Numerical Integration of the Generalized Euler Equations

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NUMERICAL INTEGRATION OF THE GENERALIZED EULER EQUATIONS

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Abstract. For the generalized Euler equations on arbitrary finite dimensional Lie groups explicit numerical integration schemes that preserve either the underlying Lie–Poisson structure or the Hamiltonian (energy) of the problem are derived. The concept of energy preservation is generalized to so–called M–orthogonal schemes and it is shown that certain energy preserving schemes are actually M–orthogonal. We also provide a backward error analysis for those schemes.

Key words. Euler equations, numerical integration, Lie–Poisson integrator, preservation of energy, Hamiltonian systems, backward error analysis

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1. Introduction. Recently a lot of attention has been devoted to the numerical integration of Hamiltonian systems of the type

$$x' = \{x, H\}$$

where H denotes the Hamiltonian of the system and $\{\ ,\ \}$ is the corresponding Poisson bracket [17] defined by

$$\{F, G\} = F_x J(x) G_x^T$$

Here $J(x)$ is the skew–symmetric structure matrix of the bracket and $F, G : \mathbb{R}^n \to \mathbb{R}$ are arbitrary smooth functions. The two most important types of Poisson brackets are given by (i) $J(x)$ a constant skew–symmetric matrix and (ii) $J(x)$ skew–symmetric and linear in x. In the latter case the structure matrix $J(x)$ is derived from a Lie algebra associated with the phase space $\mathbb{R}^n$ and the corresponding bracket is called a Lie–Poisson bracket [17]. It has been shown that numerical integrators that preserve the Poisson bracket exist in both cases and that those schemes possess better long–term stability properties than standard integration codes [19],[11],[16],[6]. While these schemes are implicit in general, explicit schemes for separable Hamiltonians and

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

have been derived in [18],[15],[16],[10]. In this paper we derive explicit schemes for Lie–Poisson systems with a quadratic Hamiltonian which we call generalized Euler equations [2]. We first derive a second order symmetric method and, based on this method, we construct higher order methods by a proper composition of the second order scheme as suggested in [4],[15],[25].

While these integrators preserve the Poisson structure of the problem they do not, in general, preserve the Hamiltonian of the systems [11]. Therefore, attention has also been devoted to energy preserving schemes [3],[21],[19],[8]. Especially it has been shown that the implicit midpoint rule is energy preserving for the rigid body equations [3],[21]. In this paper we show that there exist explicit energy preserving schemes (in the sense that they do not require the solution of a nonlinear system of equations) and that those schemes (as well as the implicit midpoint rule) possess the stronger property of M–orthogonality. This property implies that the numerical solutions do not only stay on level curves of constant energy but that the numerical schemes is also non–dissipative on these level curves. An example of an energy preserving scheme that is not M–orthogonal is given. Finally we also provide a backward error analysis in terms of an asymptotic expansion. A similar result in terms of P–series [13] was given in [12] for Hamiltonian systems with a constant structure matrix J.

Applications of generalized Euler equations include rigid body dynamics [2], certain Riccati equations [24], and finite dimensional truncations of ideal hydrodynamics [26]. As a numerical example we consider the Euler equations on the Lie algebra $A_{3,7}^a$ [24] and the Euler equations for the free rigid body [2].

2. The Generalized Euler Equations. Eulerian motion of a rigid body can be described as motion along geodesics in the group of rotations of three dimensional euclidian space provided with a left–invariant riemannian metric. A significant part of Euler's theory depends only upon this invariance, and therefore can be extended to other groups (see, e.g., [2],[17]). In this section we summarize a few results on such a generalization which are needed throughout this paper (see [2],[17] for details).

Let G be a real Lie group and $\mathbf{g}$ its Lie algebra, i.e., the tangent space to the group at the identity provided with the Lie bracket operation $[\,,\,]$. We also consider the dual vector space $\mathbf{g}^*$ to the Lie algebra $\mathbf{g}$. This is the space of real linear functionals on the Lie algebra. Next we introduce the Lie–Poisson bracket on $\mathbf{g}^*$. For that reason let $F, G : \mathbf{g}^* \to I\!R$ be any two smooth functions. Their gradient is an element of $(\mathbf{g}^*)^* \simeq \mathbf{g}$ at any point $\xi \in \mathbf{g}^*$. Then the Lie–Poisson bracket of the two functions F and G is defined by

$$\{F, G\}(\xi) \;=\; \langle \xi\,;\, [\nabla F(\xi), \nabla G(\xi)]\rangle$$

where $\langle\,;\,\rangle$ is the natural pairing between $\mathbf{g}$ and $\mathbf{g}^*$.

