{9}$$

In general the mass matrix $M(q)$ may be singular, meaning that more constraints are actually acting on the system. It can be supposed only that the matrix

$$\begin{pmatrix} M(q) & G^T(q) \\ G(q) & 0 \end{pmatrix} \text{ is invertible} \ . \tag{10}$$

Nevertheless, under the assumption that

$$\begin{pmatrix} M(q) & G^T(q) - f_\lambda(q,v,\lambda) \\ G(q) & 0 \end{pmatrix} \text{ is invertible} \tag{11}$$

we still have an overdetermined index one system, since we can implicitly express v' and λ from (8b)–(8e) (explicitly if $f_\lambda(q,v,\lambda)) \equiv 0$). We will discuss hereafter how this situation can be treated.

Conservative mechanical systems are mechanical systems where the generalized forces $f(q,v,\lambda)$ are given by the sum of Coriolis forces $-M_q(q)(v,v)$, of *momental (centrifugal) inertia forces* $\frac{1}{2}(v^T M(q)v)_q^T$, and of *conservative forces* $-U_q^T(q)$ (i.e., forces coming from a *potential* $U(q)$):

$$f(q,v,\lambda) = -M_q(q)(v,v) + \frac{1}{2}(v^T M(q)v)_q^T - U_q^T(q) \ . \tag{12}$$

In this situation the dynamics (8) with (12) can also be derived from a *constrained Lagrange–Hamilton variational principle*

$$q' = v \ , \qquad \min \int_{t_0}^{t_1} L(q(\tau), v(\tau))d\tau \ , \qquad 0 = g(q),$$

where $L(q,v) = T(q,v) - U(q)$ is the *Lagrangian*, $T(q,v) = \frac{1}{2}v^T M(q)v$ is the *kinetic energy*, and $U(q)$ is the *potential energy*. Necessary conditions for this variational problem are given by the *constrained Euler–Lagrange equations*

$$q' = v \ , \qquad \frac{d}{dt}\left(\overline{L}_v^T(q,v,\lambda)\right) = \overline{L}_q^T(q,v,\lambda) \ , \qquad 0 = g(q)$$

with $\overline{L}(q,v,\lambda) = L(q,v) - g(q)^T\lambda$. We thus get

$$(M(q)v)' = \frac{1}{2}(v^T M(q)v)_q^T - U_q^T(q) - G^T(q)\lambda \ ,$$

showing that for conservative mechanical systems the formulation (8f) actually corresponds to the direct expression of the above Euler–Lagrange equations. If the generalized mass matrix $M(q)$ is invertible, then the equations can be rewritten in Hamiltonian form by defining the generalized momenta $p := M(q)v$ and by using the *Legendre transformation* of the Lagrangian with respect to v given by $H(q,p) = p^T v(q,p) - L(q,v(q,p))$. Thus the properties of Hamiltonian systems can be transfered to conservative mechanical systems. It can be easily shown that $H = T + U$, the total energy of the system. More generally, under the assumption (10), e.g., when the generalized mass matrix $M(q)$ is noninvertible, a trick is to consider the *augmented system*

$$\begin{pmatrix} q' \\ r' \end{pmatrix} = \begin{pmatrix} v \\ w \end{pmatrix} \ , \tag{13a}$$

$$\begin{pmatrix} M(q) & G^T(q) \\ G(q) & 0 \end{pmatrix} \begin{pmatrix} v' \\ w' \end{pmatrix} = \begin{pmatrix} f(q,v,\lambda) - G^T(q)\lambda \\ -G_q(q)(v,v) - \mu \end{pmatrix} \ , \tag{13b}$$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} g(q) \\ r \end{pmatrix} \ , \tag{13c}$$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} G(q)v \\ w \end{pmatrix} \ , \tag{13d}$$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} G_q(q)(v,v) + G(q)v' \\ w' \end{pmatrix} \ . \tag{13e}$$

This system possesses exactly the same structure as (8) by considering the augmented variables $Q = (q,r)$, $V = (v,w)$, and $\Lambda = (\lambda,\mu)$. In this formulation the augmented

mass matrix in (13b) is invertible by the assumption (10). The exact solution of the augmented system satisfies trivially $r = 0$, $w = 0$, and $\mu = 0$. Therefore, the properties of Hamiltonian systems can still be transfered to conservative mechanical systems with a noninvertible mass matrix. Hence, four properties of conservative mechanical systems with holonomic constraints are the following:

1. Any solution must lie on the *manifold of constraints*

$$W = \{(q, v) \in \mathbf{R}^n \times \mathbf{R}^n \mid 0 = g(q),\ 0 = G(q)v\} \ .$$

2. The total energy is invariant along a solution, i.e., $T(q(t), v(t)) + U(q(t)) =$ Const.

Proof. The result is trivial when the mass matrix is invertible. The total energy of the augmented system is given by

$$\frac{1}{2} \begin{pmatrix} v \\ w \end{pmatrix}^T \begin{pmatrix} M(q) & G^T(q) \\ G(q) & 0 \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} + U(q) \ .$$

Because of $w = 0$ we get the desired result. ∎

3. The flow $\psi_\tau : (q(t), v(t)) \mapsto (q(t+\tau), v(t+\tau))$ preserves the *symplectic* 2-form $dq \wedge d(M(q)v)$ on the manifold of constraints W.

Proof. When the mass matrix is invertible the result directly follows from the preservation of $dq \wedge dp$ in Hamiltonian form, where $p = M(q)v$. For the augmented system we have

$$d \begin{pmatrix} q \\ r \end{pmatrix} \wedge d \left(\begin{pmatrix} M(q) & G^T(q) \\ G(q) & 0 \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} \right) \text{ is preserved .} \tag{14}$$

Since $r = 0, w = 0$, and $G(q)v = 0$, we get the desired result. ∎

4. The flow is γ-*reversible* with respect to a reflection of the generalized velocities $\gamma : (q, v) \mapsto (q, -v)$, i.e., $\psi_\tau = \gamma^{-1} \circ \psi_\tau^{-1} \circ \gamma$.

For more general mechanical systems we assume that the forces appearing on the right-hand side of (8f) can be decomposed in classes modeling different physical effects:

$$M_q(q)(v, v) + f(q, v, \lambda) - G^T(q)\lambda = f^{(1)}(q, v) + \sum_{m=2}^{4} f^{(m)}(q, v, \lambda) \ . \tag{15}$$

As mentioned before, the term $M_q(q)(v, v)$ cancels out with its opposite contained in $f(q, v, \lambda)$. We do not pretend that the forces of any given system can be easily decomposed, but we think that it is likely to be possible for many engineering problems of interest (see, e.g., the system (1)). The term $f^{(2)}$ should contain momental (centrifugal) inertia forces $\frac{1}{2}(v^T M(q)v)_q^T$ and conservative forces $-U_q^T(q)$. The term $f^{(3)}$ should contain *dissipative forces*, e.g., friction forces and forces due to the presence of dampers. The term $f^{(4)}$ should contain *explosive forces*, i.e., forces increasing the energy of the system, e.g., forces due to external excitation. Similarly, for the augmented system we can decompose the expression coming from (13b) and (4) as

$$\begin{aligned} \begin{pmatrix} M_q(q)(v, v) + G_q^T(q)(v, w) + f(q, v, \lambda) - G^T(q)\lambda \\ -\mu \end{pmatrix} &= F^{(1)}(q, v, w) \\ &\quad + \sum_{m=2}^{4} F^{(m)}(q, v, w, \lambda, \mu) \ . \end{aligned} \tag{16}$$

4. SPARK methods. When applying a numerical method, it will be seen in the linear situation in section 5 that different types of terms (e.g., the force terms for a mechanical system) require different numerical stability properties. As a unique Runge–Kutta (RK) method possessing all these stability properties cannot exist, this is one motivation of the forthcoming combination of different RK methods. Another motivation comes from the preservation of diverse nonlinear structures and invariants as described in section 6. Once again, there cannot exist a unique RK method possessing all desired properties.

4.1. Definition of SPARK methods. The general definition of SPARK methods is as follows.

DEFINITION 4.1. *One step of an* s-stage SPARK method *applied to the overdetermined partitioned differential-algebraic system* (2) *with decomposition* (4)–(5)*, consistent initial values* (y_0, z_0, u_0)*, and stepsize* h *is read as*

$$Y_i = y_0 + h \sum_{m=1}^{4} \sum_{j=1}^{s} a_{ij}^{(m)} f^{(m)}(Y_j, Z_j) \quad \text{for } i = 1, \dots, s \ , \tag{17a}$$

$$M(Y_i)Z_i = M(y_0)z_0 + h \sum_{j=1}^{s} a_{ij}^{(1)} k^{(1)}(Y_j, Z_j) + h \sum_{m=2}^{4} \sum_{j=1}^{s} a_{ij}^{(m)} k^{(m)}(Y_j, Z_j, U_j) \quad \text{for } i = 1, \dots, s \ , \tag{17b}$$

$$0 = g\left(y_0 + h \sum_{j=1}^{s} a_{ij}^{(1)} f(Y_j, Z_j) \right) \quad \text{for } i = 1, \dots, s \ , \tag{17c}$$

$$y_1 = y_0 + h \sum_{m=1}^{4} \sum_{i=1}^{s} b_i^{(m)} f^{(m)}(Y_i, Z_i) \ , \tag{17d}$$

$$0 = g(y_1) \ , \tag{17e}$$

$$M(y_1)z_1 = M(y_0)z_0 + h \sum_{i=1}^{s} b_i^{(1)} k^{(1)}(Y_i, Z_i) + h \sum_{m=2}^{4} \sum_{i=1}^{s} b_i^{(m)} k^{(m)}(Y_i, Z_i, U_i) \ , \tag{17f}$$

$$0 = g_y(y_1) f(y_1, z_1) \ , \tag{17g}$$

$$0 = g_{yy}(y_1)(f(y_1, z_1), f(y_1, z_1)) + g_y(y_1) f_y(y_1, z_1) f(y_1, z_1) + g_y(y_1) f_z(y_1, z_1) M^{-1}(y_1) k(y_1, z_1, u_1) \ . \tag{17h}$$

The coefficients $(b_i^{(m)}, a_{ij}^{(m)})$ *for* $m = 1, \dots, 4$ *are the coefficients of four RK methods.*

REMARK 4.2.

