A Note on the Numerical Solution of the Heavy Top Equations *

K. Engø (kenth.engo@ii.uib.no)
Department of Informatics, University of Bergen, Norway

A. Marthinsen (arne.marthinsen@math.ntnu.no)
Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway

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Abstract. In [Multibody System Dynamics 2, 71–88], we described the Munthe-Kaas and Crouch–Grossman methods for integrating ordinary differential equations numerically on Lie groups. We used the heavy top as a special test problem, and showed that the numerical solution respects the configuration space TSO(3). We were, however, not able to generate numerical solutions that preserved the first integrals of the top. In this paper, we formulate the heavy top equations on a more natural configuration space, and show that both the Munthe-Kaas and the Crouch–Grossman methods with suitable coefficient sets can generate numerical solutions that render first integrals to machine accuracy. As a partial answer to the comment in "Concluding Remarks" in [Multibody System Dynamics 2, 71–88], we also argue that for Hamiltonian systems on the dual space of a Lie algebra, the infinitesimal generator map describing the differential equation for the coadjoint action is the functional derivative of the Hamiltonian.

Keywords: geometric integration, numerical integration of ordinary differential equations on manifolds, numerical analysis, Lie groups, Lie algebras, heavy top, Lagrangian top

AMS Subject Classification: 65L06, 34A50

1. Introduction

In [5], we described two approaches for numerical integration of ordinary differential equations on Lie groups. The methods, named Munthe-Kaas [10] and Crouch–Grossman [2] methods, are constructed so that they generate numerical solutions that respect the Lie group on which the exact solution evolves. This means, e.g., that if the problem has a solution that evolves on $\mathrm{SO}(n)$, the Lie group of orthogonal matrices with unit determinant, the numerical approximation will also consist of matrices in $\mathrm{SO}(n)$. Taking steps of size h, the methods approximate

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the true solution to a certain order p, meaning that the local error after one step is $\mathcal{O}(h^{p+1})$, but the qualitative property that the true solution evolves in $\mathrm{SO}(n)$ is rendered also by the numerical approximation. Classical solvers view the Lie group as a manifold embedded in a Euclidean space. This has the implication that, even though the initial value is an orthogonal matrix, the orthogonality is instantly lost when using methods that do not preserve quadratic constraints, e.g. explicit Runge–Kutta methods.

In [5], we used the heavy top as one of the test problems. Although we showed that the configuration space $\mathrm{TSO}(3)$ was respected by the numerical solution, we were not able to produce numerical approximations that preserved the first integrals of the top. A first integral is a constant function along the true solution of the differential system. In this paper we formulate the heavy top equations on a more natural configuration space, and we show that both the Munthe-Kaas and the Crouch–Grossman methods implemented with carefully chosen coefficients generate numerical approximations that, in addition to respect the configuration space itself, also render first integrals to machine precision. Section 2 introduces some definitions and results needed in Section 3, which describes the formulation of the governing equations. Section 4 includes some results from numerical simulations, and we conclude the paper in Section 5.

2. Some Preliminaries

It is well-known, see e.g. [1], that the tangent bundle of a Lie group is, as a manifold, isomorphic to the direct product of the Lie group with its Lie algebra; e.g. $\mathrm{TSO}(3) \simeq \mathrm{SO}(3) \times \mathfrak{so}(3)$. A 'trivial' Lie group structure on this direct product can be introduced by choosing the group multiplication of $\mathrm{SO}(3)$ as operation in the first component and vector addition in the second component. This choice was made in [5]. The space $\mathrm{TSO}(3)$ is a Lie group, and is perfectly valid as a configuration space for the heavy top. The numerical solutions respect the configuration space, but it seems that $\mathrm{SO}(3) \times \mathfrak{so}(3)$ equipped with the trivial group structure does not provide the structure necessary for the Munthe-Kaas or Crouch–Grossman methods to generate numerical solutions that render correctly the first integrals of the true solution.

