Symplectic Integrators for Systems of Rigid Bodies

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March 23, 1995

Abstract

Recent work reported in the literature suggest that for the long-term integration of Hamiltonian dynamical systems one should use methods that preserve the symplectic structure of the flow. This has especially been shown for the numerical treatment of conservative many-particle systems as they arise, e.g., in molecular dynamics and astronomy. In this paper we use recent results by McLachlan [10] and Reich [13] on the symplectic integration of Lie-Poisson systems to derive an explicit symplectic integrator for rigid bodies moving under the influence of external forces. In case that rigid bodies are interconnected by joints, the resulting holonomic constraints can be treated in the same way as described by Reich [12] for general Hamiltonian systems with holonomic constraints.

Keywords: Hamiltonian systems, symplectic discretization, multibody systems

AMS(MOS) Subject Classifications: 65L05, 70-08, 70F20

1 Introduction

Much recent research has gone into developing numerical discretization schemes that inherit the symplectic structure of a Hamiltonian vector field. It has been observed that symplectic methods with fixed step-size possess better long-term stability properties than non-symplectic methods or symplectic methods with varying step-size. It has also been shown that these methods often preserve the Hamiltonian to high accuracy over long periods of time.

So far most applications of symplectic schemes are related to many-particle systems; i.e., systems of bodies moving under the influence of conservative forces such that the bodies can be modeled as point particles. Such problems arise, e.g., in astronomy and molecular dynamics.

Only a few results are available for conservative rigid body systems. In [5], Ge and Marsden derived integrators that preserve the natural Lie-Poisson structure on the duals of Lie algebras. Based on this, an implicit algorithm for the Euler equation of rigid body dynamics was given. More recently, McLachlan and Scovel [11] and Reich [14] showed that Lie-Poisson integrators can also be obtained from the symplectic integration of Hamiltonian systems with holonomic constraints. Using this result, symplectic integrators were obtained, e.g., for the free rigid body and the heavy top. An altogether different approach has been taken by Barth and Leimkuhler in [3]. They replace a given rigid body by a system of point particles whose mutual distances are kept constant.

This so called particulation of a rigid body reduces the symplectic integration of a multi-body system to the symplectic integration of a constrained many-particle system which, e.g., can be done by means of the RATTLE variant of the Verlet scheme [1]. This approach allows very easily to include various types of joints and is not restricted to special classes of rigid bodies. It has the disadvantage that additional constraints and variables have to be introduced. In addition to this, the particulation of a rigid body is not unique and an optimal choice seems to depend on the particular problem to be solved. Still another approach to the symplectic integration of rigid bodies is provided by the use of Euler angles [9]. This approach, however, has the disadvantage that the resulting Hamiltonian function is not separable and that, therefore, the symplectic integration of the corresponding equations of motion requires implicit methods such as the Gauss Runge-Kutta methods [6]. It is also not obvious how to include joints such that the schemes remain symplectic and preserve the resulting constraints.

In this paper we follow the idea of Barth and Leimkuhler to derive a symplectic integrator for general multi-body systems. However our starting point is a different one: It is well-known that the motion of a rigid body is characterized by the superposition of a translation and a rotation and that the differential equations describing the translation of the center of mass and the rotation about the center of mass are Hamiltonian. Based on this Hamiltonian formulation, we derive an explicit symplectic scheme for rigid bodies moving under the influence of external conservative forces. The interconnection of several rigid bodies by joints can then be handled as described by Barth and Leimkuhler [3]; i.e., we model joints by linear or quadratic holonomic constraints and solve the corresponding constrained equations of motion by a proper modification of the unconstrained scheme as described by Reich [12] for general Hamiltonian systems with holonomic constraints.

2 Equations of Motion for a Single Rigid Body

In this section we give the Hamiltonian formulation for the equations of motion for a single rigid body moving in R^3 under the influence of an external force. This result naturally extends to unconstrained systems of rigid bodies moving in an external force field.