1. *When the mass matrix* $M(y)$ *is not constant, it is not equivalent in general to apply a SPARK method using*

$$z' = M(y)^{-1} k(y, z, u) =: \widetilde{k}(y, z, u)$$

instead of (2b)*.*

2. *When the mass matrix* $M(q)$ *in* (8b) *is invertible, it is not equivalent to apply a SPARK method to the augmented system* (13) *instead of* (8) *since in general the internal stages* W_i *correponding to the variables* w *do not vanish.*

Using the new variables

$$Y := y \ , \qquad Z := M(y)z \ , \qquad U := u \tag{18}$$

and defining

$$\begin{aligned} F(Y,Z) &:= f(Y, M(Y)^{-1}Z) \ , \\ K(Y,Z,U) &:= \widehat{k}(Y, M(Y)^{-1}Z, U) \ , \\ G(Y) &:= g(Y) \ , \end{aligned}$$

the whole system (2) can be rewritten in an equivalent way:

$$Y' = F(Y,Z) \ , \tag{19a}$$

$$Z' = K(Y,Z,U) \ , \tag{19b}$$

$$0 = G(Y) \ , \tag{19c}$$

$$0 = G_Y(Y)F(Y,Z) \ , \tag{19d}$$

$$\begin{aligned} 0 = {} & G_{YY}(Y)(F(Y,Z),F(Y,Z)) + G_Y(Y)F_Y(Y,Z)F(Y,Z) \\ & + G_Y(Y)F_Z(Y,Z)K(Y,Z,U) \ . \end{aligned} \tag{19e}$$

Hence, the definition of SPARK methods is such that it is invariant under the nonlinear change of variables (18). It is by definition equivalent to formally apply a SPARK method to the modified formulation (19) and then to rewrite it in terms of the original variables (y,z,u). When the mass matrix $M(y)$ is not constant, this simply means that the numerical scheme is applied differently than the usual way by making use of (4) instead of (2b), which is even less costly for mechanical systems (see subsection 3.2). The convergence analysis is also simplified since it can be assumed in the proofs that the mass matrix $M(y)$ is equal to I_p the identity matrix in $\mathbf{R}^{p\times p}$.

The words *partitioned* and *additive* for the above methods can be justified from the fact that the partitioning and the splitting of the equations are taken into account in the definition. Moreover, the components y in the constraints $0 = g(y)$ are integrated differently than the differential equation (2a) for y itself, so strictly speaking the method is not a pure additive and partitioned RK method which would impose $0 = g(Y_i)$ in the definition; this is one justification for the additional word *super*. The idea of exploiting additivity by using different methods to treat different terms can be found in [22, 23], where the goal of the authors was rather to take advantage of the linearity of one term. Some general linear multistep implicit-explicit schemes treating terms of different types differently are presented in [5]. The idea of exploiting the partitioning in different variables for semiexplicit index three systems was introduced in [44, 46].

In the following susbsections we analyze SPARK methods. We first give some simplifying assumptions which are heavily used in results about existence, uniqueness, and convergence of SPARK methods. The usual way to determine the order of global convergence of RK type methods is to study the local error and then the error propagation. For SPARK methods, the same techniques as those given in [44, Chapter 5] for PRK methods can be applied. Only slight changes must be made concerning the local error.

4.2. Simplifying assumptions. In this article, we consider SPARK methods based on a unique quadrature formula, i.e.,

$$b_i^{(m)} = b_i \quad \text{for } m = 1,\dots,4, \ i = 1,\dots,s \ , \tag{20a}$$

$$c_i^{(m)} = c_i \quad \text{for } m = 1,\dots,4, \ i = 1,\dots,s \ . \tag{20b}$$

We also consider the following *simplifying assumptions*:

$$
\begin{aligned}
B(p): &\quad \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k} \quad \text{for } k = 1,\dots,p\ ,\\
C^m(q^m): &\quad \sum_{j=1}^{s} a_{ij}^{(m)} c_j^{k-1} = \frac{c_i^k}{k} \quad \text{for } i = 1,\dots,s \text{ and } k = 1,\dots,q^m\ ,\\
D^m(r^m): &\quad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij}^{(m)} = \frac{b_j}{k}\big(1 - c_j^k\big) \quad \text{for } j = 1,\dots,s \text{ and } k = 1,\dots,r^m\ ,\\
C^mC^n(Q^{mn}): &\quad \sum_{j=1}^{s}\sum_{l=1}^{s} a_{ij}^{(m)} a_{jl}^{(n)} c_l^{k-2} = \frac{c_i^k}{k(k-1)} \quad \text{for } i = 1,\dots,s \text{ and } k = 2,\dots,Q^{mn}\ ,\\
D^mD^n(R^{mn}): &\quad \sum_{i=1}^{s}\sum_{j=1}^{s} b_i c_i^{k-2} a_{ij}^{(m)} a_{jl}^{(n)} = \frac{b_l}{k} - \frac{b_l c_l}{k-1} + \frac{b_l c_l^k}{k(k-1)} \quad \text{for } l = 1,\dots,s \text{ and } k = 2,\dots,R^{mn}\ ,\\
(S^m): &\quad a_{sj}^{(m)} = b_j \quad \text{for } j = 1,\dots,s,
\end{aligned}
$$

where $m, n \in \{1,\dots,4\}$. From now on we denote the RK matrices $A^{(m)} := (a_{ij}^{(m)})_{i,j=1}^{s}$ and the weight vector $b := (b_1,\dots,b_s)^T$.

4.3. Existence and uniqueness. Generally there does not exist a solution to the nonlinear system of Definition 4.1 without any assumption on the coefficients of the SPARK method. For SPARK methods satisfying the simplifying assumption (S^1) and

$$a_{1j}^{(1)} = 0 \quad \text{for } j = 1,\dots,s\ , \tag{21a}$$

$$A^{(1)}A^{(2)} = A^{(1)}A^{(3)} = A^{(1)}A^{(4)} =: \begin{pmatrix} 0 & \dots & 0 \\ & N & \end{pmatrix}\ , \tag{21b}$$

$$\operatorname{rank}\begin{pmatrix} N \\ b^T \end{pmatrix} = s\ , \tag{21c}$$

existence and uniqueness for the nonlinear system can be shown under some additional assumptions (see Theorem 4.3 below). Assuming (21a) and $0 = g(y_0)$, (17c) for $i = 1$ is automatically satisfied. By (20a) and the simplifying assumption (S^1) we get $y_1 = y_0 + h\sum_{j=1}^{s} a_{sj}^{(1)} f(Y_j, Z_j)$. Therefore by (17c) for $i = s$ (17e) is also automatically satisfied. A very accurate value for u_1 may be unnecessary. For a consistent SPARK method by the simplifying assumption (S^1) we have $c_s = 1$. Hence, instead of computing u_1 by solving (17h), a fairly good choice is given by $u_1 := U_s$ if one is not interested to enforce the constraints (2e). The accuracy of the numerical u-component does not influence the convergence of the (y, z)-components and the properties of the SPARK method anyway.

THEOREM 4.3. *Suppose that*

$$
\begin{aligned}
0 &= g(y_0)\ ,\\
O(h^2) &= g_y(y_0)f(y_0, z_0)\ ,\\
O(h) &= g_{yy}(y_0)(f(y_0, z_0), f(y_0, z_0)) + g_y(y_0)f_y(y_0, z_0)f(y_0, z_0)\\
&\quad + g_y(y_0)f_z(y_0, z_0)M^{-1}(y_0)k(y_0, z_0, u_0)\ ,
\end{aligned}
$$

(3) *is satisfied in a neighborhood of* (y_0, z_0, u_0)*, the simplifying assumption* (S^1) *and* (20)–(21) *hold, and the simplifying assumptions* $C^1C^n(2)$ *are satisfied for* $n = 1, \dots, 4$*. Then for* $h \le h_0$ *there exists a locally unique SPARK solution of Definition* 4.1 *which satisfies*

$$\begin{aligned} Y_i - y_0 &= O(h) \quad \text{for } i = 1, \dots, s\ , \qquad & y_1 - y_0 &= O(h)\ , \\ Z_i - z_0 &= O(h) \quad \text{for } i = 1, \dots, s\ , \qquad & z_1 - z_0 &= O(h)\ , \\ U_i - u_0 &= O(h) \quad \text{for } i = 1, \dots, s\ , \qquad & u_1 - u_0 &= O(h)\ . \end{aligned}$$

REMARK 4.4. *If the mass matrix* $M(y)$ *is not invertible, existence and uniqueness of the SPARK solution cannot be shown in general.*

The proof of this theorem is quite similar to that of [44, Theorem V.4.1] and is therefore omitted. The condition (21b) is essential in order to use assumption (3) to apply the implicit function theorem in the proof of Theorem 4.3.

4.4. Local and global error. For the local error of SPARK methods we have the following result.

THEOREM 4.5. *Consider the overdetermined partitioned differential-algebraic system of index one* (2) *satisfying* (3) *in a neighborhood of the exact solution, with consistent initial values* (y_0, z_0, u_0) *at* t_0*, and a SPARK method with coefficients satisfying the hypotheses of Theorem* 4.3 *and the simplifying assumptions* $B(p)$*,* (S^1)*,* $C^m(q^m)$ *and* $D^m(r^m)$ *for* $m = 1, \dots, 4$*,* $C^1C^n(Q)$*, and* $D^1D^n(R)$ *for* $n = 2, 3, 4$*. Then we have*

$$y_1 - y(t_0 + h) = O(h^{\mu+1}), \quad z_1 - z(t_0 + h) = O(h^{\nu+1}), \quad u_1 - u(t_0 + h) = O(h^{\nu+1}),$$

where

$$\begin{aligned} \mu &= \min(p, 2q + 2, q + r + 2, \kappa + 1, Q + r', 2Q - 1, Q + R)\ , \\ \nu &= \min(\mu, 2Q - 2) \end{aligned}$$

with $q := \min_{m=1}^{4} q^m$*,* $r := \min_{m=1}^{4} r^m$*,* $\kappa := \min_{m=1}^{4}(q^m + r^m)$*,* $r' := \min_{m=2}^{4} r^m$*. If the function* $k(y, z, u)$ *of* (2b) *is linear in* u *then the values* $2Q - 1$ *in* μ *and* $2Q - 2$ *in* ν *can be raised by one.*

The proof of this theorem is rather long and technical, but it is similar to that given in [44, Theorem V.4.3]. It makes use of a "rooted-tree type" theory about the Taylor expansion of the exact and the numerical solutions. The most difficult part is to estimate the local error of the z-component.

