Global modified Hamiltonian for constrained symplectic integrators

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Abstract

We prove that the numerical solution of partitioned Runge-Kutta methods applied to constrained Hamiltonian systems (e.g., the Rattle algorithm or the Lobatto IIIA–IIIB pair) is formally equal to the exact solution of a constrained Hamiltonian system with a globally defined modified Hamiltonian. This property is essential for a better understanding of their longtime behaviour. As an illustration, the equations of motion of an unsymmetric top are solved using a parameterization with Euler parameters.

Keywords. Constrained Hamiltonian systems, symplectic integrators, partitioned Runge-Kutta methods, generating functions, backward error analysis, modified Hamiltonian.

1 Introduction

It is well-known that symplectic integrators applied to Hamiltonian systems have an improved long-time behaviour (no secular terms in the preservation of the Hamiltonian, linear error growth for generic integrable systems). This is explained by a backward error analysis which states that the numerical solution is exponentially close to the exact solution of a modified Hamiltonian system which is given by a formal series

$$\widetilde{H}(p,q) = H(p,q) + hH_2(p,q) + h^2 H_3(p,q) + \ldots$$

in powers of the step size h (see for example [3, Chap. IX]). For this explanation it is crucial that all $H_j(p,q)$ of the modified Hamiltonian are globally defined, i.e., they have to be single-valued. This holds true for all known symplectic integrators.

For constrained Hamiltonian systems, a backward error analysis has first been elaborated by Reich [13]. It is based on an extension of the integrator to an open neighbourhood of $\mathcal{M}$ so that standard techniques can be applied. For simple methods such as the Rattle algorithm (Table 1) and the symplectic Euler method (Table 2) this extension is given explicitly in [4, Sect. VII.8] and a globally defined modified Hamiltonian is obtained in this way. In the general case, however, Darboux' Theorem on the transformation of a Poisson structure to canonical form is involved, and only the local existence of a modified Hamiltonian is guaranteed.

A different approach (considered in [3]) is based on the use of a parameterization of the constrained manifold, which transforms the constrained Hamiltonian system to an unconstrained Poisson system. Backward error analysis can be applied in the parameter space and the results can be rewritten in the original variables. Also this approach is in general of a local character.

The main contribution of the present article is to derive a globally defined modified Hamiltonian for all partitioned Runge-Kutta methods including the Lobatto IIIA–IIIB pair of arbitrary order. In Sect. 2 we present Hamiltonian systems that are subject to holonomic constraints, we give the formulas for partitioned Runge-Kutta methods, and we state the main result of this article. The key for the proof is an extension of the approach of Lasagni (unpublished manuscript with the same title as [9], see also Sanz-Serna & Calvo [14, Sect. 11.4]) to partitioned Runge-Kutta methods for constrained Hamiltonian systems (Sect. 3). We give in Sect. 4 a constructive derivation of the globally defined modified Hamiltonian. An illustrative numerical experiment (Sect. 5) solving the equations of motion for an unsymmetric top concludes this study.

2 Problem, Numerical Method, and Main Result

We consider the numerical integration of constrained Hamiltonian systems

$$\begin{aligned} \dot p &= -\nabla_q H(p,q) - \nabla_q g(q)\lambda \\ \dot q &= \nabla_p H(p,q), \qquad 0 = g(q). \end{aligned} \tag{2.1}$$

Here, p and q are vectors in $\mathbb{R}^n$, $g(q) = \big(g_1(q),\dots,g_m(q)\big)^T$ is the vector of constraints, $\nabla_p H$ and $\nabla_q H$ are column vectors of partial derivatives, $\nabla_q g = \big(\nabla_q g_1,\dots,\nabla_q g_m\big)$ is the transposed Jacobian matrix of $g(q)$, and $\lambda \in \mathbb{R}^m$ is the vector of Lagrange multipliers.