Consider a rigid body free to move in R^3. A reference configuration $\mathfrak{B}$ of the body is the closure of an open set in R^3. Points in $\mathfrak{B}$, denoted by $X \in \mathfrak{B}$, are called material points. A configuration of $\mathfrak{B}$ is a mapping $\phi : \mathfrak{B} \to R^3$ which is smooth, orientation preserving, and invertible on its image. The points of the target space R^3 of ϕ are called spatial points and denoted by $x \in R^3$. A motion of $\mathfrak{B}$ is a time dependent family of configurations, written $x(t) = \phi(X,t) = \phi_t(X)$. Rigidity of the body means that the distance between points of the body are fixed as the body moves. Let us assume that the center of mass of $\mathfrak{B}$ is at the origin and let us denote the motion of the center of mass by $q(t) = \phi_t(0)$. Then any motion of $\mathfrak{B}$ is the superposition of $q(t)$ and a rotation about the center of mass; i.e.

$$x(t) = Q(t)X + q(t) \tag{1}$$

where $Q(t) \in SO(3)$.

Let $m \in R^+$ be the total mass of the rigid body and $M \in R^{3\times 3}$ the inertial tensor which, for simplicity, we assume to be diagonal. Furthermore, let a conservative force

$$F(x_o(t)) = \nabla V(x_o(t)) \tag{2}$$

$V : R^3 \to R$, act on the rigid body where

$$x_o(t) = Q(t)X_o + q(t)$$

and $X_o \in \mathfrak{B}$ is a fixed point in $\mathfrak{B}$. Upon introducing canonical momenta $p = m\dot{q}$ and $P = \dot{Q}J$ where the diagonal matrix $J \in R^{3\times 3}$ is defined by

$$M_{ii}^{-1} = \frac{1}{2}\sum_{i\neq j} J_{jj}^{-1},$$

the motion of the rigid body in R^3 is Hamiltonian with the Hamiltonian function

$$H_c(q,p,Q,P) = \tfrac{1}{2}(p^t m^{-1} p) + \tfrac{1}{2}\mathrm{tr}(PJ^{-1}P^t) + V(q,Q) + \tfrac{1}{2}\mathrm{tr}\left(\{Q^tQ - I\}\Lambda\right) \tag{3}$$

where tr denotes the trace operator and $\Lambda \in R^{3\times 3}$ is a symmetric matrix implicitly determined by the holonomic constraint $Q \in SO(3)$, i.e.

$$0 \quad = \quad Q^tQ - I\,. \tag{4}$$

[9],[11]. Thus the motion for the center of mass is simply given by

$$\begin{aligned} \dot{q} &= m^{-1}p \\ \dot{p} &= -\nabla_q V(q,Q) \end{aligned} \tag{5}$$

where $V(q,Q)$ is defined by

$$V(q,Q) \quad = \quad V(QX_o + q)\,.$$

and the corresponding equations of motion for the variable Q are

$$\begin{aligned} \dot{Q} &= PJ^{-1} \\ \dot{P} &= -\nabla_Q V(q,Q) - Q\Lambda \\ 0 &= Q^tQ - I \end{aligned} \tag{6}$$

which define a Hamiltonian vector field on the phase space

$$\mathcal{M} \quad = \quad \{(Q,P) : Q^tQ - I = 0,\, Q^tPJ^{-1} + J^{-1}P^tQ = 0\,\}$$

Note that $\nabla_q V(q,Q) = F(q,Q)$ and $\nabla_Q V(q,Q) = F(q,Q)X_o^t$.

Now $\mathcal{M} \neq T^*SO(3)$ in general. However, as shown by McLachlan and Scovel [11], the motion on $T^*SO(3)$ can be obtained from the motion on $\mathcal{M}$ by putting $\tilde{Q} = Q$ and $\tilde{P} = \mathrm{Pr}(Q)P$ where $\mathrm{Pr}(Q)$ is the orthogonal projector onto $T_Q^*SO(3) \subset R^{3\times 3}$.

To make the equations (6) more transparent, let us rewrite them on $SO(3)\times \mathfrak{so}(3)^*$. Here $\mathfrak{so}(3)^*$ denotes the dual of the Lie algebra of skew-symmetric matrices [16]. This transformation can be achieved by introducing the body angular momentum $\Pi = Q^tP \in \mathfrak{so}(3)^*$ [9]. Using the standard isomorphism between R^3 and $\mathfrak{so}(3)^*$ denoted by skew : $R^3 \to \mathfrak{so}(3)^*$, we identify $\Pi \in \mathfrak{so}(3)^*$ with $\pi \in R^3$, $\{Q^tF(q,Q)X_o^t - X_oF(q,Q)^tQ\}/2$ with $Q^tF(q,Q)\times X_o$, and $\{J^{-1}\Pi + \Pi J^{-1}\}/2$ with $M^{-1}\pi$ where M is the inertial tensor. Then we obtain the equations

$$\dot{\pi} \quad = \quad \pi \times M^{-1}\pi - \{Q^tF(q,Q)\}\times X_o \tag{7}$$

and

$$\dot{Q} \quad = \quad Q\,\mathrm{skew}\,(M^{-1}\pi) \tag{8}$$

Note that for $F = 0$, (7) becomes the standard Euler equation for the free rigid body [9].