There is also another way of turning $\mathrm{TSO}(3)$ into a Lie group. By using this alternative construction, one can capture more of the original geometric structure of the Lie group $\mathrm{SO}(3)$. A natural binary operation on the tangent bundle is obtained by considering the lift of the binary operation on the Lie group. We find that $\mathrm{TSO}(3)$ is isomorphic to a semidirect product of SO(3) and its Lie algebra $\mathfrak{so}(3)$. This semidirect product will take on different forms depending on whether we use left or right trivialization of the tangent bundle. In this paper, we use left trivialization of TSO(3) and we are hence working in 'body' coordinates.

Figure 1 shows a schematic picture of the relations used in deriving the natural lift of the binary operation from G = SO(3) to TG = TSO(3). We denote by L and R the left and right multiplication maps, respectively [8]. TL and TR are their tangent mappings. The binary operation on TSO(3) with respect to left trivialization of the bundle is

$$(a, v) \cdot_{\mathrm{TSO(3)}} (b, w) = \big(ab, b^{-1}vb + w\big). \tag{1}$$

We view SO(3) as a matrix Lie group, hence v and w are skew-symmetric matrices and the product $b^{-1}vb$ is obtained by ordinary matrix multiplication. The inverse of an element $(a, v) \in \mathrm{TSO(3)}$ is hence

$$(a, v)^{-1} = \big(a^{-1}, -ava^{-1}\big).$$

We write $\mathrm{TSO(3)} \simeq \mathrm{SO(3)} \rtimes \mathfrak{so}(3)$, where $\rtimes$ denotes the semidirect product structure given by (1).

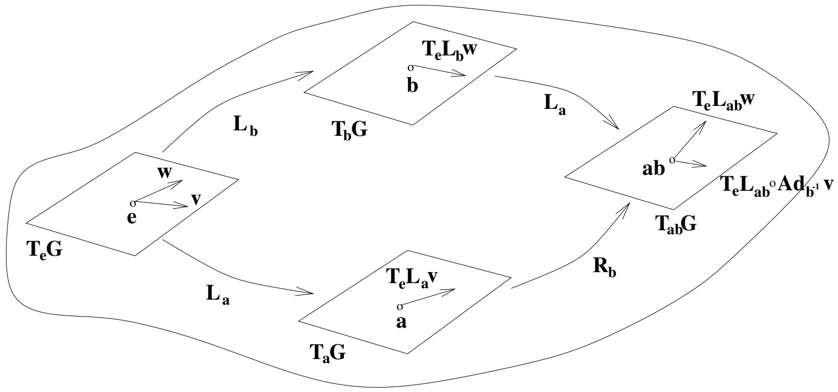

Figure 1. A schematic drawing of the relations used in deriving the natural lift of the binary operation from G to TG.

It turns out that the natural space for describing the dynamics of the heavy top is the dual space of TSO(3), denoted by $\mathrm{T^*SO(3)}$. The reason for this is that the heavy top can be described as a Hamiltonian system, and Hamiltonian differential systems are most naturally described on cotangent bundles. This cotangent bundle of SO(3) is also a Lie group, and gets a semidirect structure similar to that of TSO(3). This structure can be derived in the same manner as for TSO(3). The binary operation with respect to the left trivialization is in this case

$$(a,\alpha)\cdot_{\mathrm{T^*SO(3)}}(b,\beta)=\big(ab,\alpha+a^{-1}\beta a\big),\quad a,b\in\mathrm{SO}(3),\ \alpha,\beta\in\mathfrak{so}(3)^*.$$

The inverse of an element $(a,\alpha)\in\mathrm{T^*SO(3)}$ is

$$(a,\alpha)^{-1}=\big(a^{-1},-a\alpha a^{-1}\big).$$

Throughout the rest of this paper denote the Lie group $\mathrm{T^*SO(3)}\simeq\mathrm{SO}(3)\rtimes\mathfrak{so}(3)^*$ by G, its Lie algebra $\mathrm{T}_e(\mathrm{T^*SO(3)})\simeq\mathfrak{so}(3)\rtimes\mathfrak{so}(3)^*$ by $\mathfrak{g}$, and the dual Lie algebra $\mathrm{T}_e^*(\mathrm{T^*SO(3)})\simeq\mathfrak{so}(3)^*\rtimes\mathfrak{so}(3)$ by $\mathfrak{g}^*$.