Differentiating the constraint $0 = g\big(q(t)\big)$ with respect to time yields

$$0 = \nabla_q g(q)^T \nabla_p H(p,q) \tag{2.2}$$

(the so-called hidden constraint) which is an invariant of the flow of (2.1). A second differentiation gives the relation

$$\begin{aligned} 0 \;=\; &\frac{\partial}{\partial q}\Big(\nabla_q g(q)^T \nabla_p H(p,q)\Big)\nabla_p H(p,q) \\ &-\nabla_q g(q)^T \nabla_p^2 H(p,q)\Big(\nabla_q H(p,q) + \nabla_q g(q)\lambda\Big), \end{aligned} \tag{2.3}$$

which allows us to express λ in terms of (p,q), if the matrix

$$\nabla_q g(q)^T \nabla_p^2 H(p,q) \nabla_q g(q) \qquad \text{is invertible} \tag{2.4}$$

($\nabla_p^2 H$ denotes the Hessian matrix of H). Inserting the so-obtained function $\lambda(p,q)$ into (2.1) gives a differential equation for (p,q) on the manifold

$$\mathcal{M} = \big\{(p,q) \mid g(q) = 0,\ \nabla_q g(q)^T \nabla_p H(p,q) = 0\big\}. \tag{2.5}$$

Partitioned Runge-Kutta Methods. For the numerical integration of problem (2.1) with initial value $(p_0, q_0) \in \mathcal{M}$ we consider the discretization

$$P_i = p_0 - h \sum_{j=1}^{s} a_{ij} \Big(\nabla_q H(P_j, Q_j) + \nabla_q g(Q_j) \Lambda_j \Big) \tag{2.6}$$

$$Q_i = q_0 + h \sum_{j=1}^{s} \widehat{a}_{ij} \nabla_p H(P_j, Q_j), \qquad 0 = g(Q_i) \tag{2.7}$$

$$p_1 = p_0 - h \sum_{i=1}^{s} b_i \Big(\nabla_q H(P_i, Q_i) + \nabla_q g(Q_i) \Lambda_i \Big) \tag{2.8}$$

$$q_1 = q_0 + h \sum_{i=1}^{s} b_i \nabla_p H(P_i, Q_i). \tag{2.9}$$

Due to the conditions $0 = g(Q_i)$ in (2.7), which have to be satisfied by choosing suitably the Λ_i, the existence of the numerical solution is not guaranteed without any assumptions on the coefficients of the method. Following Jay [7] (see also [4, Sect. VII.8]) we assume that

$$\begin{array}{lll} \widehat{a}_{1j} = 0, & \widehat{a}_{sj} = b_j, & a_{is} = 0 \\ b_s \neq 0, & \big(\sum_{k=1}^{s} \widehat{a}_{ik} a_{kj}\big)_{i,j=2}^{s} & \text{invertible.} \end{array} \tag{2.10}$$

The assumptions $\widehat{a}_{1j} = 0$ and $\widehat{a}_{sj} = b_j$ imply $Q_1 = q_0$ and $Q_s = q_1$, so that $g(Q_1) = 0$ gives no extra condition and $g(q_1) = 0$ is automatically satisfied because of $g(Q_s) = 0$. Since $a_{is} = 0$, the equation (2.6) does not depend on Λ_s, and the invertibility of the matrix in (2.10) together with (2.4) allow us to determine $\Lambda_1, \dots, \Lambda_{s-1}$ in such a way that $g(Q_i) = 0$ for $i = 2, \dots, s$. If $b_s \neq 0$, the freedom in choosing Λ_s can be exploited to satisfy $\nabla_q g(q_1)^T \nabla_p H(p_1, q_1) = 0$. Consequently, the numerical solution (p_1, q_1) after one step remains in the manifold $\mathcal{M}$.

Example 2.1 (Rattle Algorithm) The most prominent example is the so-called Rattle algorithm, developed by Ryckaert, Ciccotti & Berendsen and by Andersen for separable Hamiltonians, and extended to general constrained Hamiltonian systems by Jay. It is defined by (2.6)–(2.9) with $s = 2$ and coefficients $\widehat{a}_{ij}$ (left tableau), a_{ij} (right tableau), and b_i (bottom rows) given in Table 1. This method is symmetric and of order two.

Table 1: Coefficients of the Rattle algorithm

$$
\begin{array}{c|cc} & 0 & 0 \\ & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}
\qquad\qquad
\begin{array}{c|cc} & 1/2 & 0 \\ & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}
$$

Example 2.2 (Lobatto IIIA–IIIB Pair) A natural extension of the Rattle algorithm to higher order has been found by Jay [7]. The idea is to take for b_i the weights of the Lobatto quadrature of order $2s-2$, for the coefficients $\widehat{a}_{ij}$ the Lobatto IIIA collocation method, and for a_{ij} the Lobatto IIIB method. For details of the coefficients we refer to [4] and to [3, Chap. II]. With these coefficients the method (2.6)–(2.9) is symmetric and of order $2s-2$. A new proof of the order of convergence is presented in [3, Sect. VII.1].