Now let $A : \mathbf{g}^* \to \mathbf{g}$ be a symmetric positive definite linear operator. Then A defines a scalar product $(\,,\,)$ on $\mathbf{g}^*$ by

$$(\xi, \eta) \;=\; \langle \xi; A\eta\rangle$$

and a kinetic energy T by the formula

$$T(\xi) \;=\; \frac{1}{2}(\xi, \xi)$$

With this terminology, the generalized Euler equations become

$$\xi' \;=\; \{\xi, T\}$$

Introducing proper coordinates $x = (x^1, \ldots, x^n)$ in $\mathbf{g}^*$, these equations can be rewritten as

$$x' = J(x)\nabla T(x) \tag{1}$$

with

$$T(x) \;=\; \frac{1}{2}x^T M x$$

where M is a matrix with entries only in the main diagonal and $J(x)$ is the structure matrix of the Lie–Poisson bracket in the coordinates x defined by

$$J_{ij} \;=\; \sum_{r=1}^{n} c_{ij}^{r} x_r$$

Here c_{ij}^{r} are the structure constants of the Lie group $\mathbf{g}$ relative to the coordinates x in $\mathbf{g}^*$ [17]. Due to the special structure of the matrix M, (1) simplifies furthermore to

$$x' \;=\; \sum_{i=1}^{n} J(x)\nabla T_i(x)$$

with

$$T(x) \;=\; \sum T_i(x) = \sum \frac{1}{2} x_i m_{ii} x_i \tag{2}$$

where m_{ii} is the corresponding entry in the main diagonal of M.

The flow ϕ_t of (1), which can be written as

$$\phi_t(x) \quad = \quad B_t(x)\,x$$

with

$$\frac{\partial}{\partial \tau} B_\tau(x)_{|\tau=t} \quad = \quad J(B_t(x)x)\,M\,B_t(x)$$

has two important properties: (i) ϕ_t preserves the Poisson bracket, i.e.

$$\frac{\partial}{\partial x}\phi_t^T(x)\,J(x)\frac{\partial}{\partial x}\phi_t(x) \quad = \quad J(\phi_t(x))$$

and (ii) ϕ_t is M–orthogonal, i.e.

$$B_t^T(x)\,M\,B_t(x) = M$$

The second property can be easily shown by differentiating $B_t^T(x)\,M B_t(x)$ with respect to time and using the fact that $J(x)$ is skew–symmetric. Note that M–orthogonality implies the preservation of the Hamiltonian T; i.e. $T \cdot \phi_t = T$.

REMARK 2.1. *By means of the coordinate transformation* $\tilde{x} = M^{1/2}x$, *the Euler equation* (1) *can be transformed into*

$$\tilde{x}' \quad = \quad \tilde{J}(\tilde{x})\tilde{x}$$

where $\tilde{J}(\tilde{x})$ *is again skew–symmetric. Thus the corresponding flow* $\tilde{\phi}_t(\tilde{x}) = \tilde{B}_t(\tilde{x})\tilde{x}$ *satisfies now* $\tilde{B}_t(\tilde{x}) \in SO(n)$.

In the subsequent sections we will discuss discretizations of (1) which preserve either the Lie–Poisson structure or the M–orthogonality of the flow. Numerical schemes that preserve either the energy T or the Lie–Poisson structure have been discussed in the literature before (see, e.g., [11],[6],[21]). It turns out that some of the energy T preserving schemes, such as the implicit midpoint rule, are automatically M–orthogonal. However, the schemes discussed so far are implicit in the sense that they require the solution of nonlinear systems of equations. In contrast to this we will exploit the special structure of the Euler equations (1) and, based on this, derive explicit schemes.