The Lie algebra of G has also a commutator structure expressible by matrix commutators. This commutator on $\mathfrak{g}$ is given as

$$[(u,\alpha),(w,\beta)]_{\mathfrak{g}}=([u,w],[\alpha,w]-[\beta,u]).$$

The exponential map $\exp_{\mathrm{SO(3)}}:\mathfrak{so}(3)\to\mathrm{SO}(3)$ can be lifted to $\mathrm{T^*SO(3)}$ as $\exp_{\mathrm{T^*SO(3)}}:\mathfrak{g}\to G$. It is given by

$$\exp_{\mathrm{T^*SO(3)}}(u,\alpha)=(\exp_{\mathrm{SO(3)}}(u),\mathrm{dexp}_u(\alpha)),\tag{2}$$

where the operator dexp is defined as (see e.g. [9])

$$\mathrm{dexp}_u(\alpha)=\sum_{i=0}^{\infty}\frac{1}{(j+1)!}\,\mathrm{ad}_u^i(\alpha).$$

Here, ad is the matrix commutator, this since we work in a matrix Lie group. If we represent matrices in $\mathfrak{so}(3)$ or $\mathfrak{so}(3)^*$ as vectors in $\mathbb{R}^3$, the ad-operator takes the form of the cross product.

It should be noted that the exponential map $\exp_{\mathrm{SO(3)}}$ has a closed form called the Euler–Rodrigues formula. This formula can be used to derive a closed-form expression for the dexp function, hence there exists an exact closed-form expression for (2).

3. Formulation of the Governing Equations

It is well-known that the Hamiltonian equation on $\mathfrak{g}^*$ is (see e.g. [8, p. 360])

$$\frac{d\mu}{dt}=\mathrm{ad}^*_{\frac{\delta\mathrm{H}}{\delta\mu}}(\mu),\qquad \mu(0)=\mu_0,\tag{3}$$

where $\frac{\delta\mathrm{H}}{\delta\mu}$ is the functional derivative defined in [8, p. 11]. Let $\mu=(\mathbf{\Pi},\mathbf{\Gamma})\in\mathfrak{g}^*$, where $\mathbf{\Pi}\in\mathfrak{so}(3)^*$ is the angular momentum and $\mathbf{\Gamma}\in\mathfrak{so}(3)$ is the gravity vector as seen in local coordinates. We have suppressed explicit time-dependence to simplify the exposition. Since both $\mathfrak{so}(3)^*$ and $\mathfrak{so}(3)$ are isomorphic to $\mathbb{R}^3$, we represent $\mathbf{\Pi}$ and $\mathbf{\Gamma}$ as 3-vectors. The heavy top can be described as a Hamiltonian system on $\mathfrak{g}^*$, the Hamiltonian being

$$\mathrm{H}(\mathbf{\Pi},\mathbf{\Gamma}) = \frac{1}{2}\mathbf{\Pi}\cdot\mathrm{I}^{-1}\mathbf{\Pi} + Mgl\,\mathbf{\Gamma}\cdot\boldsymbol{\chi}, \tag{4}$$

where I denotes the inertia tensor and $\boldsymbol{\chi}$ is the constant unit vector along the line segment of length l connecting the fixed point (origin) and the center of gravity of the top. M is the mass of the top, and g is the gravitational constant. We refer to [8] for background and notation. The first part of the Hamiltonian H in (4) is kinetic energy and the second part is potential energy.

We now want to derive the differential equations given by (3) for the heavy top. Throughout, we will use the Lie algebra isomorphism from skew-symmetric 3×3 matrices and matrix-commutators to three-vectors and cross-products. The functional derivative of H with respect to μ is

$$\begin{aligned}\frac{\delta \mathrm{H}}{\delta \mathbf{\Pi}} &= \mathrm{I}^{-1}\mathbf{\Pi} \;=\; \mathbf{\Omega},\\ \frac{\delta \mathrm{H}}{\delta \mathbf{\Gamma}} &= Mgl\,\boldsymbol{\chi},\end{aligned} \tag{5}$$

where $\mathbf{\Omega}$ is the angular velocity of the top. By definition, $\mathrm{Ad}_g : \mathfrak{g} \to \mathfrak{g}$, $g \in G$, is given by