For the study of the error propagation we need a result on the influence of perturbations. This technical result and its proof are similar to [44, Theorem V.4.2] for PRK methods, it is therefore omitted. For the global error of SPARK methods we have then the following result.

THEOREM 4.6. *Under the same hypotheses stated in Theorem* 4.5*, the global error of a SPARK method satisfies for* $t_n - t_0 = nh \le \text{Const}$

$$y_n - y(t_n) = O(h^\nu), \quad z_n - z(t_n) = O(h^\nu), \quad u_n - u(t_n) = O(h^\nu)\ .$$

This result remains valid in case of variable stepsizes with $h = \max_i |h_i|$*.*

The proof of this theorem is identical to that of [44, Theorem V.4.6]. In the next section we analyze the linear stability properties of SPARK methods. For nonlinear systems a linear stability analysis is generally inadequate; therefore, in section 6 we look at the preservation of some nonlinear structures and invariants by SPARK methods.

5. Linear stability. As mentioned in section 4, different types of forces in (15) require different numerical stability properties. We discuss in the following subsections three fundamental linear stability properties: L-stability, P-stability, and the new concept of explosivity. Roughly speaking, it means that for Dahlquist's test equation [24]

$$z' = \lambda z \ , \tag{22}$$

three different situations are analyzed: $\mathrm{Re}(\lambda) < 0$, $\mathrm{Re}(\lambda) = 0$, and $\mathrm{Re}(\lambda) > 0$, more importantly when $|\mathrm{Re}(\lambda)|$ or $|\mathrm{Im}(\lambda)|$ is large. Since there cannot exist a unique RK method possessing all desired stability properties in these three situations, this is one of the main motivations of the definition of SPARK methods.

5.1. L-stability. We consider Dahlquist's test equation (22). The exact solution to this simple equation with initial value z_0 at t_0 is given by

$$z(t_0 + h) = e^{\mu} z_0, \tag{23}$$

where $\mu = \lambda h$. The application of a RK method with coefficients (b_i, a_{ij}) to (22) leads to

$$z_1 = R(\mu) z_0, \tag{24}$$

where $R(\mu)$ is the *stability function* of the RK method,

$$R(\mu) = 1 + \mu b^T (I - \mu A)^{-1} \mathbb{I}_s, \tag{25}$$

and $\mathbb{I}_s$ is the s-dimensional vector $(1, \ldots, 1)^T$. For $\mathrm{Re}(\mu) < 0$ we have $|e^{\mu}| < 1$, and for $\mathrm{Re}(\mu) \to -\infty$ we obtain $|e^{\mu}| \to 0$. Hence, it is desirable that the stability function (25) possesses the same properties.

DEFINITION 5.1 (see [35, Section IV.3]). *An RK method is said to be* A-stable *if*

$$|R(\mu)| < 1 \quad \textit{for} \quad \mathrm{Re}(\mu) < 0 \ . \tag{26}$$

A-stable RK methods which additionally satisfy

$$|R(\mu)| \to 0 \quad \textit{for} \quad \mathrm{Re}(\mu) \to -\infty \tag{27}$$

are called L-stable.

It is well known that RK methods for which the stability function $R(\mu)$ is equal to $R_{j-1,j}(\mu)$ or $R_{j-2,j}(\mu)$, where $R_{kj}(\mu)$ is the (k, j)-Padé approximation to the exponential function are L-stable [35, sections IV.3 and IV.4] (see the Ehle conjecture in [35, Theorem IV.4.12]). In the family of Lobatto methods, the stability function of the s-stage Lobatto IIIC method is given by $R_{s-2,s}(\mu)$. Therefore, we have the following well-known result.

THEOREM 5.2. *The Lobatto* IIIC *RK methods are L-stable.*

In the decomposition (15) the term $f^{(3)}(q, v, \lambda)$ should contain dissipative forces ($\partial f^{(3)}/\partial v(q, v, \lambda)$ negative definite), e.g., like $-Cv$ in (1b) with C positive definite. In order to take large stepsizes regardless the strength of the damping, L-stable coefficients such as the s-stage Lobatto IIIC coefficients are the most appropriate to treat such forces.

5.2. P-stability. *Highly oscillatory systems* are systems with large eigenvalues of the Jacobian matrix on or near the imaginary axis of the complex plane. A simple model problem is given by the equations of the harmonic oscillator

$$\begin{pmatrix} y' \\ z' \end{pmatrix} = \begin{pmatrix} z \\ -\lambda^2 y \end{pmatrix}, \tag{28}$$

where by definition $\lambda \in \mathbf{R}^+$. This is one of the simplest systems where the eigenvalues of the Jacobian matrix $(\pm\lambda i)$ are purely imaginary. The exact solution to this problem with initial values y_0 and z_0 at t_0 is given by

$$\begin{pmatrix} y(t_0+h) \\ z(t_0+h) \end{pmatrix} = D_\lambda \Theta(\mu) D_\lambda^{-1} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix}, \quad \Theta(\mu) = \begin{pmatrix} \cos(\mu) & \sin(\mu) \\ -\sin(\mu) & \cos(\mu) \end{pmatrix}, \tag{29}$$

where $\mu = \lambda h$ and $D_\lambda = \mathrm{diag}(1, \lambda)$. The application of a PRK method with coefficients $(b_i, a_{ij}^{(m)})$ and $(b_i, a_{ij}^{(n)})$ to (28) yields

$$\begin{pmatrix} y_1 \\ z_1 \end{pmatrix} = D_\lambda M(\mu) D_\lambda^{-1} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix},$$

where the 2×2 *stability matrix* $M(\mu)$ is given by

$$M(\mu) = I_2 + \mu \begin{pmatrix} O & b^T \\ -b^T & O \end{pmatrix} \begin{pmatrix} I_s & -\mu A^{(m)} \\ \mu A^{(n)} & I_s \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{I}_s & O \\ O & \mathbb{I}_s \end{pmatrix}. \tag{30}$$

We are interested in methods preserving the norm (equal to one) of the eigenvalues of the rotation matrix $\Theta(\mu)$ in (29) for all μ, motivating the following concept of P-stability [16, 19, 29, 47].

Definition 5.3. *For a PRK method, an interval I with $\{0\} \subset I \subset \mathbf{R}$, is an* interval of periodicity *if for all $\mu \in I$ the eigenvalues $\lambda_i(\mu)$ $(i = 1, 2)$ of the stability matrix $M(\mu)$ (30) satisfy $|\lambda_i(\mu)| = 1$ $(i = 1, 2)$ and if $\lambda_1(\mu) = \lambda_2(\mu) = \pm 1$, then this eigenvalue must possess two distinct eigenvectors. A PRK method is said to be* P-stable *if $\mathbf{R}$ is an interval of periodicity.*

The following results are well known.

Theorem 5.4. *Symmetric RK methods are P-stable.*

Corollary 5.5. *The Lobatto* IIIA *RK methods are P-stable.*

Corollary 5.6. *The Lobatto* IIIB *RK methods are P-stable.*

However, the combination of the Lobatto IIIA and Lobatto IIIB methods leads to this somehow surprising result [47].

Theorem 5.7. *The Lobatto* IIIA-B *PRK methods are not P-stable.*

For ODEs the *trapezoidal rule* (the 2-stage Lobatto IIIA RK method) and the *(Rattle–)Verlet algorithm* (the 2-stage Lobatto IIIA-B PRK method) can be seen as particular cases of the 2-stage Lobatto IIIA-B-C-C* SPARK method (see section 8 and the coefficients in Table 1). For nonlinear highly oscillatory Hamiltonian and mechanical systems and for sufficiently small amplitudes in the oscillations, both methods do not converge when taking stepsizes larger than the shortest period of oscillation. For the (Rattle–)Verlet algorithm this is because it is not P-stable according to Theorem 5.7, its interval of periodicity being equal to $]-2, 2[$. For the trapezoidal rule the reason is less obvious; P-stability is not sufficient. The convergence of the method is dictated by its behavior when applied to a nearby holonomically constrained system, which is a differential-algebraic system of index three [31, 44, 47, 52]. That is

the reason why the trapezoidal rule, although P-stable, fails when applied with large stepsizes to these highly oscillatory systems, because it does not converge for index three problems [47]. We emphasize the fact that the (Rattle–)Verlet algorithm and the trapezoidal rule fail for large stepsizes even if the amplitudes of the oscillations are negligible (smooth motion). To overcome these problems, we propose the use of the s-stage P-stable Lobatto IIIA ($s \geq 3$) or L-stable Lobatto IIIC ($s \geq 2$) coefficients to treat the terms which are responsible of oscillations with high frequencies of sufficiently small amplitude (ensuring existence and uniqueness of the numerical solution [52, Lemma 5.1]). L-stable methods are appropriate to damp out high-frequency oscillations. Although these schemes suffer from some order reduction when applied to highly oscillatory Hamiltonian and mechanical systems [31, 47], a common phenomenon when stiffness is encountered, this order reduction is not drastic. An order reduction can also be observed for other numerical methods like the Radau IIA RK schemes [52] and also for other types of stiffness, e.g., in the B-convergence theory [35, sections IV.15, V.8, and V.9].

5.3. Explosivity. We again consider Dahlquist's test equation (22) (see subsection 5.1). For $\mathrm{Re}(\mu) > 0$ we have $|e^{\mu}| > 1$, and for $\mathrm{Re}(\mu) \to \infty$ we get $|e^{\mu}| \to \infty$. Hence, it is desirable that the stability function (25) possesses the same properties.

DEFINITION 5.8. *A RK method is said to be* explosive *if*

$$|R(\mu)| > 1 \quad \textit{for} \quad \mathrm{Re}(\mu) > 0 \ . \tag{31}$$

Explosive RK methods which satisfy in addition

$$|R(\mu)| \to \infty \quad \textit{for} \quad \mathrm{Re}(\mu) \to \infty \tag{32}$$

are called unconditionally explosive.