Example 2.3 (Methods with $\mathbf{b}_s = 0$: Symplectic Euler) If the conditions of (2.10) are satisfied with the exception of $b_s \neq 0$, the numerical solution still exists and satisfies $g(q_1) = 0$, but in general $(p_0, q_0) \notin \mathcal{M}$. To achieve $(p_0, q_0) \in \mathcal{M}$ we subtract the term $h\nabla_q g(q_1)\Lambda_s$ to (2.8) and determine Λ_s such that $\nabla_q g(q_1)\nabla_p H(p_1, q_1) = 0$ holds. An important special case is given by the coefficients of Table 2. The order of the resulting method is one.

Table 2: Symplectic Euler for Constrained Systems

$$
\begin{array}{c|cc} & 0 & 0 \\ & 1 & 0 \\ \hline & 1 & 0 \end{array}
\qquad\qquad
\begin{array}{c|cc} & 1 & 0 \\ & 1 & 0 \\ \hline & 1 & 0 \end{array}
$$

Backward Error Analysis. We are now in the position to formulate and discuss the main result of this article. We denote by $\varphi_t : \mathcal{M} \to \mathcal{M}$ the exact flow of the system (2.1), and by $\Phi_h : \mathcal{M} \to \mathcal{M}$ the discrete flow of one of the above methods applied with step size h to (2.1).

Theorem 2.4 *Let $H(p,q)$ and $g(q)$ be defined and smooth on a neighbourhood D of $\mathcal{M}$ and let (2.4) be there fulfilled. Assume that the method (2.6)–(2.9) satisfies (2.10) and the symplecticity condition*

$$b_i \widehat{a}_{ij} + b_j a_{ji} = b_i b_j \qquad \textit{for all } i, j. \tag{2.11}$$

Then, there exist functions $H_k(p,q)$ defined and smooth on D, satisfying

$$\nabla_q g(q)^T \nabla_p H_k(p,q) = 0 \qquad \textit{for } (p,q) \in \mathcal{M}, \tag{2.12}$$

such that for arbitrary $N \geq 1$ and with

$$\widetilde{H}(p,q) \;=\; H(p,q) + hH_2(p,q) + \ldots + h^{N-1}H_N(p,q) \tag{2.13}$$

we have

$$\Phi_h(y) - \widetilde{\varphi}_h(y) = \mathcal{O}(h^{N+1}),$$

where $\widetilde{\varphi}_t : \mathcal{M} \to \mathcal{M}$ denotes the exact flow of

$$\begin{aligned} \dot p &= -\nabla_q \widetilde{H}(p,q) - \nabla_q g(q)\lambda \\ \dot q &= \nabla_p \widetilde{H}(p,q), \qquad 0 \;=\; g(q). \end{aligned} \tag{2.14}$$

The proof of this theorem is the subject of this article.

3 Generating Function

The numerical solution of (2.6)–(2.8) is well-defined only for $(p_0.q_0) \in \mathcal{M}$. However, if we replace the condition "$0 = g(Q_i)$" in (2.7) by

$$0 \;=\; g(Q_i) - g(q_0) - h\widehat{c}_i \nabla_q g(q_0)^T \nabla_p H(p_0,q_0) \tag{3.1}$$

$(i = 2, \ldots, s)$ and the condition "$0 = \nabla_q g(q_1)^T \nabla_p H(p_1,q_1)$" defining Λ_s by

$$0 \;=\; \nabla_q g(q_1)^T \nabla_p H(p_1,q_1) - \nabla_q g(q_0)^T \nabla_p H(p_0,q_0), \tag{3.2}$$

then the numerical solution is well-defined for all (p_0,q_0) in an open neighbourhood of $\mathcal{M}$ (cf. [4, page 546]). Unfortunately, the so-obtained extension of (2.6)–(2.8) is not symplectic.