In the following section we will discuss numerical methods for the symplectic integration of the constrained Hamiltonian system corresponding to (3)-(4).

3 Symplectic Integration of a Single Rigid Body

A Hamiltonian system on $R^n \times R^n$ with holonomic constraints of the form $g(q) = 0$, where $g : R^n \to R^m$ is a smooth map with full rank Jacobian in the neighborhood of its zero-set $g^{-1}(0)$, is characterized by the equations

$$\begin{aligned} \dot{q} &= \nabla_p H(q,p) \\ \dot{p} &= -\nabla_q H(q,p) - G(q)^t \lambda \\ 0 &= g(q) \end{aligned} \tag{9}$$

where $H : R^n \times R^n \to R$ is the Hamiltonian of the unconstrained system, $G(q) = g_q(q)$, and

$$H_c = H + \lambda^t g$$

the Hamiltonian of the constrained system. The solutions of (9) define a symplectic flow [2] on the constraint manifold

$$\mathcal{M} = \{(q,p) :\, g(q) = 0,\, G(q)\nabla_p H(q,p) = 0\}$$

Recently it has been shown by Jay [7] and Reich [12] that for arbitrary Hamiltonian functions H there exist discretizations of (9) which preserve the constraint manifold $\mathcal{M}$ and are symplectic. Even more recently, McLachlan and Scovel [11] extended this result to the symplectic integration of the corresponding constrained system on the cotangent manifold

$$T^*\mathcal{N} = \{\,(q,p) :\, g(q) = 0,\, G(q)p = 0\,\}$$

In case that the Hamiltonian H is separable, i.e. of the form

$$H(q,p) = T(p) + V(q)\,,$$

we can, e.g., use the scheme RATTLE [1] which is a generalization of the Verlet scheme for unconstrained systems. It was shown to be symplectic and constraint-preserving by Leimkuhler and Skeel [8].

Since the Hamiltonian (3) is separable, the RATTLE discretization can be directly applied to the symplectic integration of the corresponding constrained Hamiltonian system. To see this, we have to use the correspondences $q \mapsto (q,Q)$ and $p \mapsto (p,P)$ and the constraint function g is given by (4). Thus we obtain the following

Algorithm 3.1 *Step 1.*

$$\begin{aligned} q_{n+1} &= q_n + hm^{-1}p_{n+1/2} \\ p_{n+1/2} &= p_n - (h/2)F(q_n,Q_n) \end{aligned}$$

Step 2.

$$\begin{aligned} Q_{n+1} &= Q_n + hP_{n+1/2}J^{-1} \\ P_{n+1/2} &= P_n - (h/2)\,\{F(q_n,Q_n)X_o^t + Q_n\Lambda_n\} \\ 0 &= Q_{n+1}^t Q_{n+1} - I \end{aligned}$$

Step 3.

$$\begin{aligned} P_{n+1} &= P_{n+1/2} - (h/2)\left\{F(q_{n+1},Q_{n+1})X_o^t + Q_{n+1}\mu_{n+1}\right\} \\ 0 &= Q_{n+1}^t P_{n+1} + P_{n+1}^t Q_{n+1} \end{aligned}$$

Step 4.

$$p_{n+1} = p_{n+1/2} - (h/2)F(q_{n+1},Q_{n+1})$$

where $F(q,Q) = \nabla V(q + QX_o)$*.*

Step 2 requires the solution of a nonlinear system of equations in 6 variables (since Λ is assumed to be symmetric). This can be avoided by applying recent results by McLachlan [10] and Reich [13] on the explicit symplectic integration of the Euler equations on the $so(3)^*$. Specifically:

Step 2 and 3 represent a second order symplectic integrator for the Hamiltonian

$$H_r(Q,P) = \frac{1}{2}\mathrm{tr}\,(PJ^{-1}P^t) + V(q,Q) + \frac{1}{2}\mathrm{tr}\,(\{Q^tQ - I\}\Lambda)$$

where q is treated as a parameter. Upon rewriting H_r as

$$H_r(Q,P) = H_e(Q,P,\Lambda) + V(q,Q) \tag{10}$$

with

$$H_e(Q,P,\Lambda) = \frac{1}{2}\mathrm{tr}\,(PJ^{-1}P^t) + \frac{1}{2}\mathrm{tr}\,(\{Q^tQ - I\}\Lambda)$$

we see that H_e is the Hamiltonian of a free rigid body fixed at the origin and the potential V corresponds to an external force acting on the body. Using the notation introduced in Section 2, the equations of motion of a free rigid body in terms of the body angular momentum are

$$\dot{\pi} = \pi \times M^{-1}\pi \tag{11}$$

where the Hamiltonian is now the kinetic energy of the body; i.e.

$$T(\pi) = \frac{1}{2}\pi^t M^{-1}\pi$$

As pointed out by McLachlan [10] and Reich [13], (11) can be integrated numerically by rewriting (11) as the sum of three Euler equations $\dot{\pi} = \pi \times \nabla T_i(\pi)$ where $T_i(\pi) = \frac{1}{2}\pi_i^2 M_{ii}^{-1}$. For each of these equations we have $\pi_i = const.$ and therefore each equation can be solved exactly. The solutions, denoted by $\exp\,(tD_{T_i})\,\pi$, are rotations about the π_i-axis with constant angular velocity $\pi_i M_{ii}^{-1}$. For example, for $i = 1$, we have to solve the system of linear differential equations

$$\begin{aligned} \dot{\pi}_1 &= 0 \\ \dot{\pi}_2 &= +\pi_1 M_{11}^{-1}\,\pi_3 \\ \dot{\pi}_3 &= -\pi_1 M_{11}^{-1}\,\pi_2 \end{aligned}$$

By applying the Baker-Campbell-Hausdorff formula [16], one can show that the scheme

$$\pi_{n+1} \;=\; A_h(\pi_n)\,\pi_n$$

with

$$A_h(\pi) \;=\; \exp\big(\frac{h}{2}D_{T_1}\big)\circ\exp\big(\frac{h}{2}D_{T_2}\big)\circ\exp\big(hD_{T_3}\big)\circ\exp\big(\frac{h}{2}D_{T_2}\big)\circ\exp\big(\frac{h}{2}D_{T_1}\big)$$

is of second order in the step-size h and naturally preserves the Lie-Poisson structure of the Euler equation [9]. Let us now return to the symplectic integration of the corresponding Hamiltonian system on $T^*SO(3)$. We make use of the same splitting of the kinetic energy $T(\pi)$. But now we have to solve for each $T_i(\pi)$ the system of linear differential equations

$$\begin{aligned}\dot\pi &= \pi\times\nabla T_i(\pi)\\ \dot Q &= Q\,\mathrm{skew}\,(\nabla T_i(\pi))\end{aligned}$$

Composing the single steps as done above for the Euler equation, we finally obtain the second-order symplectic scheme

$$\begin{aligned}Q_{n+1} &= Q_n\,B_h(\pi_n)\\ \pi_{n+1} &= A_h(\pi)\,\pi_n\end{aligned}\tag{12}$$

with A_h as above and B_h properly defined.

The motion due to the potential V in (10) is given by the differential equation

$$\begin{aligned}\dot\pi &= -\{Q^tF(q,Q)\}\times X_o\\ \dot Q &= 0\end{aligned}\tag{13}$$

This differential equation can be solved exactly and Step 2 and 3 in Algorithm 3.1 can now be replaced by a proper composition of (12) and the exact time-h-flow of the differential equation (13). Thus we obtain the following explicit

Algorithm 3.2 *Step 1.*

$$\begin{aligned}q_{n+1} &= q_n + hm^{-1}p_{n+1/2}\\ p_{n+1/2} &= p_n - (h/2)F(q_n,Q_n)\end{aligned}$$

Step 2.

$$\bar\pi_n \;=\; \pi_n - (h/2)\{Q_n^tF(q_n,Q_n)\}\times X_o$$

$$\begin{aligned}Q_{n+1} &= Q_nB_h(\bar\pi_n)\\ \bar\pi_{n+1} &= A_h(\bar\pi_n)\,\bar\pi_n\end{aligned}$$

$$\pi_{n+1} \;=\; \bar\pi_{n+1} - (h/2)\{Q_{n+1}^tF(q_{n+1},Q_{n+1})\}\times X_o$$