By symmetry with the L-stability concept it is trivial to show that a RK method is unconditionally explosive if and only if its stability function $R(\mu)$ is equal to $R_{k,k-1}(\mu)$ or $R_{k,k-2}(\mu)$, where $R_{kj}(\mu)$ is the (k,j)-Padé approximation to the exponential function. In the family of Lobatto methods, the stability function of the s-stage Lobatto IIIC* method is given by $R_{s,s-2}(\mu)$ (see section 8). We call the *Lobatto* IIIC* methods (a notation suggested by R. P. K. Chan) the RK schemes due to J. Butcher initially known as the Lobatto III processes [10] (see also [33, section II.7]). Therefore, we have the following result.

THEOREM 5.9. *The Lobatto* IIIC* *RK methods are unconditionally explosive.*

Although explosivity is not a stability concept in the usual sense, it may be of interest for systems where the exploding modes need not be resolved accurately. From a shadowing perspective it is not important to solve these modes accurately anyway because of their intrinsic instability. We quote from [68]: *In the scenario studied in numerical analysis textbooks it is assumed that when integrating problems such as* $y' = y$, $y(0) = 1$, $0 \leq t \leq T_{\max}$ *the goal is to accurately compute the value of* $y(t)$, $0 \leq t \leq T_{\max}$. *Due to the exponential growth of the errors, this goal is not realistic when* $T_{\max}$ *is not small.* Large stepsizes for exploding modes with explosive methods can therefore be appropriate. Another justification for explosive methods comes from the use of L-stable methods for stiff systems. Integrating in the forward direction with L-stable RK coefficients is equivalent to integrate backward with their adjoint explosive RK coefficients, and vice versa. Thus, explosive methods are as much justified as L-stable methods from the viewpoint of backward error analysis.

In the decomposition (15) the term $f^{(4)}(q,v,\lambda)$ should contain *exploding* forces ($\partial f^{(4)}/\partial v(q,v,\lambda)$ positive definite), i.e., forces increasing the energy of the system,

e.g., like Lv with L positive definite. Unconditionally explosive RK coefficients can be appropriate to treat such forces.

6. Structure preservation for nonlinear systems. Linear stability properties are usually not adequate for nonlinear systems. In this section we characterize SPARK methods preserving different (generally nonlinear) structures (see section 3) when they are present, namely, the manifold of constraints, symplecticness, reversibility, contractivity, dilatation, energy, momentum, and quadratic invariants. For mechanical systems, we emphasize that these properties can be preserved directly in terms of generalized coordinates q and of generalized velocities v without reformulating the system using generalized momenta p.

6.1. Constraint preservation. By construction the numerical solution (y_1, z_1) of the SPARK methods considered in Theorem 4.3 lies on the manifold of constraints

$$X = \{(y,z) \in \mathbf{R}^n \times \mathbf{R}^p \mid 0 = g(y),\ 0 = g_y(y) f(y,z)\} \ . \tag{33}$$

If one defines the numerical u-component u_1 by (17h), then the constraint (2e) is also enforced. However, as discussed in subsection 4.3, a very accurate value for u_1 may be unnecessary. A fairly good choice is given by $u_1 := U_s$.

The definition of SPARK methods and the convergence results of section 4 can be extended to include the presence of *nonholonomic constraints*

$$0 = h(y,z) \ .$$

Such constraints do not derive from holonomic constraints. More precisely, there does not exist a function $\ell(y)$ such that $h(y,z) = \ell_y(y) f(y,z)$ with f of (2a). However, when such constraints are present, the flow is, in general, nonsymplectic and may possess no reversibility property.

6.2. Symplecticness. To preserve the symplecticness property of Hamiltonian systems, we consider the decompositions (5) (see (6ab)) with $f^{(1)}(y,z) \equiv H_p^T(q,p)$, $k^{(2)}(y,z,u) \equiv -H_q^T(q,p) - G^T(q)\lambda$, and the other terms identically zero.

For conservative mechanical systems, the symplecticness property can be preserved directly in terms of the variables (q,v) without explicitly reformulating the system in Hamiltonian form. Another advantage is that the equation $q' = v$ is simpler to integrate than $q' = M(q)^{-1}p$ for a pure Hamiltonian formulation. When the mass matrix is invertible, we consider the decompositions (5) (see (8)–(12)) with $f^{(1)}(y,z) \equiv v$, $k^{(2)}(y,z,u) \equiv \frac{1}{2}(v^T M(q) v)_q^T - U_q^T(q) - G^T(q)\lambda$, and the other terms identically zero. Under the assumption (10) we consider similar decompositions for the augmented system (see (13a), (13b))

$$f^{(1)}(y,z) \equiv \begin{pmatrix} v \\ w \end{pmatrix} \ , \tag{34a}$$

$$k^{(2)}(y,z,u) \equiv \begin{pmatrix} G_q^T(q)(v,w) + \frac{1}{2}(v^T M(q) v)_q^T - U_q^T(q) - G^T(q)\lambda \\ -\mu \end{pmatrix} \ . \tag{34b}$$

THEOREM 6.1. *With the above decompositions a SPARK method satisfying* (20a) *is symplectic for Hamiltonian systems and conservative mechanical systems if*

$$b_i a_{ij}^{(2)} + b_j a_{ji}^{(1)} - b_i b_j = 0 \quad \text{for} \ \ i,j = 1,\dots,s \ . \tag{35}$$

REMARK 6.2.

1. *The symplecticness condition* (35) *and the assumption* (21a) *imply* $a^{(2)}_{i1} = b_1$ *for* $i = 1, \ldots, s$.

2. *The symplecticness condition* (35) *and the simplifying assumption* (S^1) *imply* $a^{(2)}_{is} = 0$ *for* $i = 1, \ldots, s$.

Proof. For Hamiltonian systems this theorem has been proved in [44, Theorem V.3.1] and [46]. For conservative mechanical systems with an invertible mass matrix the result comes directly from the definition of SPARK methods, because the application of a SPARK method is equivalent to its application to the corresponding Hamiltonian form with $p := M(q)v$ and $H = T + U$. For the augmented system (13) the same argument holds, and the 2-form in (14) is preserved. Since $r_1 = 0$, $w_1 = 0$, and $G(q_1)v_1 = 0$, the 2-form $dq \wedge d(M(q)v)$ is preserved. □

The idea of applying indirectly a symplectic method to conservative mechanical systems can be extended to other systems in nonstandard Hamiltonian form. For example, if a 2-form $dY(y,z) \wedge dZ(y,z)$ is preserved where the transformation $(y,z,u) \mapsto (Y(y,z), Z(y,z), U(u))$ is a diffeomorphism, a symplectic method can be applied to the differential-algebraic system corresponding to (Y,Z,U) expressed in terms of (y,z,u), thus allowing the direct preservation of the 2-form. This holds for Lagrangian systems, and this gives rise to *Lagrangian integrators* [45]. For the simple Lotka–Volterra system a different unconventional symplectic integrator is presented in [66].

6.3. Reversibility. Reversibility of Hamiltonian systems and of conservative mechanical systems has been mentioned in subsections 3.1 and 3.2. Here we consider more generally the overdetermined partitioned differential-algebraic system (2) and we assume that there exist three linear maps $\sigma^y : \mathbf{R}^n \to \mathbf{R}^n$, $\sigma^z : \mathbf{R}^p \to \mathbf{R}^p$, and $\sigma^u : \mathbf{R}^m \to \mathbf{R}^m$ such that

$$\begin{aligned} (\sigma^y y)' &= -f(\sigma^y y, \sigma^z z) \ , \\ M(\sigma^y y)(\sigma^z z)' &= -k(\sigma^y y, \sigma^z z, \sigma^u u) \ , \end{aligned}$$

and $\sigma(y,z) := (\sigma^y y, \sigma^z z) \in X$ if $(y,z) \in X$ (see (33)). Then the flow $\chi_\tau : (y(t), z(t)) \mapsto (y(t+\tau), z(t+\tau))$ is *σ-reversible*, i.e.,

$$\chi_\tau = \sigma^{-1} \circ \chi_\tau^{-1} \circ \sigma \ .$$

Consequently, the time direction of the flow is reversed by the transformation σ. If we denote by Φ_h the numerical flow induced by a SPARK method, by "linearity" of these methods we have $\sigma \circ \Phi_h = \Phi_{-h} \circ \sigma$. Therefore, a SPARK method preserves the σ-reversibility of the flow if $\Phi_{-h} = \Phi_h^{-1}$; i.e., the SPARK method must be *symmetric*. A variable stepsize strategy preserving the reversibility property is discussed in section 9.

THEOREM 6.3. *Suppose that for* $m = 3, 4$ *we have* $f^{(m)}(y,z) \equiv 0$ *and* $k^{(m)}(y,z,u) \equiv 0$ *in* (5). *Then a SPARK method satisfying* (20a) *is symmetric if*

$$a^{(m)}_{s+1-i,s+1-j} + a^{(m)}_{ij} = b_j = b_{s+1-j} \quad \text{for} \ \ m = 1, 2 \ \ \text{and} \ \ i, j = 1, \ldots, s \ . \tag{36}$$

REMARK 6.4.

1. *The symmetry condition* (36) *for* $m = 1$ *and the simplifying assumption* (S^1) *imply* (21a).

2. *The symmetry condition* (36) *for* $m = 2$ *and the assumption* $a^{(2)}_{is} = 0$ *for* $i = 1, \ldots, s$ *imply* $a^{(2)}_{i1} = b_1$ *for* $i = 1, \ldots, s$.

Proof. We consider consistent initial values

$$\begin{aligned}
0 &= g(y_0)\ ,\\
0 &= g_y(y_0)f(y_0,z_0)\ ,\\
0 &= g_{yy}(y_0)(f(y_0,z_0),f(y_0,z_0)) + g_y(y_0)f_y(y_0,z_0)f(y_0,z_0)\\
&\quad + g_y(y_0)f_z(y_0,z_0)M^{-1}(y_0)k(y_0,z_0,u_0)\ .
\end{aligned}$$

Exchanging $(y_0,z_0,u_0) \leftrightarrow (y_1,z_1,u_1)$ and $h \leftrightarrow -h$ in Definition 4.1 and above, we obtain the *adjoint* method (y_1^*,z_1^*,u_1^*). Since by definition a symmetric method is equal to its adjoint, the conclusion follows. ∎

For the augmented system (13), since $w=0$ it is possible to discard the expression $G_q^T(q)(v,w)$ in (16) (see also (34b)) to avoid extra computation. This does not destroy the reversibility property, only the preservation of symplecticness.