Inspired by the formulas of Lasagni for the generating functions of (unconstrained) symplectic Runge-Kutta methods, we define

$$\begin{aligned} S(p_1,q_0,h) \;=\; & h \sum_{i=1}^{s} b_i \Big(H(P_i,Q_i) + g(Q_i)^T \Lambda_i \Big) \\ & - \; h^2 \sum_{i,j=1}^{s} b_i\, \widehat{a}_{ij} \Big(\nabla_q H(P_i,Q_i) + \nabla_q g(Q_i)\Lambda_i \Big)^T \nabla_p H(P_j,Q_j), \end{aligned} \tag{3.3}$$

where P_i, Q_i and Λ_i are considered as functions of (p_1,q_0), what is possible because $p_1 = p_0 + \mathcal{O}(h)$. This function S permits us to find a symplectic extension of our method on the manifold $\mathcal{M}$.

Lemma 3.1 *Let the coefficients $b_i, a_{ij}, \widehat{a}_{ij}$ satisfy (2.10) and (2.11). Then, the numerical method given by*

$$p_0 = p_1 + \nabla_{q_0} S(p_1,q_0,h), \qquad q_1 = q_0 + \nabla_{p_1} S(p_1,q_0,h) \tag{3.4}$$

defines a symplectic extension of the partitioned Runge-Kutta method (2.6)–(2.9) to an open neighbourhood of $\mathcal{M}$.

Proof. As a consequence of the theory of generating functions the transformation $(p_0, q_0) \mapsto (p_1, q_1)$, given implicitly by (3.4), is a symplectic mapping for every smooth $S(p_1, q_0, h)$.

We still have to prove that (3.4) is an extension of the partitioned Runge-Kutta method (2.6)–(2.9). For this we compute the partial derivatives of $S(p_1, q_0, h)$. Observing that the derivatives of P_i, Q_i, p_0 with respect to p_1 and q_0 can be obtained from (2.6)–(2.8) by implicit differentiation, and using the symplecticity condition (2.11), a straightforward computation yields

$$\begin{aligned}
\nabla_{q_0} S &= h \sum_{i=1}^{s} b_i \Big(\nabla_q H(P_i, Q_i) + \nabla_q g(Q_i) \Lambda_i \Big) + h \sum_{i=1}^{s} b_i \big(\nabla_{q_0} \Lambda_i \big) g(Q_i) \\
\nabla_{p_1} S &= h \sum_{i=1}^{s} b_i \nabla_p H(P_i, Q_i) + h \sum_{i=1}^{s} b_i \big(\nabla_{p_1} \Lambda_i \big) g(Q_i).
\end{aligned}$$

Since $g(Q_i) = 0$ for $(p_0, q_0) \in \mathcal{M}$ (cf. (3.1)), this proves that the method (3.4) is on the manifold $\mathcal{M}$ the same as (2.6)–(2.9). □

For methods satisfying (2.11) and (2.10) with the exception of $b_s \neq 0$ we have to include the term $-h \nabla_q g(q_1) \Lambda_s$ in formula (2.8) to be able to fulfill (3.2). In this case the statement of Lemma 3.1 holds true, if the expression

$$h g(Q_s)^T \Lambda_s - h^2 \sum_{j=1}^{s} \widehat{a}_{sj} \Big(\nabla_q g(Q_s) \Lambda_s \Big)^T \nabla_p H(P_j, Q_j) \tag{3.5}$$

is added to S of (3.3).

We observe, and this is crucial for the rest of this paper, that the generating function can be written as

$$S(p, q, h) = h S_1(p, q) + h^2 S_2(p, q) + h^3 S_3(p, q) + \dots\ , \tag{3.6}$$

where the functions $S_j(p, q)$ are smooth and well-defined on D (the domain where $H(p, q)$ and $g(q)$ are defined and where (2.4) holds). In fact, they are composed of derivatives of H and g, and of multiplications with the inverse of the matrix (2.4). This is illustrated with the following example.