Step 3.

$$p_{n+1} \;=\; p_{n+1/2} - (h/2)F(q_{n+1},Q_{n+1})$$

If necessary, P_{n+1} can be computed from Q_{n+1} and π_{n+1} by means of

$$P_{n+1} \;\; = \;\; Q_{n+1}\Pi_{n+1}$$

where, using the standard isomorphism between R^3 and $\mathfrak{so}(3)^*$, we transform $\pi_{n+1} \in R^3$ back into $\Pi_{n+1} \in \mathfrak{so}(3)^*$. Let us denote the resulting scheme by

$$\begin{pmatrix} q_{n+1} \\ Q_{n+1} \\ p_{n+1} \\ P_{n+1} \end{pmatrix} \;\; = \;\; \Psi_h \begin{pmatrix} q_n \\ Q_n \\ p_n \\ P_n \end{pmatrix} \qquad (14)$$

Note that this scheme is now explicit in Q and P. The scheme is of second order. This can be seen from the time reversibility of the scheme. Furthermore, by construction, the scheme is symplectic and preserves the constraint $Q \in SO(3)$.

4 Equations of Motion for Constrained Systems of Rigid Bodies

So far we have considered the motion of unconstrained rigid bodies under the influence of external forces. In this and the following section we generalize this to the situation that rigid bodies are interconnected by joints.

There are two classes of joints; those that do not allow for a relative translation and those that do not allow for a relative rotation. The first type of joints is obtained whenever two bodies are joined at a single location. If no further constraints are imposed, the resulting joint is called a free or spherical joint. Other types of joints include the universal, revolve, prismatic etc. joint [3]. In this paper we only consider the simplest form of a joint; the spherical joint. As discussed by Barth and Leimkuhler in [3], any other, more complicated joint can be treated in a similar fashion.

Let us consider two rigid bodies with Hamiltonian H_i, $i = 1, 2$, with, for simplicity of exposition, no external forces acting on them; i.e., the Hamiltonian functions H_i are of the form

$$H_i(q_i, p_i, Q_i, P_i) \;\; = \;\; \frac{1}{2}\mathrm{tr}\,(P_i J_i^{-1} P_i^t) + \frac{1}{2} p_i^t m_i^{-1} p_i + \frac{1}{2}\mathrm{tr}\,(\{Q_i^t Q_i - I\}\Lambda_i)$$

together with the constraint

$$0 \;\; = \;\; Q_i^t Q_i - I$$

Let us assume that these two rigid bodies are linked by a spherical joint. The position of the joint relative to the reference configurations $\mathfrak{B}_i$ shall be given by the vectors $X_i \in \mathfrak{B}_i$. Thus we obtain the linear holonomic constraint

$$0 \;\; = \;\; Q_1 X_1 + q_1 - Q_2 X_2 - q_2 \qquad (15)$$

and the corresponding constraint function is

$$g(q_1, q_2, Q_1, Q_2) \;\; := \;\; Q_1 X_1 + q_1 - Q_2 X_2 - q_2$$

As for constrained many-particle systems, the modified Hamiltonian, describing the motion of the two interconnected rigid bodies, is then given by

$$H_c \;\; = \;\; H_1 + H_2 + \lambda^t g$$

where $\lambda \in R^3$. Following (9) and applying the correspondences $q \mapsto (q_1, q_2, Q_1, Q_2)$, $p \mapsto (p_1, p_2, P_1, P_2)$, and $H \mapsto H_1 + H_2$, the resulting equations of motion are

$$\begin{array}{rcll} \dot{q}_i &=& m_i^{-1} p_i & \\ \dot{p}_i &=& (-1)^i \lambda & \\ \dot{Q}_i &=& P_i J_i^{-1} & i = 1,2 \\ \dot{P}_i &=& -Q_i \Lambda_i + (-1)^i \lambda X_i^t & \\ 0 &=& Q_i^t Q_i - I & \\ & & & \\ 0 &=& Q_1 X_1 + q_1 - Q_2 X_2 - q_2 & \end{array} \tag{16}$$

The Lagrange multiplier λ can be obtained by differentiating the constraint (15) twice with respect to time. This yields the equation

$$\Big(\sum_i X_i^t J_i^{-1} X_i + m_i^{-1}\Big)\, \lambda \;=\; -Q_1 \Lambda_1 J_1^{-1} X_1 + Q_2 \Lambda_2 J_2^{-1} X_2$$

which, since $(\sum_i X_i^t J_i^{-1} X_i + m_i^{-1}) > 0$, can be solved for $\lambda \in R^3$.