3. M–Orthogonal Integrators. In [9], the numerical integration of matrix differential equations of the type

$$U' \quad = \quad A(U)U \tag{3}$$

with $A(U) \in I\!R^{n\times n}$ skew symmetric for all $U \in I\!R^{n\times q}$, $n \geq q \geq 1$, was discussed under the aspect of the preservation of the following solution behavior: If the matrix solution satisfies $U^T(t)U(t) = I$ at $t = 0$ then this holds for all t; i.e., the solution $U(t)$ is orthogonal for all t. As was shown in [9], Gauss–Legendre RK methods [14] preserve this property; i.e. $U_n^T U_n = I$ if $U_o^T U_o = I$. Furthermore, in case $U \in I\!R^{n\times n}$, a projection method was proposed with the effect that any integration scheme can be turned into a so–called unitary integrator [9]. This method consists basically of a QR decomposition of the numerical solution U_n and a subsequent substitution of U_n by the corresponding Q_n.

In this section we apply and generalize these results to vector valued differential equations of the type

$$x' = J(x)Mx \tag{4}$$

where the matrix $J(x)$ is the structure matrix of a Lie–Poissón bracket and M is a symmetric matrix corresponding to the quadratic Hamiltonian T.

With a simple modification of the proof given in [22], it is straightforward to show that the Gauss–Legendre methods lead to iteration schemes

$$x_k = B_h(x_k)x_k$$

where B_h is M–orthogonal for all x, i.e.

$$B_h(x)^T M B_h(x) = M$$

REMARK 3.1. *It has been observed before (see, e.g.,* [7],[19],[21]*) that Gauss–Legendre methods preserve quadratic Hamiltonians such as T for the generalized Euler equations* (1). *Note however that energy preservation does not automatically imply the M-orthogonality of the scheme. As an example consider the formulation*

$$\begin{aligned} x' &= J(x)Mx + \lambda x \\ 0 &= T(x) - T(x(0)) \end{aligned}$$

which is a differential–algebraic equation of index two [5]. *The discretization of this formulation by an implicit Radau Runge–Kutta method* [14] *results in a scheme that preserves the energy T but, in general, will not be M-orthogonal. Thus the numerical solutions stay on level curves of constant energy but on these level curves artificial dissipation might be introdced by the numerical integration scheme. This numerically introduced dissipation might lead to a destabilization of the numerical solution in a long–term integration.*

In the remainder of this section we discuss a modification of Gauss–Legendre methods which leads to schemes that avoid the solution of nonlinear equations while preserving the M–orthogonality of the original method.

Let us consider the discretization of (4) by a Runge–Kutta method

$$\begin{aligned} x_{k+1} &= x_k + h \textstyle\sum_{i=1}^{s} b_i J(X_i) M X_i \\ X_i &= x_k + h \textstyle\sum_{j=1}^{s} a_{ij} J(X_j) M X_j \qquad (i = 1, \ldots, s) \end{aligned} \tag{5}$$

For non–stiff differential equations and implicit Runge–Kutta methods (such as the Gauss–Legendre methods), the following function iteration in the variables X_i with $X_i^o = x_k$ proves to be very efficient:

$$X_i^l = x_k + h \textstyle\sum_{j=1}^{s} a_{ij} J(X_j^{l-1}) M X_j^{l-1} \qquad (l = 1, \ldots, m) \tag{6}$$

By comparing the solution X_i of (5) with the solution X_i^l of (6) it is easy to show that

$$X_i = X_i^l + O(h^{l+1})$$

and thus the modified scheme (6) is of the same order, p, $p \geq 1$, as the corresponding RK method (5) provided $X_i^o = x_k$ and $m = p$. However, even if (5) is M–orthogonal, the scheme corresponding to (6) will not, in general, be M–orthogonal. To ensure the M–orthogonality of a scheme (6) corresponding to a Gauss–Legendre method the following modification of (6) has to be made: Let us replace the mth iteration step by the following linear system of equations

$$X_i^m = x_k + h\sum_{j=1}^{s} a_{ij} J(X_j^{m-1}) M X_j^m \qquad (i = 1, \ldots, s) \tag{7}$$

For the resulting iteration together with the output map

$$x_{k+1} = x_k + h\sum_{i=1}^{s} b_i J(X_i^{m-1}) M X_i^m \tag{8}$$

we obtain

LEMMA 3.1. *Let* (5) *be the scheme corresponding to a Gauss–Legendre method of order* p. *Then the iteration* (6)–(7) *with* $m = p$ *together with the output equation* (8) *results in a* M*–orthogonal integrator for differential equations of the type* (4) *of order* p.