Example 3.2 For the symplectic Euler method of Table 2 it follows from (3.3) and (3.5) that

$$\begin{aligned}
S(p_1, q_0, h) &= h \left(H(P_1, q_0) + g(q_0)^T \Lambda_1 + g(q_1)^T \Lambda_2 \right) \\
&- h^2 \, \nabla_p H(P_1, q_0)^T \nabla_q g(q_1) \Lambda_2,
\end{aligned}$$

where $P_1, q_1, \Lambda_1, \Lambda_2$ have to be interpreted as functions of (p_1, q_0). This generating function has an expansion of the form (3.6) with

$$\begin{aligned}
S_1(p, q) &= H(p, q) + g(q)^T \left(\lambda_1^0(p, q) + \lambda_2^0(p, q) \right) \\
S_2(p, q) &= \nabla_p H(p, q)^T \nabla_q g(q) \lambda_2^0(p, q) + g(q)^T \left(\lambda_1^1(p, q) + \lambda_2^1(p, q) \right),
\end{aligned}$$

where $\lambda_i^j(p_1,q_0)$ are the coefficients of the h-expansion of $\Lambda_i(p_1,q_0,h)$. In fact, $\lambda_1^0(p,q)+\lambda_2^0(p,q)$ equals the function $\lambda(p,q)$ defined in (2.3), the function λ_2^0 is given by

$$\big(\nabla_q g^T\,\nabla_p^2 H\,\nabla_q g\big)\lambda_2^0 \;=\; g''\,(\nabla_p H)^2+\nabla_q g^T\,\nabla_{pq}H\,\nabla_p H,$$

(the obvious argument (p,q) is omitted in this formula), and for $\lambda_1^1+\lambda_2^1$ we have a similar formula with a much more complicated right-hand side.

Remark 3.3 (Symmetric Extension) For symmetric partitioned Runge-Kutta methods (2.6)–(2.9), i.e., methods for which $a_{ij}+a_{s+1-i,s+1-j}=b_j$ and $\widehat a_{ij}+\widehat a_{s+1-i,s+1-j}=b_j$ hold, the extension (3.4) is not symmetric. This is due to the unsymmetric relation (3.1) and can easily be repaired by replacing it with

$$0 \;=\; g(Q_i)-\frac{1}{2}\big(g(q_0)+g(q_1)\big)-h\big(\widehat c_i-\frac{1}{2}\big)\nabla_q g(q_0)^T\nabla_p H(p_0,q_0). \qquad (3.7)$$

Examples of symmetric methods are the Rattle algorithm (Table 1) and the Lobatto IIIA–IIIB pair.

4 Global Modified Hamiltonian

For numerical methods (3.4) with a globally defined generating function the modified Hamiltonian can be obtained from the Hamilton-Jacobi differential equation (see Benettin & Giorgilli [2], the thesis of Murua [11, p. 100], and also [3, Sect. IX.3.2]). We briefly recall this construction of the modified Hamiltonian. It consists of three steps:

First Step. We consider a formal modified Hamiltonian

$$\widetilde H(p,q)=H_1(p,q)+h\,H_2(p,q)+h^2H_3(p,q)+\dots \qquad (4.1)$$

and use the fact that the exact solution $(P,Q)=\widetilde\varphi_t(p_0,q_0)$ of the Hamiltonian system with $\widetilde H(p,q)$ is formally given by

$$p_0=P+\nabla_q\widetilde S(P,q_0,t),\qquad Q=q_0+\nabla_p\widetilde S(P,q_0,t),$$

where $\widetilde S(p,q,t)$ is the solution of the Hamilton-Jacobi differential equation

$$\frac{\partial\widetilde S}{\partial t}(p,q,t) \;=\; \widetilde H\big(p,q+\nabla_p\widetilde S(p,q,t)\big),\qquad \widetilde S(p,q,0)=0 \qquad (4.2)$$

We express $\widetilde S(p,q,t)$ as a series (observe that $\widetilde H$ and hence $\widetilde S$ depend on h)

$$\widetilde S(p,q,t) \;=\; t\,\widetilde S_1(p,q,h)+t^2\widetilde S_2(p,q,h)+t^3\widetilde S_3(p,q,h)+\dots\;,$$

insert it into (4.2), expand $\widetilde H(p,q+\dots)$ into a Taylor series, and compare like powers of t. This yields recurrence relations for $\widetilde S_j(p,q,h)$ expressed in terms of derivatives of $\widetilde{H}$: for example, we obtain $\widetilde{S}_1(p,q,h) = \widetilde{H}(p,q)$ and $2\,\widetilde{S}_2(p,q,h) = \big(\nabla_q \widetilde{H}^T \nabla_p \widetilde{S}_1\big)(p,q,h)$, etc.