It could be argued that symmetric schemes present a potential risk when applied to differential-algebraic equations [4]. But here the situation is different. Symmetric RK schemes are not used for terms destroying the reversibility property since there is no advantage of doing so. We rather make use of nonsymmetric methods like the Lobatto IIIC and Lobatto IIIC* methods to treat such terms (see sections 5 and 8 and the next subsection).

Even if the partitioned differential-algebraic system (2) does not possess any σ-reversibility, its flow always possesses the *time-reversibility* property

$$\chi_\tau^{-1} = \chi_{-\tau}\ .$$

Obviously, this property is directly preserved under the assumptions of Theorem 6.3. Nevertheless, using nonsymmetric methods has also several advantages, especially for stiff problems. Unfortunately, the time-reversibility property cannot be preserved directly with nonsymmetric SPARK methods. Although direct σ-reversibility preservation is of importance, it is unclear whether direct time-reversibility preservation does play a role or not. However, it might still be useful in practice to preserve this property indirectly when integrating a system backward in time. To do so when $f^{(m)}(y,z) \not\equiv 0$ or $k^{(m)}(y,z,u) \not\equiv 0$ for $m=3,4$ and the corresponding RK coefficients $(b_i, a_{ij}^{(m)})$ are not symmetric, these two sets of coefficients should be symmetrically conjugate, i.e.,

$$a^{(3)}_{s+1-i,s+1-j} + a^{(4)}_{ij} = b_j = b_{s+1-j} \quad \text{for } i=1,\dots,s, \text{ and } j=1,\dots,s\ . \tag{37}$$

When reversing the time direction of integration, the RK coefficients $(b_i, a_{ij}^{(3)})$ and $(b_i, a_{ij}^{(4)})$ should be exchanged, or equivalently for the terms $f^{(3)}(y,z)$, $f^{(4)}(y,z)$, and $k^{(3)}(y,z,u)$, $k^{(4)}(y,z,u)$.

6.4. Contractivity and dilatation. A generalization of the concept of A-stability to nonlinear systems is given by B-stability (see [35, Chapter IV] and the references therein).

Definition 6.5. *An RK method applied to $z' = k(z)$ is said to be* B-stable *if the* contractivity *condition*

$$\langle k(z) - k(\widehat{z}), z - \widehat{z}\rangle \le 0$$

implies that for all $h \ge 0$

$$\|z_1 - \widehat{z}_1\| \le \|z_0 - \widehat{z}_0\|,$$

where z_1 and $\widehat{z_1}$ are the numerical approximations after one step starting with initial values z_0 and $\widehat{z_0}$, respectively, and $\|z\| := \sqrt{\langle z, z\rangle}$.

A sufficient condition for B-stability is given by the criteria of algebraic stability.

DEFINITION 6.6 (see [35, section IV.12]). *If the RK coefficients satisfy the following:*

1. *$b_i \geq 0$ for $i = 1, \ldots, s$,*
2. *the matrix $(m_{ij})_{i,j=1}^{s} = (b_i a_{ij} + b_j a_{ji} - b_i b_j)_{i,j=1}^{s}$ is nonnegative definite,*

then the method is called algebraically stable.

In the family of Lobatto methods we have the following well-known result.

THEOREM 6.7 (see [35, Theorem IV.12.9]). *The Lobatto* IIIC *RK methods are algebraically stable.*

In parallel with A-stability and explosivity, by symmetry with B-stability we can consider the new concept of *dilatation* by simply reversing the inequality signs in Definition 6.5. It is trivial to show that symmetrically conjugate methods to B-stable methods preserve the dilatation property. Such methods can be called *dilative*. In the family of Lobatto methods we thus have the following result.

THEOREM 6.8. *The Lobatto* IIIC* *RK methods are dilative.*

6.5. Energy. It has been proved in [82] that symplectic integrators cannot preserve energy exactly in general, unless the numerical flow is exact. Hence, for conservative systems the class of *energy-momentum-conserving algorithms* has been proposed in [25, 28, 72, 73]. Such methods obviously cannot be symplectic. Another drawback of such methods is that they may introduce an undesirable spurious coupling. This is easily understandable when considering the theoretical case where a system is decoupled into several subsystems. Although the total energy of the whole system can be preserved, the energy of each subsystem is in general not preserved, and an artificial coupling is introduced between the different subsystems. An attempt to minimize the effects of this drawback for this class of methods has been made in [62].

Nevertheless, with respect to energy preservation, symplectic methods can possess good properties. Although they do not preserve energy exactly in general, they can quasi preserve it over long-time intervals provided the energy surfaces of the system are bounded in the phase space. This property is closely related to the preservation of symplecticness by backward error analysis arguments [30]: for Hamiltonian systems, symplectic methods can be interpreted as being exponentially close to the exact solution of a nearby perturbed Hamiltonian system. This result has been partly extended to Hamiltonian systems with holonomic constraints in [63]. Moreover, unlike energy-momentum conserving algorithms, for a system decoupled into subsystems they also naturally quasi preserve the energy of each subsystem without any artificial coupling. The numerical solution may be projected onto the correct energy surfaces in a post processing step if desired, though the time integration should still be carried with the unprojected values to keep the good long-time behavior of the method.

6.6. Momentum and quadratic invariants. Symplectic PRK methods preserve also certain momentum maps [60] such as angular momentum [81]. It has been proved in [21] that symplectic RK methods preserve exactly quadratic first integrals of differential systems. By a simple generalization of another similar result in [60], it can be seen that for the system (2), symplectic PRK methods preserve exactly quadratic first integrals of the form $y^T S M(y) z = \text{Const}$, where S is a matrix in $\mathbf{R}^{n\times p}$. Moreover, as in [49], it can be shown that for the system (2) the Lobatto IIIA-B PRK methods even preserve quadratic weak invariants of the form $y^T T y = \text{Const}$, where T is a symmetric matrix in $\mathbf{R}^{n\times n}$.

7. Numerical damping. In structural dynamics, linear systems of the form

$$\begin{aligned} q' &= v \ , \\ Mv' &= F(t) - Cv - Kq \end{aligned}$$

are usually considered (see also the introduction). Good methods in structural dynamics must introduce some controllable numerical dissipation to damp out spurious high frequencies without affecting the low frequencies of the system and the accuracy of the method. With this respect some methods have been proposed in the literature for unconstrained linear structural dynamics systems: the Newmark method [55], the Hilber–Hughes–Taylor α-method [37, 38, 40], the θ_1-method of Hoff and Pahl [39], the generalized α-method [20], and the SDIRK methods of Owren and Simonsen [56]. Most of these methods are of order two. For constrained systems few results have been reported [14, 15].

SPARK methods can achieve certain goals of structural dynamics, especially for constrained systems (1), and even go further. The main idea is that each term of each component $f_k^j(q,v,\lambda)$ entering in the forces (15) can be formally decomposed as

$$f_k^j(q,v,\lambda) = \sum_{m=1}^{4} \beta_k^{j,m} f_k^j(q,v,\lambda)$$

with $\sum_{m=1}^4 \beta_k^{j,m} = 1$ and can be treated differently. More generally, for the system (2)–(4)–(5), $f_l^i(y,z)$ entering in the ith component of (5a) and $k_k^j(y,z,u)$ entering in the jth component of (5b), we can consider the decompositions

$$\begin{aligned} f_l^i(y,z) &= \sum_{m=1}^{4} \alpha_l^{i,m} f_l^i(y,z) \ , \\ k_k^j(y,z,u) &= \sum_{m=1}^{4} \beta_k^{j,m} k_k^j(y,z,u) \end{aligned}$$

with $\sum_{m=1}^4 \alpha_l^{i,m} = 1 = \sum_{m=1}^4 \beta_k^{j,m}$ ($\beta_k^{j,1} = 0$ if $k_k^j(y,z,u)$ depends on u). According to Definition 4.1 four RK schemes are used for each of these expressions. The RK coefficients $(b_i, a_{ij}^{(1)})$ and $(b_i, a_{ij}^{(2)})$ will introduce no numerical damping since they will be chosen to satisfy the symplecticness conditions (35) and the symmetry conditions (36). The RK coefficients $(b_i, a_{ij}^{(3)})$ will introduce numerical damping since they will be chosen to satisfy the L-stability condition (see Definition 5.1). The RK coefficients $(b_i, a_{ij}^{(4)})$ will introduce no numerical damping but numerical explosivity since they will be chosen to satisfy the unconditional explosivity condition (see Definition 5.8). With this approach the numerical damping for each different term in each component can be tuned with different coefficients $\alpha_l^{i,m}$ for each i, l, and m, and $\beta_k^{j,m}$ for each j, k, and m, without affecting the overall accuracy. Moreover, these coefficients controlling the stability behavior of the numerical scheme may depend on the solution itself. Therefore, they might be adjusted automatically via certain criteria to obtain certain desired effects.

8. The Lobatto IIIA-B-C-C* SPARK methods. In this section we present a class of SPARK methods based on the same underlying quadrature formula (see (20)) and which satisfy all desired requirements: the simplifying assumption (S^1), the assumptions (21), the hypotheses of Theorem 4.3, the symplecticness conditions

(35), the symmetry conditions (36)–(37), L-stability and algebraic stability for the RK coefficients $(b_i, a_{ij}^{(3)})$, P-stability for the RK coefficients $(b_i, a_{ij}^{(1)})$, and unconditional explosivity and the dilative property for the RK coefficients $(b_i, a_{ij}^{(4)})$. In a certain sense such methods track the energy level of the system without introducing unnecessary numerical damping where it is not needed, whereas pure L-stable methods introduce numerical damping and are therefore not suited for conservative systems, especially for mid- and long-time integration. These methods are the s-stage Lobatto IIIA-B-C-C* SPARK methods ($s \geq 2$). The nodes c_i of the Lobatto quadrature formula of order $2s-2$ are the roots of the polynomial of degree s:

$$\frac{d^{s-2}}{dx^{s-2}}\left(x^{s-1}(x-1)^{s-1}\right) .$$

The weights b_i are chosen such that $B(s)$ holds. For the coefficients $a_{ij}^{(1)}$ we take the coefficients of the s-stage Lobatto IIIA RK method defined by $C^1(s)$. For the coefficients $a_{ij}^{(2)}$ we take the coefficients of the s-stage Lobatto IIIB RK method defined by $D^2(s)$. For the coefficients $a_{ij}^{(3)}$ we take the coefficients of the s-stage Lobatto IIIC RK method defined by $C^3(s-1)$ and $a_{i1}^{(3)} = b_1$ for $i = 1, \ldots, s$. For the coefficients $a_{ij}^{(4)}$ we take the coefficients of the s-stage Lobatto IIIC* RK method defined by $C^4(s-1)$ and $a_{is}^{(4)} = 0$ for $i = 1, \ldots, s$. These SPARK methods satisfy the simplifying assumptions $B(2s-2)$, (S^1), $C^1(s)$, $D^1(s-2)$, $C^2(s-2)$, $D^2(s)$, (S^3), $C^3(s-1)$, $D^3(s-1)$, $C^4(s-1)$, $D^4(s-1)$, $C^1C^n(s)$, and $D^1D^n(s)$ for $n = 2, 3, 4$ (see [44, Lemma V.5.3] and [46]). A detailed presentation of the construction of implicit RK methods can be found in [35, Section IV.5].