Proof: The equations (7) together with (8) can be written as

$$x_{k+1} = B(X^{m-1}) x_k$$

and can be considered as the discretization of a time–dependent differential equation

$$x' = J(t) M x \tag{9}$$

with $J(t_j) = J(X_j^{m-1})$ by a Gauss–Legendre method. Again a straightforward modification of the proof given in [9] for matrix differential equations of the type

$$U' = A(t) U$$

shows that Gauss–Legendre methods are M–orthogonal for time–dependent problems of type (9) and, consequently, $B(X^{m-1})$ is M–orthogonal. □

A similar iteration method was proposed in [9] for matrix differential equations (3). However, the iteration considered there requires the solution of a linear system of equations of type (7) in each step. Also no results are stated on the number of iterations that are needed to obtain a certain order of convergence.

As an example, let us consider the second order scheme corresponding to the implicit midpoint rule. Following Lemma 3.1 and after reformulating the resulting equations, we obtain

$$x_{k+1} = (I - (h/2)J(X)M)^{-1}(I + (h/2)J(X)M) x_k \tag{10}$$

$$X = x_k + (h/2) J(x_k) M x_k \tag{11}$$

Note that this scheme is no longer symmetric.

REMARK 3.2. *The Gauss–Legendre Runge–Kutta methods also preserve quadratic Casimir functions* [17] *corresponding to the Lie–Poisson bracket of the problem under consideration (see* [7] *for a proof). This is no longer true for the modified Gauss–Legendre methods discussed in this section. However, if one choses* m *in Lemma 3.1 such that* $m \geq p$, *then the resulting scheme preserves quadratic Casimir functions up to terms of order* m.

From a practical point of view it might also often be sufficient to choose m in (6) *large enough and not to replace the mth iteration by* (7). *The method obtained this way will be of order p in the variable x and M-orthogonal of order m, $m > p$.*

EXAMPLE 3.1. *Let us assume that $x \in \mathbb{R}^3$ and that the structure matrix $J(x)$ corresponds to the $so(3)$; i.e.*

$$J(x) = \begin{pmatrix} 0 & x_3 & -x_2 \\ -x_3 & 0 & x_1 \\ x_2 & -x_1 & 0 \end{pmatrix}$$

Then, since

$$J(x)y = -J(y)x$$

the Gauss–Legendre methods are both M- and I-orthogonal (I the identity matrix). This is in contrast to the modified Gauss–Legendre schemes discussed in this section which, depending on wether the formulation

$$x' = J(x)Mx$$

is integrated or

$$x' = -J(Mx)x\,,$$

are either M- or I-orthogonal.

4. Lie–Poisson Integrators. In this section we consider the discretization of the Euler equations (1) under the aspect of preservation of the Lie–Poisson bracket. So-called Lie–Poisson integrators have been discussed before for systems (1) with arbitrary Hamiltonian T [11],[6]. Here we make use of the fact that for the Euler equations the Hamiltonian T is quadratic and derive an explicit Lie–Poisson integrator.

Assuming that the coordinate system was chosen such that the matrix M has entries in the main diagonal only, (1) can be rewritten as

$$\begin{aligned} x' &= \textstyle\sum_{i=1}^n x_i m_{ii} J_i(x) \\ &= \textstyle\sum_{i=1}^n X^i \end{aligned} \tag{12}$$

with $X^i = x_i m_{ii} J_i(x)$ where $J_i(x)$ denotes the ith column of $J(x)$. Since $J_{ii}(x) = 0$, x_i is constant for each vector field X^i and, thus, X^i is linear and the flow X_t^i can be computed analytically. This allows us to apply an idea first used for Hamiltonian systems with separable Hamiltonian (see, e.g, [25]) to derive a Lie–Poisson integrator for the Euler equations (1).