Second Step. We write $\widetilde{S}_j$ as a formal series

$$\widetilde{S}_j(p,q,h) = \widetilde{S}_{j1}(p,q) + h\,\widetilde{S}_{j2}(p,q) + h^2\widetilde{S}_{j3}(p,q) + \ldots\ ,$$

insert it and the expansion (4.1) for $\widetilde{H}$ into the relations obtained in the first step, and compare like powers of h. This yields $\widetilde{S}_{1k}(p,q) = H_k(p,q)$, $2\widetilde{S}_{2k} = \sum_{l=1}^{k-1} \nabla_q H_l^T \nabla_p H_{k-l}$, and also for $j \geq 3$ the function $\widetilde{S}_{jk}(p,q)$ is expressed in terms of derivatives of H_l with $l < k$.

Third Step. To obtain the modified Hamiltonian for our extended method (3.4) we require that the generating function (3.6) is equal to $\widetilde{S}(p,q,h)$. This gives $S_1(p,q) = \widetilde{S}_{11}(p,q)$, $S_2(p,q) = \widetilde{S}_{12}(p,q) + \widetilde{S}_{21}(p,q)$, etc., and hence

$$\begin{aligned}
S_1 &= H_1 \\
S_2 &= H_2 + \frac{1}{2}\nabla_q H_1^T \nabla_p H_1 \\
S_3 &= H_3 + \frac{1}{2}\nabla_q H_1^T \nabla_p H_2 + \frac{1}{2}\nabla_q H_2^T \nabla_p H_1 \\
&+ \frac{1}{6}\nabla_q H_1^T \nabla_p \big(\nabla_q H_1^T \nabla_p H_1\big) + \frac{1}{3}\nabla_p H_1^T \nabla_q^2 H_1 \nabla_p H_1
\end{aligned} \tag{4.3}$$

so that $S_j(p,q)$ is seen to be equal to $H_j(p,q)$ plus terms containing derivatives of $H_k(p,q)$ with $k < j$. For a given generating function (3.6), this recurrence relation allows us to determine successively the $H_j(p,q)$. We see from these explicit formulas that the functions H_j are defined on the same domain as the S_j.

Properties of the Modified Hamiltonian. We consider a consistent partitioned Runge-Kutta method satisfying the assumptions of Theorem 2.4. The modified Hamiltonian (4.1) constructed above has the following properties:

(a) The Hamiltonian system

$$\dot{p} = -\nabla_q \widetilde{H}(p,q), \qquad \dot{q} = \nabla_p \widetilde{H}(p,q), \tag{4.4}$$

where $\widetilde{H}$ is an arbitrary truncation of the series (4.1), defines a differential equation on the manifold $\mathcal{M}$, i.e., for all $k \geq 1$ the vector $\big(-\nabla_q H_k(p,q), \nabla_p H_k(p,q)\big)$ lies in the tangent space of $\mathcal{M}$ at (p,q). This is seen by induction on the truncation index (starting with the zero-vector field), because the numerical method (3.4) has $\mathcal{M}$ as invariant manifold (cf. [3, Sect. IX.5]).

(b) As a consequence of property (a), all functions $H_k(p,q)$ satisfy

$$\nabla_q g(q)^T \nabla_p H_k(p,q) = 0 \qquad \text{for} \quad (p,q) \in \mathcal{M} \tag{4.5}$$

(c) On the manifold $\mathcal{M}$ the differential equation (4.4) is equivalent to

$$\begin{aligned} \dot p &= -\nabla_q \widetilde H(p,q) - \nabla_q g(q)\lambda \\ \dot q &= \nabla_p \widetilde H(p,q), \qquad 0 = g(q) \end{aligned} \tag{4.6}$$

with a function λ that vanishes identically.

(d) In the formulation (4.6), terms of the form

$$g(q)^T \mu(p,q)$$

can be removed from the functions H_k without changing the problem on $\mathcal{M}$. This makes the function λ non-zero. After this modification the function $H_1(p,q)$ can be assumed to be equal to the original Hamiltonian $H(p,q)$ of (2.1).