$$\begin{aligned}\mathrm{Ad}_{(a,\alpha)}(v,\beta) &= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} I_{(a,\alpha)}\big(\exp_{\mathrm{T}^*\mathrm{SO}(3)}(tv,t\beta)\big) && \text{(Definition)}\\ &= \big(ava^T, a^T\beta a + [v,\alpha]\big) && \text{(Matrix form)}\\ &= \big(a\vec{v}, a^T\vec{\beta} + \vec{v}\times\vec{\alpha}\big), && \text{(Vector form)}\end{aligned}$$

where $(a,\alpha) \in G,\ (v,\beta) \in \mathfrak{g}$, and I_g is the inner automorphism on G. Define the pairing $\langle\cdot,\cdot\rangle$ between $\mathfrak{g}^*$ and $\mathfrak{g}$ as $\langle(\alpha,w),(v,\beta)\rangle = \langle\alpha,v\rangle_{\mathfrak{so}} + \langle\beta,w\rangle_{\mathfrak{so}}$, where the pairing with subscript $\mathfrak{so}$ indicates the pairing between $\mathfrak{so}(3)^*$ and $\mathfrak{so}(3)$. We can now compute, for $g \in G$, the coadjoint action $\mathrm{Ad}^*_{g^{-1}} : \mathfrak{g}^* \to \mathfrak{g}^*$. It should be said that this computation is most easily done in a coordinate-free manner using operators. The result is

$$\begin{aligned}\mathrm{Ad}^*_{(a,\alpha)^{-1}}(\beta,v) &= \big(a\beta a^T - [a\alpha a^T, v], a^T v a\big) && \text{(Matrix form)}\\ &= \big(a\vec{\beta} - \vec{\alpha}\times\vec{v}, a^T\vec{v}\big), && \text{(Vector form)}\end{aligned}$$

where $(a,\alpha) \in G$ and $(\beta, v) \in \mathfrak{g}^*$. Furthermore, the infinitesimal generator of the coadjoint action is given as

$$\begin{aligned}
\mathrm{ad}^*_{(u,\alpha)}(\beta, v) &= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \mathrm{Ad}^*_{\exp_{\mathrm{T}^*\mathrm{SO}(3)}(-tu,-t\alpha)}(\beta, v) && \text{(Definition)}\\
&= \big([\beta, u] + [v, \alpha], [v, u]\big) && \text{(Matrix form)}\\
&= \big(\vec{\beta} \times \vec{u} - \vec{\alpha} \times \vec{v}, \vec{v} \times \vec{u}\big). && \text{(Vector form)}
\end{aligned}$$

Hence,

$$\mathrm{ad}^*_{(\frac{\delta \mathrm{H}}{\delta \Pi}, \frac{\delta \mathrm{H}}{\delta \Gamma})}(\mathbf{\Pi}, \mathbf{\Gamma}) = \begin{pmatrix} \mathbf{\Pi} \times \frac{\delta \mathrm{H}}{\delta \Pi} + \mathbf{\Gamma} \times \frac{\delta \mathrm{H}}{\delta \Gamma} \\ \\ \mathbf{\Gamma} \times \frac{\delta \mathrm{H}}{\delta \Pi} \end{pmatrix} = \begin{pmatrix} \mathbf{\Pi} \times \mathbf{\Omega} + Mgl\mathbf{\Gamma} \times \boldsymbol{\chi} \\ \\ \mathbf{\Gamma} \times \mathbf{\Omega} \end{pmatrix}.$$

The equations defining the configuration of the heavy top follow from (3):

$$\begin{aligned}
\frac{d\mathbf{\Pi}}{dt} &= \mathbf{\Pi} \times \mathbf{\Omega} + Mgl\mathbf{\Gamma} \times \boldsymbol{\chi}, \\
\frac{d\mathbf{\Gamma}}{dt} &= \mathbf{\Gamma} \times \mathbf{\Omega}.
\end{aligned} \tag{6}$$

In the setting of Munthe-Kaas and Crouch–Grossman methods, the ordinary differential equation (3) must be cast in the form of an infinitesimal generator with infinitesimal generator map $f : \mathfrak{g}^* \to \mathfrak{g}$ [3].