Two conditions of Theorem 4.3 are shown in the following lemma.

LEMMA 8.1. *For the s-stage Lobatto IIIA-B-C-C* SPARK methods, the conditions (21bc) on the RK matrices $A^{(m)}$ for $m = 1, \ldots, 4$ hold.*

Proof. The matrix equalities in (21b) can be proved by the use of the W-transformation. For details about this transformation we refer the reader to [35, Section IV.5] and [18, 27]. The aim here is to express the condition (21b) in term of the transformed matrices $X^{(m)} := W^T B A^{(m)} W$ for $m = 1, \ldots, 4$, where $B = \mathrm{diag}(b_1, \ldots, b_s)$ and the coefficients of the matrix W are given by $w_{ij} = P_{j-1}(c_i)$ with $P_{j-1}(x)$ the $(j-1)$th shifted Legendre polynomial. These matrices for the Lobatto IIIA, Lobatto IIIB, Lobatto IIIC, and Lobatto IIIC* coefficients are given respectively by

$$X^{(1)} = \begin{pmatrix} 1/2 & -\zeta_1 & & & O \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ & & \zeta_{s-2} & 0 & 0 \\ O & & & \zeta_{s-1}\sigma & 0 \end{pmatrix},$$

$$X^{(2)} = \begin{pmatrix} 1/2 & -\zeta_1 & & & O \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ & & \zeta_{s-2} & 0 & -\zeta_{s-1}\sigma \\ O & & & 0 & 0 \end{pmatrix},$$

$$X^{(3)} = \begin{pmatrix} 1/2 & -\zeta_1 & & & O \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ & & \zeta_{s-2} & 0 & -\zeta_{s-1}\sigma \\ O & & & \zeta_{s-1}\sigma & \sigma/(2s-2) \end{pmatrix},$$

$$X^{(4)} = \begin{pmatrix} 1/2 & -\zeta_1 & & & O \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ & & \zeta_{s-2} & 0 & -\zeta_{s-1}\sigma \\ O & & & \zeta_{s-1}\sigma & -\sigma/(2s-2) \end{pmatrix},$$

where $\zeta_k = 1/\left(2\sqrt{4k^2-1}\right)$ and $\sigma = \sum_{i=1}^{s} b_i P_{s-1}^2(c_i) = (2s-1)/(s-1)$. The condition $A^{(1)}A^{(m)} = A^{(1)}A^{(n)}$ can be expressed equivalently in term of their W-transforms by $X^{(1)}(W^TBW)^{-1}X^{(m)} = X^{(1)}(W^TBW)^{-1}X^{(n)}$. Here we have $W^TBW = \mathrm{diag}(1,\ldots,1,\sigma)$. Hence, since the last column of $X^{(1)}$ vanishes, we get $X^{(1)}(W^TBW)^{-1} = X^{(1)}$. Thus, because $X^{(2)}, X^{(3)}$, and $X^{(4)}$ differ only in their last row, the matrix products $X^{(1)}(W^TBW)^{-1}X^{(m)}$ give rise to the same matrix for $m = 2,3,4$. Because of $\mathrm{rank}(A^{(1)}) = s-1$ and $\mathrm{rank}(A^{(3)}) = s$, we necessarily have $\mathrm{rank}(N) = s-1$. From $a_{is}^{(2)} = 0$ we get $n_{is} = 0$; therefore, from $b_s \neq 0$ we finally conclude that (21c) holds. □

It is easily seen that the Lobatto IIIC* methods are symmetrically conjugate to the Lobatto IIIC methods; i.e., they satisfy (37), since the symmetrically conjugate methods to the Lobatto IIIC methods must satisfy $C^4(s-1)$, $D^4(s-1)$, and

$$\begin{aligned} a_{1j}^{(4)} &= b_{s+1-j} - a_{s,s+1-j}^{(3)} = 0 \quad \text{for } j = 1,\ldots,s\ , \\ a_{is}^{(4)} &= b_1 - a_{s+1-i,1}^{(3)} = 0 \quad \text{for } i = 1,\ldots,s\ . \end{aligned}$$

By symmetry with the Lobatto IIIC methods, the stability function of the Lobatto IIIC* methods is given by the $(s,s-2)$-Padé approximation to the exponential function $R_{s,s-2}(\mu)$ (see [35, Theorem IV.3.12 and Exercise IV.3.1]). Moreover, the symplectically conjugate methods to the Lobatto IIIC schemes must satisfy $C^4(s-1)$, $D^4(s-1)$, and

$$\begin{aligned} a_{1j}^{(4)} &= b_j\left(1 - \frac{a_{j1}^{(3)}}{b_1}\right) = 0 \quad \text{for } j = 1,\ldots,s\ , \\ a_{is}^{(4)} &= b_s\left(1 - \frac{a_{si}^{(3)}}{b_i}\right) = 0 \quad \text{for } i = 1,\ldots,s\ . \end{aligned}$$

These are again the Lobatto IIIC* methods. However, this additional property does not seem to have any particular signification in our context.

We give in Tables 1 and 2 the coefficients of the 2-stage and 3-stage Lobatto IIIA-B-C-C* SPARK methods respectively. For Lobatto IIIX schemes we use the Butcher

TABLE 1
Coefficients of the 2*-stage Lobatto* IIIA-B-C-C* *SPARK method.*

0	0	0		0	1/2	0		0	1/2	$-1/2$		0	0	0
1	1/2	1/2		1	1/2	0		1	1/2	1/2		1	1	0
A	1/2	1/2		B	1/2	1/2		C	1/2	1/2		C^*	1/2	1/2

TABLE 2
Coefficients of the 3*-stage Lobatto* IIIA-B-C-C* *SPARK method.*

0	0	0	0		0	1/6	$-1/6$	0		0	1/6	$-1/3$	1/6		0	0	0	0
1/2	5/24	1/3	$-1/24$		1/2	1/6	1/3	0		1/2	1/6	5/12	$-1/12$		1/2	1/4	1/4	0
1	1/6	2/3	1/6		1	1/6	5/6	0		1	1/6	2/3	1/6		1	0	1	0
A	1/6	2/3	1/6		B	1/6	2/3	1/6		C	1/6	2/3	1/6		C^*	1/6	2/3	1/6

tableau notation

$$\begin{array}{c|ccc} c_1 & a_{11}^{(m)} & \dots & a_{1s}^{(m)} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1}^{(m)} & \dots & a_{ss}^{(m)} \\ \hline X & b_1 & \dots & b_s \end{array}$$

From Theorem 4.5 and Theorem 4.6 we have the following superconvergence result.

COROLLARY 8.2. *For the s-stage Lobatto* IIIA-B-C-C* *SPARK methods applied to the overdetermined partitioned differential-algebraic system of index one* (2) *satisfying* (3) *in a neighborhood of the exact solution, with consistent initial values* (y_0, z_0, u_0) *at* t_0*, the global error satisfies for* $t_n - t_0 = nh \le \text{Const}$

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

This result remains valid in case of variable stepsizes with $h = \max_i |h_i|$.

8.1. Note on the Lobatto IIID coefficients. In [18] a one-parameter family of symmetric and algebraically stable RK methods based on Lobatto quadrature formulas is constructed. Within this family the s-stage Lobatto IIID methods are of interest in our context. The RK coefficients of the s-stage Lobatto IIID method are given by $a_{ij}^{(5)} = (a_{ij}^{(3)} + a_{ij}^{(4)})/2$ where $a_{ij}^{(3)}, a_{ij}^{(4)}$ are the coefficients of the s-stage Lobatto IIIC and Lobatto IIIC* methods respectively. This comes directly from the W-transform of the Lobatto IIID coefficients:

$$X^{(5)} = \begin{pmatrix} 1/2 & -\zeta_1 & & & O \\ \zeta_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\zeta_{s-2} & \\ & & \zeta_{s-2} & 0 & -\zeta_{s-1}\sigma \\ O & & & \zeta_{s-1}\sigma & 0 \end{pmatrix} .$$

TABLE 3
Coefficients of the 2-stage and 3-stage Lobatto IIID *methods.*

0	1/4	−1/4
1	3/4	1/4
D	1/2	1/2

0	1/12	−1/6	1/12
1/2	5/24	1/3	−1/24
1	1/12	5/6	1/12
D	1/6	2/3	1/6

Therefore, results for Lobatto IIIA-B-C-C* SPARK methods directly apply to include the Lobatto IIID coefficients as well. These methods satisfy $C^5(s-1)$, $D^5(s-1)$, $C^1C^5(s)$, and $D^1D^5(s)$. They are also symplectic [27] and dilative. We give in Table 3 the coefficients of the 2-stage and 3-stage Lobatto IIID methods.