These properties altogether complete the proof of Theorem 2.4. We should mention that due to the arbitrariness in choosing the extension of the method to an open neighbourhood of the manifold $\mathcal{M}$, the functions $H_k(p,q)$ in (4.1) are not unique. However, their restriction to the manifold $\mathcal{M}$ is unique up to an additive constant (this is a consequence of the uniqueness of the modified differential equation).

5 Numerical Illustration

Let us consider the movement of a rigid body with a fixed point chosen at the origin. We express a point of the body by $a \in \mathbb{R}^3$ in the coordinate system connected to the body, and by $Q(t)a$ in a stationary coordinate system. The matrix $Q(t)$ is orthogonal and describes the movement of the body. This means that the configuration manifold is the three-dimensional rotation group $SO(3)$. If we denote by I_1, I_2, I_3 the moments of inertia of the body, its kinetic energy is

$$T = \tfrac{1}{2}\big(I_1\Omega_1^2 + I_2\Omega_2^2 + I_3\Omega_3^2\big),$$

where the angular velocity in the body $\Omega = (\Omega_1, \Omega_2, \Omega_3)^T$ is defined by

$$\widehat\Omega = \begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{pmatrix} = Q^T\dot Q,$$

(see [1, Chap. 6]). Expressed in terms of $\widehat\Omega$ or Q, the kinetic energy on the manifold $\{Q \mid Q^TQ = I\}$ becomes

$$T = \tfrac{1}{2}\,\mathrm{trace}\,(\widehat\Omega D \widehat\Omega^T) = \tfrac{1}{2}\,\mathrm{trace}\,(Q^T\dot Q D \dot Q^T Q) = \tfrac{1}{2}\,\mathrm{trace}\,(\dot Q D \dot Q^T),$$

where $D = \operatorname{diag}(d_1, d_2, d_3)$ is given by the relations $I_1 = d_2 + d_3$, $I_2 = d_3 + d_1$, and $I_3 = d_1 + d_2$. Introducing conjugate variables $P = \partial T / \partial \dot{Q} = \dot{Q} D$, we are thus concerned with

$$H(P, Q) = \frac{1}{2} \operatorname{trace}(P D^{-1} P^T) + V(Q),$$

and the constrained Hamiltonian system becomes

$$\begin{aligned} \dot{P} &= -\nabla_Q V(Q) - Q \Lambda \\ \dot{Q} &= P D^{-1}, \qquad 0 = Q^T Q - I, \end{aligned} \tag{5.1}$$

where Λ is a symmetric matrix consisting of Lagrange multipliers. This is of the form (2.1) and satisfies the regularity condition (2.4).

Every partitioned Runge-Kutta method satisfying the assumptions of Section 2 can be applied. E.g., the Rattle algorithm of Example 2.1 yields

$$\begin{aligned} P_{1/2} &= P_0 - \frac{h}{2} \nabla_Q V(Q_0) - \frac{h}{2} Q_0 \Lambda_1 \\ Q_1 &= Q_0 + h P_{1/2} D^{-1}, \qquad Q_1^T Q_1 = I \\ P_1 &= P_{1/2} - \frac{h}{2} \nabla_Q V(Q_1) - \frac{h}{2} Q_1 \Lambda_2, \quad D^{-1} P_1^T Q_1 + Q_1^T P_1 D^{-1} = 0, \end{aligned} \tag{5.2}$$

where both, Λ_1 and Λ_2, are symmetric matrices. For consistent initial values, Q_0 is orthogonal and $Q_0^T P_0 D^{-1} = \widehat{\Omega}_0$ is skew-symmetric. Working with

$$\widehat{\Omega}_0 = Q_0^T \dot{Q}_0 = Q_0^T P_0 D^{-1}, \quad \widehat{\Omega}_{1/2} = Q_0^T P_{1/2} D^{-1}, \quad \widehat{\Omega}_1 = Q_1^T P_1 D^{-1}$$

instead of P_0, $P_{1/2}$, P_1, the equations (5.2) become the following integrator $(Q_0, \widehat{\Omega}_0) \mapsto (Q_1, \widehat{\Omega}_1)$:

(i) find an orthogonal matrix $I + h\widehat{\Omega}_{1/2}$ such that

$$\widehat{\Omega}_{1/2} = \widehat{\Omega}_0 - \frac{h}{2} Q_0^T \nabla_Q V(Q_0) D^{-1} - \frac{h}{2} \Lambda_1 D^{-1}$$

holds with a symmetric matrix Λ_1;