For Hamiltonian systems on $\mathfrak{g}^*$, it turns out that a natural choice of action is the coadjoint action Ad^*. One of the main reasons for this is that Casimir functions are preserved on the coadjoint orbits. Indeed, the right-hand side of (3) is the infinitesimal generator of the coadjoint action, and hence, (5) gives us the infinitesimal generator map $f : \mathfrak{g}^* \to \mathfrak{g}$. The algorithm to compute the infinitesimal generator map $f : \mathfrak{g}^* \to \mathfrak{g}$ for general Hamiltonian functions H, is just to find the functional derivative of H.

The Lagrangian (symmetric) heavy top possesses four conserved quantities: the Hamiltonian (4); the projection of the angular momentum on the symmetry axis of the top $\mathbf{\Pi}\cdot\boldsymbol{\chi}$; the projection of the angular momentum on the gravity vector $\mathbf{\Pi} \cdot \mathbf{\Gamma}$; and, finally, the norm of the gravity vector $\|\mathbf{\Gamma}\|^2$. The two latter first integrals are Casimirs of the Poisson bracket defining the Hamiltonian structure. The Casimirs are preserved under the coadjoint action and rendered to machine accuracy in the numerical simulations.

Note that $\mathfrak{g}^*$ is a vector space. Since the conserved quantities are linear (the projection of the angular momentum on the symmetry axis of the top) or quadratic (the energy, the projection of the angular momentum on the gravity vector and the norm of the gravity vector) the symplectic Runge–Kutta methods will generate solutions that also respect the first integrals. However, the new methods also output the configuration of the top in addition to preservation of the first integrals. The full strength of the new methods is utilized for problems in which the integrals are of a non-linear and non-quadratic nature.

4. Numerical Illustrations

The Munthe-Kaas and the Crouch–Grossman methods were described in [5]. As will be seen from the numerical results, using the new action defined in Section 3 will preserve all first integrals that are Casimirs. This fact follows from the definition of coadjoint action and the fact that Casimirs are invariant under coadjoint actions. Non-Casimirs will in general not be preserved to machine accuracy. However, by using the recent flow-symmetric versions of the Munthe-Kaas methods, we are also able to render non-Casimir first integrals of the heavy top with an error confined within a bound, i.e. not increasing. The idea of these methods is to base the coordinates of the method on a geodesic or a flow midpoint between y_n and y_{n+1}. The resulting Munthe-Kaas methods, when based on classical selfadjoint Runge–Kutta schemes, are time-symmetric, a property that turns out to be advantageous when aiming at generating numerical approximations that respect the first integrals of the true solution.

The Crouch–Grossman method advances the solution from y_n to y_{n+1} through a composition of elementary flows. We will now show that the Crouch–Grossman method based on the coefficients of the classical trapezoidal rule is a time-symmetric method. Written out in all its detail, the above Crouch–Grossman method applied to the differential equation $y' = f(y)y$ on a Lie group G, is the following:

$$\begin{aligned} Y_1 &= y_n \\ Y_2 &= \exp\left(\tfrac{h}{2} f(Y_2)\right) \exp\left(\tfrac{h}{2} f(Y_1)\right) y_n \\ y_{n+1} &= \exp\left(\tfrac{h}{2} f(Y_2)\right) \exp\left(\tfrac{h}{2} f(Y_1)\right) y_n. \end{aligned} \tag{7}$$

Here, h is the stepsize, and Y_1, Y_2 are elements of the Lie group. The method given by (7) is equivalent to

$$y_{n+1} = \exp\left(\tfrac{h}{2} f(y_{n+1})\right) \exp\left(\tfrac{h}{2} f(y_n)\right) y_n. \tag{8}$$

Performing the interchanges $y_n \leftrightarrow y_{n+1}$ and $h \leftrightarrow -h$ in (8), we see that the method remains the same. Hence, the Crouch-Grossman method based on the trapezoidal rule is flow-symmetric, i.e. the numerical flow is centered at the midpoint along the flow.