9. Implementation of a reversible variable stepsize strategy. To preserve the symplecticness property, symplectic methods must be essentially applied with constant stepsizes [76]. The use of a standard variable stepsize strategy destroys this property [12]. For reversible systems a constant-stepsize application of a reversible method may be inefficient. The recent *reversible variable stepsize strategy* has been proposed in [41, 76], which allows a symmetric method to preserve the reversibility of the system and to keep its good long-time properties [11, 13, 34, 75]: the error growth is linear with time for integrable systems and for problems with periodic solutions. A reversible variable stepsize strategy is based on the construction of a *symmetric error estimator* and of a *symmetric stepsize function* [41, 76]. We can use an embedded method $(\widetilde{b}_i, c_i)$ of lower order $\widetilde{p}$ to build an error estimator of the form

$$\begin{aligned} err(h) &:= \|y_1 - \widetilde{y}_1\| + \|M(y_1)z_1 - M(\widetilde{y}_1)\widetilde{z}_1\| \\ &= \left\| h\sum_{i=1}^{s}(b_i - \widetilde{b}_i) f(Y_i, Z_i) \right\| + \left\| h\sum_{i=1}^{s}(b_i - \widetilde{b}_i)\widehat{k}(Y_i, Z_i, U_i) \right\| , \end{aligned} \tag{38}$$

Under the hypotheses of Theorem 6.3, this error estimator is symmetric provided the coefficients $e_i := b_i - \widetilde{b}_i$ are symmetric or antisymmetric, i.e., $e_i = e_{s+1-i}$ or $e_i = -e_{s+1-i}$ for $i = 1, \ldots, s$. A symmetric stepsize function can then be implicitly defined by

$$err(h) = TOL, \tag{39}$$

where TOL is the tolerance [76]. At each timestep we need to determine the stepsize h such that this nonlinear equation is satisfied. This variable stepsize strategy clearly does not destroy the reversibility property. In molecular dynamics a variable stepsize strategy may be of importance when simulating phase transitions. The stepsizes should be decreased to reproduce accurately all phenomena occuring during these transformations. For example during a first-order phase transition, latent heat is released in form of kinetic energy, and amplitudes and vibrational frequencies can increase significantly [79].

For the starting values of the simplified Newton iterations, as pointed out in [32, section 7], we can take $Y_i^{(0)} := y_0 + hc_i f(y_0, z_0) + O(h^2)$ for $i = 1, \ldots, s$, $y_1^{(0)} := y_0 + hf(y_0, z_0) + O(h^2)$, $Z_i^{(0)} := z_0 + O(h)$ for $i = 1, \ldots, s$, $z_1^{(0)} := z_0 + O(h)$, $U_i^{(0)} := u_0 + O(h)$ for $i = 1, \ldots, s$, and $u_1^{(0)} := u_0 + O(h)$. Every simplified Newton iteration improves the approximation by a factor h in the norm $\|y\| + h\|z\| + h^2\|u\|$. The equation (39) is a nonlinear equation for h which can be solved simultaneously to the

nonlinear system (17). Starting with an initial guess $h^{(0)}$ by using for example the previous stepsize or local extrapolation of previous stepsizes [76], after each simplified Newton iteration we can use the following simple iteration [11]:

$$h^{(k+1)} := h^{(k)} \cdot \left(\frac{TOL}{err(h^{(k)})} \right)^{1/(\widetilde{p}+1)} .$$

Moreover, after each simplified Newton iteration we also interpolate the values $(Y_i^{(k)}, Z_i^{(k)}, U_i^{(k)})$ and $(y_1^{(k)}, z_1^{(k)}, u_1^{(k)})$ which are approximations to the solution at $t_0 + c_i h^{(k)}$ and $t_0 + h^{(k)}$, respectively, to obtain new approximations $(Y_i^{(k+1)}, Z_i^{(k+1)}, U_i^{(k+1)})$ and $(y_1^{(k+1)}, z_1^{(k+1)}, u_1^{(k+1)})$ to the solution at $t_0 + c_i h^{(k+1)}$ and $t_0 + h^{(k+1)}$, respectively. The convergence of these iterations is nearly as fast as the standard simplified Newton iterations without modification of the stepsize [11]. A reversible variable stepsize strategy is thus a natural choice for implicit methods, since this strategy is nearly no more costly than a constant stepsize application of the method. This is an advantage of implicit methods compared to explicit methods with this respect.

Now the question arises to know the minimal precision that the nonlinear system (17) must be solved given a certain tolerance TOL for the local truncation error. It is clear that the error estimator (38) will be too pessimistic in general since $err(h) = O(h^{\widetilde{p}+1})$ and the local truncation error is of size $O(h^{p+1})$ with $p > \widetilde{p}$. Therefore, if we determine h by (39), then the local truncation error will be much smaller than TOL as it will be of the order of $TOL^{(p+1)/(\widetilde{p}+1)}$. Therefore, to have a local truncation error of the order of TOL, we propose replacing (39) by

$$err(h) = TOL^{(\widetilde{p}+1)/(p+1)} .$$

We also get "tolerance proportionality" with such a modification. To maintain an error of the order of TOL, the nonlinear system (17) must be solved at least at the precision TOL (multiplied by a safety factor, e.g., 0.01). For long-time integration more stringent conditions on the precision to solve the nonlinear system are given in [34]. The given tolerance TOL and the precision to which the nonlinear system of equations must be solved are thus related; this remark holds for any implicit integrator. Without such a modification, since the local truncation error would be of the order of $TOL^{(p+1)/(\widetilde{p}+1)}$, the nonlinear system should be solved at least at the precision $TOL^{(p+1)/(\widetilde{p}+1)}$. It is interesting to note that the order $\widetilde{p}$ of the embedded formula in (38) does not really play a significant role, low values of $\widetilde{p}$ are fine.

10. Numerical experiments. For the numerical experiments, we first consider a mechanical system consisting of seven rigid bodies, known in the literature as *Andrew's squeezing mechanism*. This system has six holonomic constraints. We do not enter into the details of the model here, thorough descriptions of this mechanism can be found in [69] and [35, section VI.9]. To illustrate the advantage of using the formulation eliminating the Coriolis forces, we compare for this system the expressions of the generalized forces with and without the presence of the Coriolis forces. Written as FORTRAN statements the expression of the generalized forces $f(q, v)$ entering into $M(q)v'$ (see (8b)) containing the Coriolis forces is given as [35, p. 537]

```
f(1) = MOM(t) - M2*DA*RR*THP*(THP + 2*BEP)*SITH
f(2) = M2*DA*RR*BEP**2*SITH
f(3) = FX*(SC*COGA - SD*SIGA) + FY*(SD*COGA + SC*SIGA)
f(4) = M4*ZT*(E - EA)*DEP**2*COPH
f(5) = - M4*ZT*(E - EA)*PHP*(PHP + 2*DEP)*COPH
```

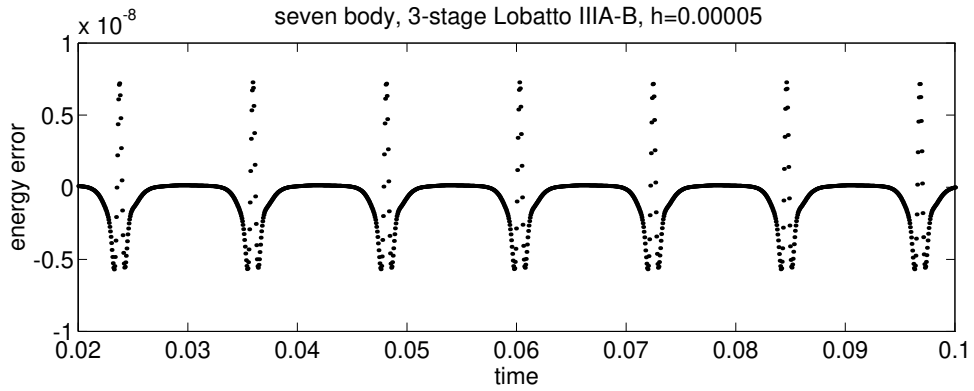

FIG. 1. *Energy error with constant stepsizes, no drive torque for* $t \geq 0.02$.

```
f(6) = - M6*U*(ZF - FA)*EPP**2*COOM
f(7) = M6*U*(ZF - FA)*OMP*(OMP + 2*EPP)*COOM ,
```

whereas for the expression $M_q(q)(v,v) + f(q,v)$ entering into $(M(q)v)'$ eliminating the Coriolis forces $-M_q(q)(v,v)$ (see (8f)) we obtain

```
F(1) = MOM(t)
F(2) = M2*DA*RR*BEP*(BEP + THP)*SITH
F(3) = FX*(SC*COGA - SD*SIGA) + FY*(SD*COGA + SC*SIGA)
F(4) = M4*ZT*(E - EA)*DEP*(DEP + PHP)*COPH
F(5) = 0
F(6) = - M6*U*(ZF - FA)*EPP*(EPP + OMP)*COOM
F(7) = 0 .
```

Comparing the number of additions and multiplications (including exponentiations) for these two expressions, we get 11 additions and 39 multiplications for the first one and 8 additions and 21 multiplications for the second one. Thus for this system the gain is drastic when using the second formulation.

To move the system a nonconstant drive torque $\texttt{MOM}(t) = 0.033 \cdot (1 - t/0.02)$ is applied during the interval $[0, 0.02]$, and then the system is let free to swing with no drive torque applied. We have applied the 3-stage Lobatto IIIA-B SPARK method to this system with constant stepsizes $h = 5 \cdot 10^{-5}$. In Fig. 1 we have plotted the energy error on the interval $[0.02, 0.1]$. We clearly observe that this error remains bounded with time and oscillates around 0, this is an illustration of the symplectic nature of the integrator.

In Fig. 2 we have plotted the energy error using a reversible variable stepsize strategy with a local error tolerance $TOL = 10^{-8}$. It can be observed that the error grows linearly with time, whereas in general for a standard variable stepsize strategy the error growth is quadratic.