(ii) compute $Q_1 = Q_0 (I + h\widehat{\Omega}_{1/2})$;

(iii) compute a skew-symmetric matrix $\widehat{\Omega}_1$ such that

$$\widehat{\Omega}_1 = \widehat{\Omega}_{1/2} - \frac{h}{2} Q_1^T \nabla_Q V(Q_1) D^{-1} - (\widehat{\Omega}_{1/2} + \widehat{\Omega}_{1/2}^T) - \frac{h}{2} \Lambda_2 D^{-1}$$

holds with a symmetric matrix Λ_2.

This algorithm for the simulation of the heavy top is proposed in [10]. A variant, based on the first order method of Table 2, is considered in [12].

We emphasize that the above algorithm can be implemented efficiently with the use of quaternions, sometimes called Euler parameters (see [8, page

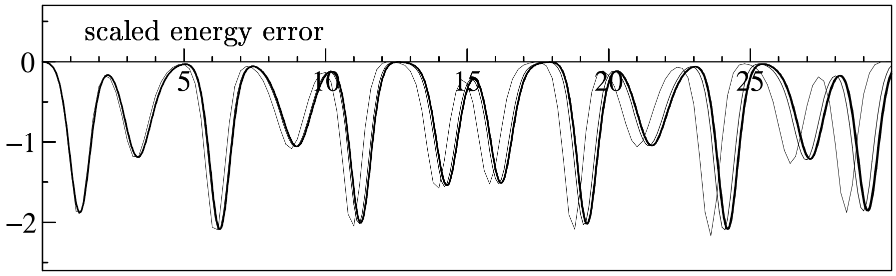

Figure 1: Scaled energy error $\big(H(p_n,q_n)-H(p_0,q_0)\big)/h^2$ as a function of the time t_n for step sizes $h = 0.2, 0.1, 0.05, 0.025$; smaller step sizes correspond to thicker lines.

76] for an introduction to quaternions, and Sections 9.3 and 11.3 of [5] for the use of Euler parameters in numerical simulations). In fact, every orthogonal matrix can be written as

$$Q = I + 2e_0\,\widehat{e} + 2\,\widehat{e}^2, \qquad \widehat{e} = \begin{pmatrix} 0 & -e_3 & e_2 \\ e_3 & 0 & -e_1 \\ -e_2 & e_1 & 0 \end{pmatrix},$$

where $e_0^2+e_1^2+e_2^2+e_3^2 = 1$. The parameters e_0, e_1, e_2, e_3 are the coordinates of a quaternion. In the above algorithm we represent the orthogonal matrices Q_0, Q_1 and $I + h\widehat{\Omega}_{1/2}$ by quaternions. This reduces the dimension of the system, simplifies the nonlinear system in step (i) of the algorithm, and due to the simple product formula of quaternions gives an efficient program. A Fortran version is available from the author.

For our numerical experiment we let $V = q_{33} = e_0^2 - e_1^2 - e_2^2 + e_3^2$ be the potential energy due to gravity, so that the above equations describe the movement of a top. We let $I_1 = 0.5$, $I_2 = 0.9$, $I_3 = 1$, and we consider initial values $e(0) = (0.4, 0.2, 0.4, 0.8)^T$, and $\Omega(0) = (0.2, 1.0, 0.4)^T$. We apply the above algorithm, and we plot in Fig. 1 the scaled error in the Hamiltonian $\big(H(p_n,q_n) - H(p_0,q_0)\big)/h^2$ as a function of the time t_n. We observe that this scaled error behaves like $H_3\big(p(t_n), q(t_n)\big) + \mathcal{O}(h^2)$, which is in agreement with (2.13) and with the fact that symmetric methods have an expansion in even powers of h. Computations on longer time intervals confirm that not only $H(p,q)$ but also $H_3(p,q)$ remains bounded along the numerical solution.

Remark 5.1 There exist several numerical approaches to the solution of the equations of motion for the heavy top. Let us just mention the widely used splitting method as described in [15], or Lie-group methods as studied in [6]. Limited numerical tests indicate that the above algorithm is comparable to the most efficient integrators among them.

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