We want to remark the following: The fact that the trapezoidal rule is classically symmetric is just a coincidence. Numerical experiments indicate that a classical symmetric Runge–Kutta method does not yield a flow-symmetric Crouch–Grossman method. The general non-commutativity of the elementary flows seems to be the reason why the classical result does not carry over to the Crouch-Grossman methods. Hence, the general construction of time-symmetric Crouch–Grossman methods is for the moment open.

We have simulated the system (6) with the following data (see [5] and [11]):

$$\mathrm{I} = \frac{1}{8}\begin{bmatrix} 7 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \quad \boldsymbol{\chi} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

and

$$(\mathbf{\Pi}_0, \mathbf{\Gamma}_0) = \left(\begin{bmatrix} 0 \\ 0 \\ 0.25 \end{bmatrix}, \begin{bmatrix} 0 \\ -0.195090 \\ 0.980785 \end{bmatrix} \right).$$

Moreover, the gravitational constant g equals 9.81, the length l equals $\frac{\sqrt{3}}{2}$, and the mass M equals 1. The stepsize of the integration was $h = 0.05$, while the interval of integration was $[0, 100]$.

Figures 2 and 3 show the results from the Munthe-Kaas method with the coefficients of the famous explicit fourth order Runge–Kutta method ([6, p. 138]) and the fourth order Gauss–Legendre method, respectively. These constellations are not time-symmetric. The Casimirs are rendered correctly, but there are linear drifts in both the Hamiltonian and the projection of the angular momentum on the symmetry axis of the top.

Consider next the *time-symmetric* Munthe-Kaas method [11] with the coefficients of the sixth order Gauss–Legendre method. The numerical results are shown in Figure 4. There is no overall drift in the Hamiltonian nor in the projection of the angular momentum on the symmetry axis of the top.

Figure 5 shows the preservation of the first integrals when applying the Munthe-Kaas method with the coefficients of the second order trapezoidal rule. We see that the projection of the angular momentum on the gravity vector oscillates within a band, and there is no growth in time. The trapezoidal Munthe-Kaas method behaves very favorably in rendering the energy, even though this is not a time-symmetric method

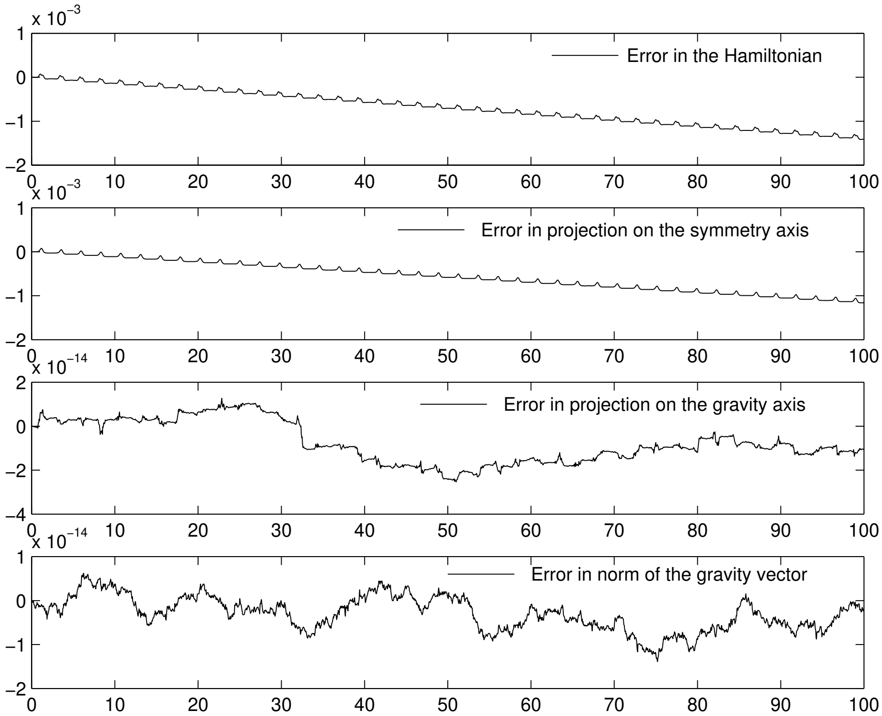

Figure 2. Preservation of first integrals: the Munthe-Kaas method with the coefficients of the famous fourth order explicit Runge–Kutta method

in the setting of Zanna et al. [11]. The reason is that it is possible to show that the trapezoidal Munthe-Kaas method is in fact energy preserving [4].