LEMMA 4.1. *Let X_t^i be the flow corresponding to the linear vector field X^i in* (12). *Then the following composition of these flows*

$$\psi_h^{2nd}(x) = \prod_{i=1}^{n} X_{h/2}^i \cdot \prod_{i=0}^{n-1} X_{h/2}^{n-i} \cdot x$$

yields a discretization of (1) *which is of second order, symmetric, and Lie-Poisson.*

Proof: The second order convergence can easily be seen by applying the Baker–Campbell–Hausdorff formula [23],[25]. The preservation of the Lie–Poisson bracket follows from the fact that each flow X_t^i is Lie–Poisson. □

EXAMPLE 4.1. *Let us again assume that $x \in \mathbb{R}^3$ and that the structure matrix $J(x)$ corresponds to the $so(3)$; i.e.*

$$J(x) = \begin{pmatrix} 0 & x_3 & -x_2 \\ -x_3 & 0 & x_1 \\ x_2 & -x_1 & 0 \end{pmatrix}$$

The vector fields X^i corresponding to (12) *are*

$$X^1 = m_{11}x_1 \begin{pmatrix} 0 \\ -x_3 \\ x_2 \end{pmatrix} \quad X^2 = m_{22}x_2 \begin{pmatrix} x_3 \\ 0 \\ -x_1 \end{pmatrix} \quad X^3 = m_{33}x_3 \begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}$$

and the corresponding flows can be computed analytically. Thus the iteration scheme

$$\psi_h^{2nd}(x) = X_{h/2}^1 \cdot X_{h/2}^2 \cdot X_h^3 \cdot X_{h/2}^2 \cdot X_{h/2}^1 \cdot x$$

is of second order and symmetric. The time–h–map ψ_h^{2nd} can be written as

$$\psi_h^{2nd}(x) = B_h(x)\, x$$

with $B_h(x) \in SO(3)$. Thus ψ_h^{2nd} can be also considered as an I–orthogonal integrator (I the identity matrix). Note however that I–orthogonality does not imply the preservation of the Lie–Poisson structure.

As shown in [25] for systems with separable Hamiltonian, the second order scheme ψ_h^{2nd} can be used to obtain higher order Lie–Poisson integrators. For example, the composed method

$$\psi_h^{4th} = \psi_{c_1 h}^{2nd} \cdot \psi_{c_2 h}^{2nd} \cdot \psi_{c_1 h}^{2nd}$$

with $2c_1 + c_2 = 1$ and $2c_1^3 + c_2^3 = 0$ is of fourth order.

Besides being Lie–Poisson integrators, the schemes introduced in this section possess another important preservation property.

LEMMA 4.2. *The Lie–Poisson integrators considered in this section preserve any Casimir function* [17] *corresponding to the Lie–Poisson structure of the problem.*
Proof: The Lie–Poisson integrators considered here are the composition of flows solving certain Euler equations on the Lie algebra exactly. Since each single flow preserves the Casimir functions, the composition of those flows also preserves Casimir functions. □

5. Numerical Experiment. In this section we apply our results to the Euler equation on the Lie algebra $A_{3,7}^a$ [24] and the Euler equation for the free rigid body [2].

5.1. Euler Equation on the $A_{3,7}^a$. The structure matrix of the Lie–Poisson bracket for the Lie algebra $A_{3,7}^a$ [24] is given by

$$J(x) = \begin{pmatrix} 0 & 0 & ax_1 - x_2 \\ 0 & 0 & x_1 + ax_2 \\ -ax_1 + x_2 & -x_1 - ax_2 & 0 \end{pmatrix}$$

where $a > 1$ is a constant. Thus the vector fields X^i, $i = 1, 2, 3$ are given by

$$\begin{aligned}
X^1 &= m_{11}x_1 \begin{pmatrix} 0 \\ 0 \\ -ax_1 + x_2 \end{pmatrix} \\
X^2 &= m_{22}x_2 \begin{pmatrix} 0 \\ 0 \\ -x_1 - ax_2 \end{pmatrix} \\
X^3 &= m_{33}x_3 \begin{pmatrix} ax_1 - x_2 \\ x_1 + ax_2 \\ 0 \end{pmatrix}
\end{aligned}$$