For more complicated joints we will, in general, obtain quadratic holonomic constraints $g = 0$ in the variables q_i and Q_i [3]. These can be treated in the same way as described above for the constraint (15).

5 Symplectic Integration of Constrained Systems of Rigid Bodies

Let Ψ_h be a first or second order symplectic integrator for the unconstrained system

$$\begin{array}{rcl} \dot{q} &=& \nabla_p H(q,p) \\ \dot{p} &=& -\nabla_q H(q,p) \end{array}$$

In [12], Reich showed that this symplectic integrator can be modified such that the resulting scheme provides a symplectic integrator for the corresponding constrained Hamiltonian systems (9). Upon substituting for Ψ_h the symplectic integrator (14) and taking (15) as the holonomic constraint $g(q) = 0$, we can generalize this method to the symplectic integration of two rigid bodies interconnected by a spherical joint. Again we have to use the correspondences $q \mapsto (q_1, q_2, Q_1, Q_2)$ and $p \mapsto (p_1, p_2, P_1, P_2)$. This results in

Algorithm 5.1 *For $i = 1, 2$:*
Step 1.

$$\begin{array}{rcl} \bar{p}_{i,n} &=& p_{i,n} + (-1)^i (h/2) \lambda_n \\ \bar{P}_{i,n} &=& P_{i,n} + (-1)^i (h/2) \lambda_n X_i^t \end{array}$$

Step 2.

$$\begin{pmatrix} q_{i,n+1} \\ Q_{i,n+1} \\ p_{i,n+1} \\ P_{i,n+1} \end{pmatrix} = \Psi_h \begin{pmatrix} q_{i,n} \\ Q_{i,n} \\ \bar{p}_{i,n} \\ \bar{P}_{i,n} \end{pmatrix}$$

with λ_n chosen such that

$$0 = Q_{1,n+1} X_1 + q_{1,n+1} - Q_{2,n+1} X_2 - q_{2,n+1}$$

The resulting nonlinear equation for the variable λ_n can be solved by a modified Newton method. For the approximate Jacobian we can simply use $A = \sum_i X_i^t J_i^{-1} X_i + m_i^{-1}$, $A \in R^+$.

It is straightforward to generalize this algorithm to multi-body systems interconnected by joints that can be modeled by holonomic constraints of the form

$$0 \;=\; g(q_l, Q_l, q_k, Q_k)$$

Here subscript l (k) denotes the lth (kth) body.

6 Symmetries and Conservation of Momentum Maps

For symplectic algorithms preservation of momentum follows from the equivariance of the algorithm with respect to the corresponding symmetry group [4]. Now the schemes considered in Section 3 are composition methods with each sub-step equivariant to a given symmetry of the Hamiltonian (3). Thus the schemes derived in Section 3 preserve the corresponding momentum map. The same is true for systems of rigid bodies interconnected by joints whenever the Hamiltonian (3) for each rigid body and the holonomic constraints due to joints are invariant under certain symmetries.

7 Heavy Top

Consider the motion of a rigid body fixed at a stationary point subject to the action of a uniform gravitational field. In terms of the reference configuration $\mathfrak{B}$, let the body be fixed at a point $x_o = QX_o + q$, $X_o \in \mathfrak{B}$. For simplicity we take $x_o = (0,0,0)$ and $X_o = (0,0,-z)$, $z > 0$. Since the point x_o can be considered as a spherical joint of the heavy top with the ground, we obtain the holonomic constraint

$$0 \;=\; g(q,Q) \;=\; QX_o + q \tag{17}$$

Furthermore, since the gravitational force acts only on the center of mass, the potential V in (3) is given by

$$V(q,Q) \;=\; c\,k^t q$$

where $k = (0,0,1)^t$ and c is the constant of gravitation. Thus the Hamiltonian of a heavy top is given by

$$\begin{aligned} H_c(q,Q,p,P) \;=\; & \frac{1}{2}\mathrm{tr}\,(PJ^{-1}P^t) + \frac{1}{2}p^t m^{-1} p + c\,k^t q + \\ & + \frac{1}{2}\mathrm{tr}\,(\{Q^tQ - I\}\Lambda) + \lambda^t(QX_o + q) \end{aligned}$$

subject to the constraints $Q \in SO(3)$ and (17).