In Figures 6 and 7 are shown results from integration using the Crouch–Grossman method. Figure 6 shows the results obtained when applying the coefficients of the fourth order method presented in [7]. The non-Casimirs are not preserved. Figure 7 shows the results from the Crouch–Grossman method using the coefficients of the second order trapezoidal rule. Observe that the error in the first integrals is bounded. This is due to the time-symmetry of the Crouch–Grossman method with the trapezoidal rule coefficients (7).

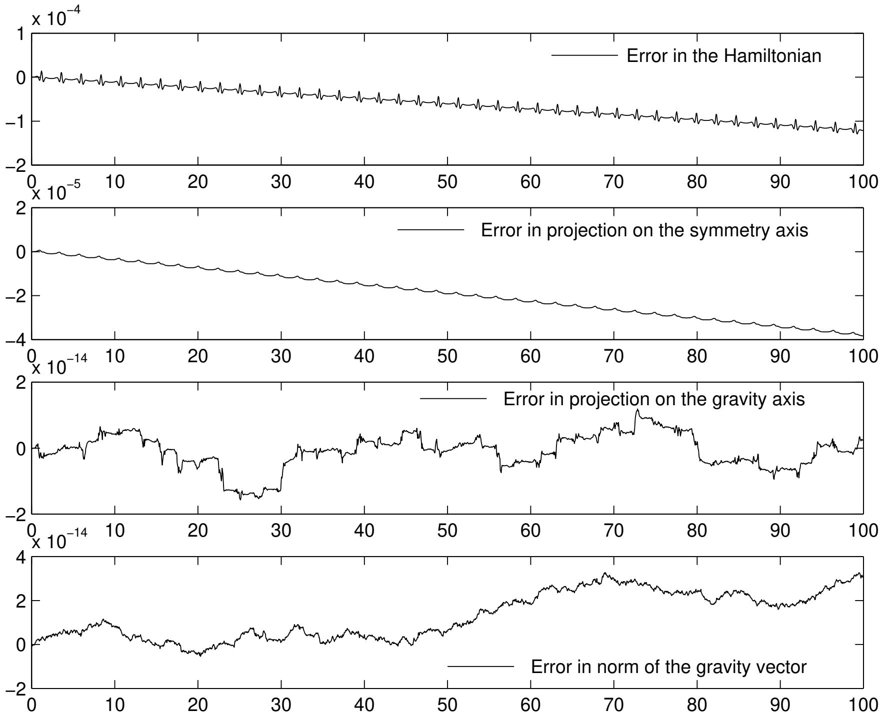

Figure 3. Preservation of first integrals: the Munthe-Kaas method with the coefficients of the fourth order Gauss–Legendre method

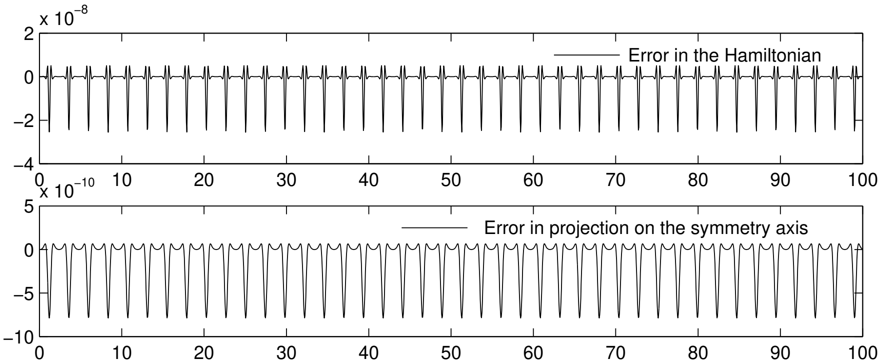

Figure 4. Preservation of first integrals: *time-symmetric* Munthe-Kaas method [11] with the coefficients of the sixth order Gauss–Legendre method