with corresponding flows

$$\begin{aligned}
X_t^1 &= \begin{pmatrix} x_1 \\ x_2 \\ x_3 + tm_{11}x_1(-ax_1 + x_2) \end{pmatrix} \\
X_t^2 &= \begin{pmatrix} x_1 \\ x_2 \\ x_3 - tm_{22}x_2(x_1 + ax_2) \end{pmatrix} \\
X_t^3 &= \begin{pmatrix} e^{\gamma t}(\cos(\omega t)x_1 - \sin(\omega t)x_2) \\ e^{\gamma t}(\sin(\omega t)x_1 + \cos(\omega t)x_2) \\ x_3 \end{pmatrix}
\end{aligned}$$

where $\gamma = am_{33}x_3$ and $\omega = m_{33}x_3$.

The Casimir function of the Lie–Poisson bracket is given by

$$C(x) = (x_1^2 + x_2^2)\exp(-2a \arctan\frac{x_2}{x_1})$$

Based on these flows the second order Lie–Poisson integrator of Section 4 was used to integrate the corresponding Euler equations. In Fig. 1 the drift in the Hamiltonian and in the Casimir function is plotted versus time. For the numerical experiment we used step–size $h = 0.01$, $a = 2.0$, and the Hamiltonian

$$H(x) = 0.5x_1^2 + x_2^2 + 0.005x_3^2$$

The same equations were integrated using the modified M–orthogonal midpoint rule (10)–(11). The drift in the Hamiltonian and the Casimir function is shown in Fig. 2.

5.2. Euler Equation for the Rigid Body. Recall that the equations of motion for a simple rigid body in three dimensions take the form [3]:

$$A' = A\,J(Mx) \tag{13}$$

$$x' = -J(Mx)\,x \tag{14}$$

where $A \in SO(3)$ is the matrix of direction cosines for a body frame attached to the rigid body as viewed in an inertial frame, $x \in I\!R^3$ is the body angular momentum,

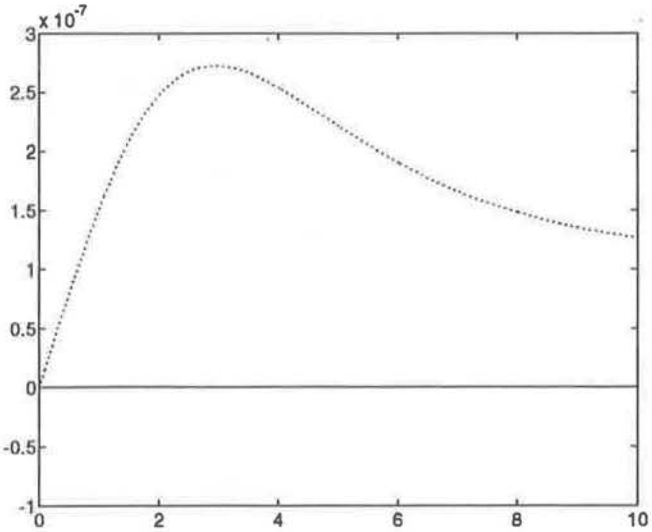

FIG. 1. *Drift in the Hamiltonian (dotted line) and in the Casimir function (solid line) for the Lie–Poisson integrator.*

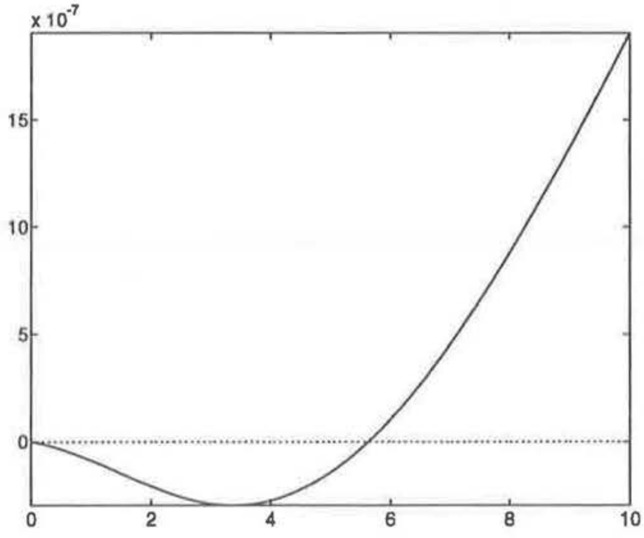

FIG. 2. *Drift in the Hamiltonian (dotted line) and in the Casimir function (solid line) for the M-orthogonal integrator.*

and M is the moment of inertia tensor of the rigid body in the body frame. $J(x)$ is defined as in Example 4.1.