It is well-known [9] that, due to symmetry, these equations can be reduced to a Lie-Poisson system on $\mathfrak{se}(3)^*$. Thus, in principle, any Lie-Poisson integrator can be applied. Here we are interested in the direct symplectic integration of the unreduced equations.

Following the approach taken in this paper, we derive first an symplectic integrator for the 'free' heavy top; i.e., for the heavy top equations of motion without the constraint (17). This can be done as described in Section 3. Then the constraint is incorporated as described in Section 5 for spherical joints. Because (17) can be considered as a spherical joint of the heavy top with the ground at $x_o = (0,0,0)$, the index i takes only the value $i = 1$ which we drop for simplicity of notation. Thus the overall scheme in the variable (q, Q, p, π) becomes

$$\begin{aligned}
\bar{p}_n &= p_n - (h/2)\lambda_n \\
\bar{\pi}_n &= \pi_n - (h/2)\{Q_n^t \lambda_n\} \times X_o \\
\\
q_{n+1} &= q_n + h\, m^{-1} p_{n+1/2} \\
p_{n+1/2} &= \bar{p}_n - (h/2)\, c\, k \\
p_{n+1} &= p_{n+1/2} - (h/2)\, c\, k \\
\\
Q_{n+1} &= Q_n\, B_h(\bar{\pi}_n) \\
\pi_{n+1} &= A_h(\bar{\pi}_n)\, \bar{\pi}_n
\end{aligned}$$

subject to the constraint

$$0 = Q_{n+1} X_o + q_{n+1}$$

Note that the above scheme also preserves the third component of angular momentum corresponding to the $SO(2)$ symmetry of the heavy top about its z-axis.

Acknowledgments. We like to thank B. Leimkuhler and Ch. Lubich for valuable discussions.

References

[1] Anderson, H.C., Rattle: A 'Velocity' Version of the Shake algorithm for Molecular Dynamics Calculations, *J. Comp. Phys.*, 52(1983), 24–34.

[2] Arnold, V.I., *Mathematical Methods of Classical Mechanics*, Springer-Verlag, NY, 1975.

[3] Barth, E., Leimkuhler, B., Symplectic Methods for Conservative Multibody Systems, this volume.

[4] Ge, Z., Symplectic Difference Schemes and Generating Functions, *Physica D*, 49(1991), 376–386.

[5] Ge, Z., Marsden, J.E., Lie-Poisson Hamilton-Jacobi Theory and Lie-Poisson Integrators, *Physics Letters A*, 133(1988)3, 134–139.

[6] Hairer, E., Nørsett, S.P., Wanner, G., *Solving Ordinary Differential Equations, I*, Springer-Verlag, 1987.

[7] Jay, L., Symplectic Partitioned Runge-Kutta Methods for Constrained Hamiltonian Systems, *SIAM J. Num. Anal.*, to appear.

[8] Leimkuhler, B. and Skeel, R.D., Symplectic Numerical Integrators in Constrained Hamiltonian Systems, *J. Comp. Phys.*, 112(1994), 117–125.

[9] Marsden, J.R., Ratiu, T., *An Introduction to Mechanics and Symmetry*, Springer-Verlag, 1994.

[10] McLachlan, R.I., Explicit Lie-Poisson Integration and the Euler Equations, *Phys. Rev. Lett.*, 71(1993), 3043–3046.

[11] McLachlan, R.I., Scovel, C., Equivariant Constrained Symplectic Integration, *J. Nonlinear Science*, to appear.

[12] Reich, S., Symplectic Integration of Constrained Hamiltonian Systems by Composition Methods, *SIAM J. Numer. Anal.*, to appear.

[13] Reich, S., Numerical Integration of the Generalized Euler Equation, Techn. Report, Univ. of British Columbia, 1993.

[14] Reich, S., Momentum Conserving Symplectic Integrators, *Physica D*, 76(1994), 375–383.

[15] Sanz-Serna, J.M., Symplectic Integrators for Hamiltonian Problems: An Overview, *Acta Numerica*, 1(1992), 243–286.

[16] Varadarajan, V.S., *Lie Groups, Lie Algebras, and Their Representation*, Prentice-Hall, Englewood Cliffs, 1994.