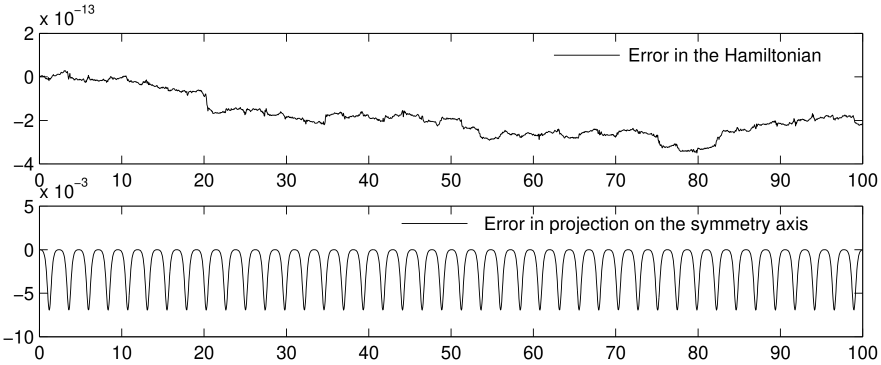

Figure 5. Preservation of first integrals: the Munthe-Kaas method with the coefficients of the second order trapezoidal rule

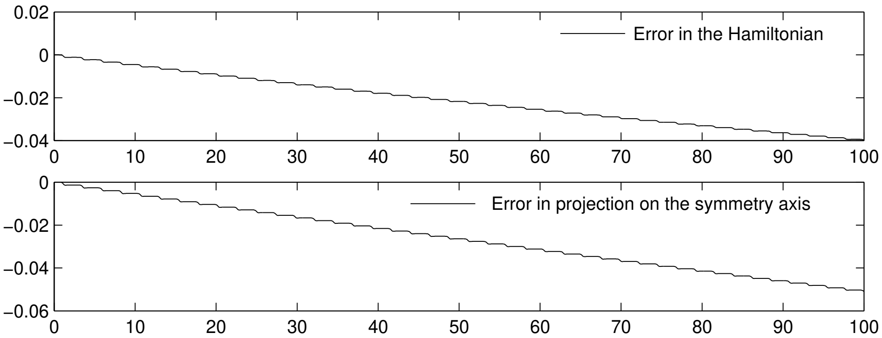

Figure 6. Preservation of first integrals: the Crouch–Grossman method with the coefficients of the fourth order method from [7]

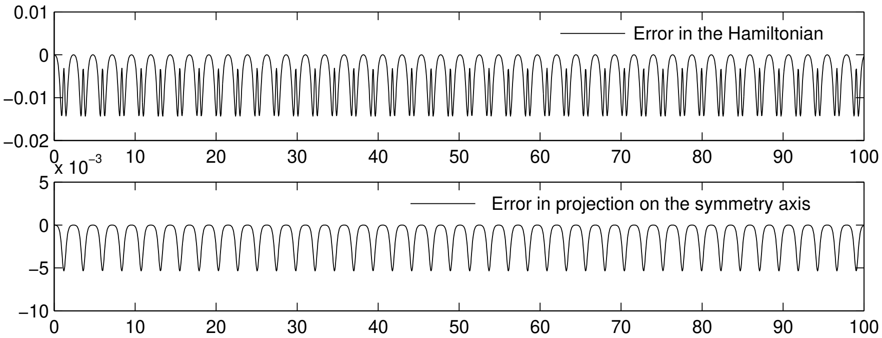

Figure 7. Preservation of first integrals: the Crouch–Grossman method with the coefficients of the second order trapezoidal rule

5. Concluding Remarks

We have shown that an appropriate choice of modeling space and group action for the heavy top lead to the conservation of more structure than the naive approach presented in [5]. Hence, finding the right setting, i.e. space and action, in the case of Munthe-Kaas and Crouch-Grossman type methods is very important. The big challenge for the future is also to apply, if possible, the numerical geometric integration techniques we now know as Lie-group methods for ordinary differential equation, on fluid flow problems and partial differential equations.

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