Let us discretize the equation (14) by a method given in Lemma 3.1. The resulting time–h–map can be written as

$$x_{k+1} = B_h(x_k)\, x_k \tag{15}$$

where $B_h(x_k)$ is I–orthogonal; i.e. $B_h(x_k) \in SO(3)$. Then, a spatial angular momentum $\pi = A\, x$ preserving update for the spatial attitude A is given by

$$A_{k+1} = A_k\, B_h^T(x_k) \tag{16}$$

Furthermore, if $A_k \in SO(3)$, then also $A_{k+1} \in SO(3)$. Note that this scheme does not preserve the energy of the system. This would be the case if (14) were discretized by a Gauss–Legendre method (since then $B_h(x_k)$ would also be M–orthogonal). The order of the overall scheme is the same as the order of the method applied to the equation (14). If (14) were discretized by a Lie–Poisson integrator of Section 4, then the iteration map could be written again as (15) with $B_h(x_k)$ I–orthogonal and the same update (16) could be used for the spatial attitude A.

The rigid body equation (13) was integrated by the second order explicit Runge method [13], the modified implicit midpoint rule (10)–(11), and the second order Lie–Poisson integrator of Lemma 4.1. The results were obtained for $M = \mathrm{diag}(1, 1/2, 1/3)$, $x(0) = (1, 10, 1)$, $A(0) = I$, and $h = 0.1$. In Fig. 3–5 the computed values of the variable $A(1,1)$ for all three methods are plotted versus time. For comparison we also plotted the "exact" numerical solution abtained by the fourth order Gauss–Legendre method with step–size $h = 0.001$.

While the explicit second order Runge method leads to unacceptable results, the other two methods both yield only small phase errors. However, the modified midpoint rule (as well as the midpoint rule itself) results in a constantly growing phase error, while for the Lie–Poisson integrator the phase drift "oscillates" around the zero value.

6. Backward Error Analysis. In this section we show that the solutions of a M–orthogonal, Lie–Poisson integrator, respectively, can be formally considered as the exact solution of a certain perturbed differential equation at time $t = h$. Throughout this section we assume that the mappings involved are smooth, i.e. C^∞ and that the step–size h is kept constant during the integration. We will also use the symbol $\approx$ instead of $=$ to indicate that two expressionsare equal only in the sense of asymptotic power expansions (nothing is said about their convergence [1]).

Following the approach taken in [25] for separable Hamiltonian systems, it is easy to show that the numerical solutions of a Lie–Poisson integrator, as discussed in Section 4, can be considered as the exact solution of a perturbed system

$$x' = J(x) \nabla \tilde{T}(x, h)$$

where $\tilde{T}(h)$ is the perturbed Hamiltonian satisfying

$$\tilde{T}(h) = T + O(h^p)$$

and p is the order of the scheme. The Taylor expansion of $\tilde{T}(h)$ is given by the Baker–Campbell–Hausdorff formula [23]. Note, however, that the perturbed Hamiltonian $\tilde{T}$

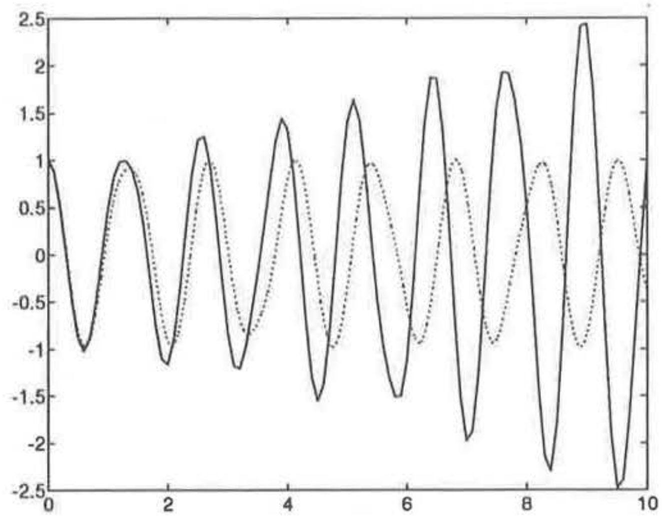

FIG. 3. *Numerical values of $A(1,1)$ for the second order Runge method (solid line) compared to the exact solution (dotted line).*