Applying a constant drive torque $\texttt{MOM}(t) = 0.033$ during the whole interval $[0, 0.1]$, we obtain the result given in Fig. 3 for the energy error versus time. This is an interesting numerical experiment since, although the method is symplectic, reversible, and applied with constant stepsizes, it can be observed that this error grows quadratically with time (though still oscillating around 0). This might seem quite surprising since in general for symplectic integrators the energy error remains bounded. Nevertheless, this unboundedness can be explained by the fact that the energy surfaces are here unbounded in the phase space, whereas this was previously not the case. The kinetic energy roughly grows with time meaning that the mechanism is moving faster and

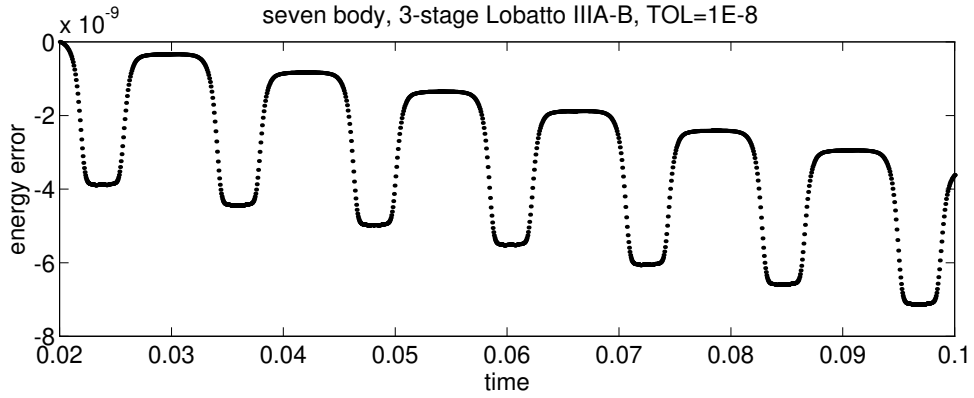

FIG. 2. *Energy error with a symmetric variable stepsize strategy, no drive torque for* $t \geq 0.02$.

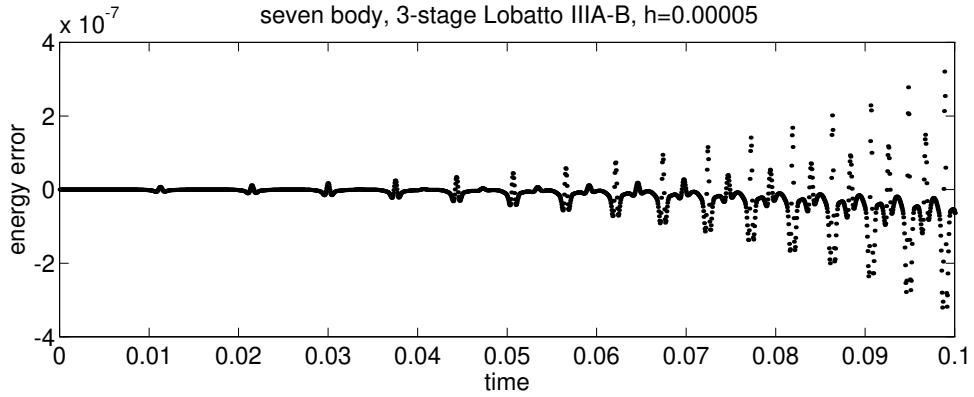

FIG. 3. *Energy error with constant stepsizes, constant drive torque.*

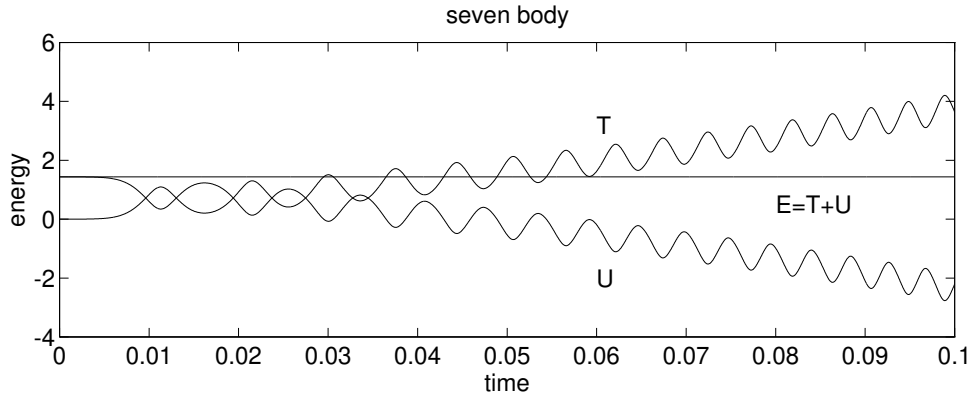

FIG. 4. *Total energy* E*, kinetic energy* T*, and potential energy* U*, constant drive torque.*

faster. We have plotted in Fig. 4 the total energy E which is constant as the sum of its kinetic part T and of its potential part U.

Finally, we consider a system composed of a rigid pendulum attached to a stiff spring pendulum undergoing some dry friction. The stiff spring pendulum consists

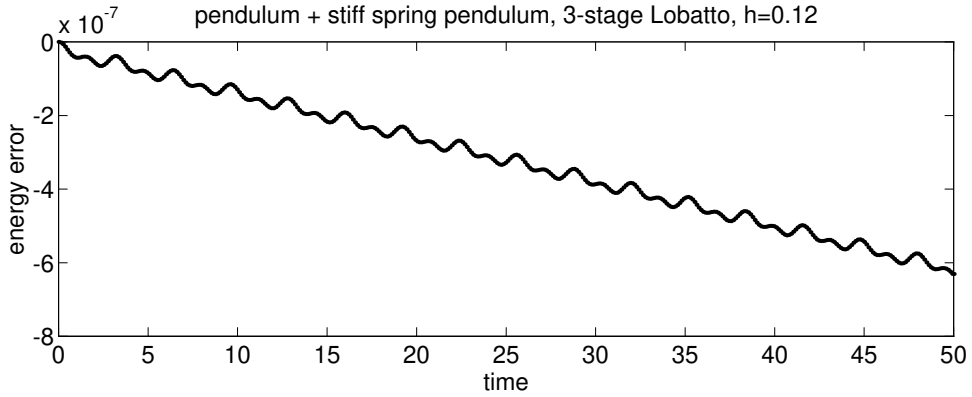

FIG. 5. *Energy error for the rigid pendulum using the Lobatto* IIIC *coefficients.*

of a mass point of unit mass suspended at a massless spring with a rest position of unit length and a large Hooke's constant $1/\varepsilon^2$. Its Cartesian coordinates are given by (q_{x_1}, q_{z_1}) and its corresponding velocities by (v_{x_1}, v_{z_1}). The rigid pendulum is of unit mass and of unit length. Its Cartesian coordinates are given by (q_{x_2}, q_{z_2}) and its corresponding velocities by (v_{x_2}, v_{z_2}). The gravitational constant is equal to one unit and the friction coefficient is denoted by γ. The equations of motion (8b) for this system are given by

$$\begin{aligned} v'_{x_1} &= -\gamma v_{x_1} - q_{x_1}\mu + (q_{x_2} - q_{x_1})\lambda \ , \\ v'_{z_1} &= -1 - \gamma v_{z_1} - q_{z_1}\mu + (q_{z_2} - q_{z_1})\lambda \ , \\ v'_{x_2} &= -(q_{x_2} - q_{x_1})\lambda \ , \\ v'_{z_2} &= -1 - (q_{z_2} - q_{z_1})\lambda \ , \end{aligned}$$

where

$$\mu := \frac{1}{\varepsilon^2}\left(1 - \frac{1}{\sqrt{q_{x_1}^2 + q_{z_1}^2}}\right) \ ,$$

and the holonomic constraint (8c) on the length of the rigid pendulum is given by

$$0 = \sqrt{(q_{x_2} - q_{x_1})^2 + (q_{z_2} - q_{z_1})^2} - 1 \ .$$

The constants $1/\varepsilon$ and γ are chosen large $1/\varepsilon = 10^8$ and $\gamma = 10^{12}$, so that the system is stiff. With a stepsize $h = 0.12$, we have first applied the 3-stage Lobatto IIIC coefficients to the differential equations, whereas the holonomic constraint is treated with the Lobatto IIIA coefficients. The energy error related to the rigid pendulum is plotted in Fig. 5. We observe that some undesirable numerical damping is introduced by the method due to the damping property of the Lobatto IIIC coefficients.

Using the Lobatto IIIA-B coefficients for the differential equations corresponding to the rigid pendulum, but still the Lobatto IIIC coefficients for the differential equations corresponding to the stiff spring pendulum, we have plotted in Fig. 6 the energy error for the rigid pendulum. This error remains now bounded with time and illustrates a clear advantage of using a SPARK method.

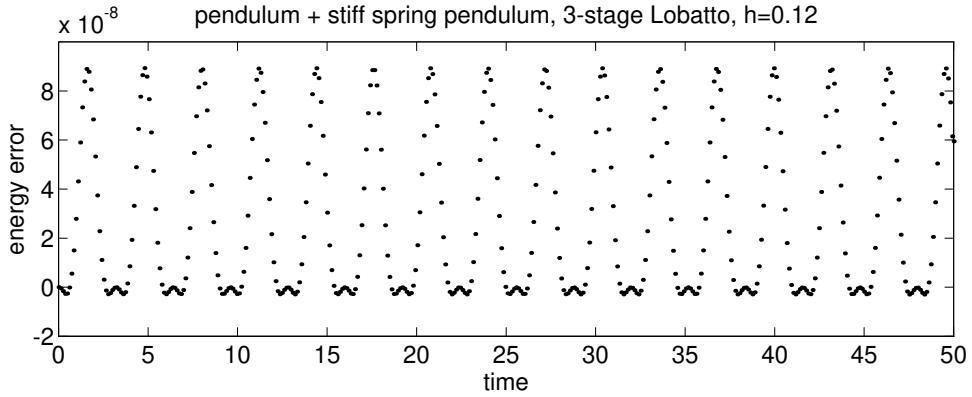

FIG. 6. *Energy error for the rigid pendulum using the Lobatto* IIIA-B *coefficients.*

11. Conclusion. We have considered a broad class of partitioned differential equations with possible algebraic constraints, including Hamiltonian and mechanical systems with holonomic constraints. For mechanical systems a formulation eliminating the Coriolis forces and closely related to the Euler–Lagrange equations has been presented. A new class of integrators has been defined: the SPARK methods. Within this class, the s-stage Lobatto IIIA-B-C-C* SPARK methods are of special interest. They can allow the direct preservation of different invariants and structures when present in the system, namely: the manifold of constraints, symplecticness, reversibility, contractivity, dilatation, momentum, and quadratic invariants. They can also quasi preserve energy. The s-stage Lobatto IIIA-B-C-C* SPARK methods are superconvergent with order $2s-2$, and they can possess good linear stability properties: L-stability, P-stability, and unconditional explosivity. The underlying idea of the new Lobatto SPARK methods is that diverse terms are treated by different coefficients of the Lobatto family. Controllable numerical damping can be introduced by the use of additional parameters. Some issues related to the implementation of a variable stepsize strategy preserving the reversibility property have been discussed.

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