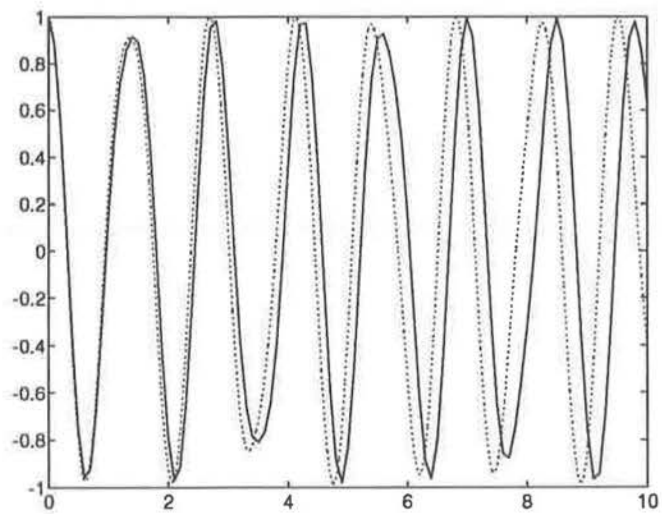

FIG. 4. *Numerical values of $A(1,1)$ for the modified midpoint rule (solid line) compared to the exact solution (dotted line).*

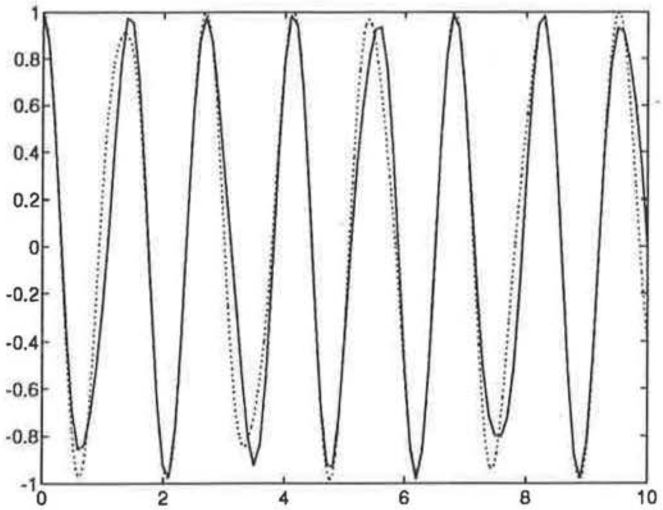

FIG. 5. *Numerical values of $A(1,1)$ for the second order Lie–Poisson integrator (solid line) compared to the exact solution (dotted line).*

is no longer quadratic in x. Let $\tilde{X}_t$ denote the flow of the perturbed Hamiltonian system and ψ_h the time–h–map corresponding to the Lie–Poisson integrator, then we have

$$\psi_h \approx \tilde{X}_h$$

Below we give a general result that can be used to show that a similar statement holds for M–orthogonal integrators. Specifically: There exists a perturbed skew–symmetric matrix $\tilde{J}(x)$ such that the flow $\tilde{X}_t$ of the perturbed system

$$x' = \tilde{J}(x,h)Mx$$

satisfies

$$\psi_h \approx \tilde{X}_h$$

and

$$\tilde{J}(h) = J + O(h^p)$$

where p is the order of the M–orthogonal scheme ψ_h. Note that the perturbed matrix will not, in general, correspond to a Lie–Poisson bracket and will not be linear in x.

Lie–Poisson integrators and M–orthogonal integrators are special cases of numerical schemes for differential equations whose corresponding vector fields X belong to a certain Lie subalgebra $\mathbf{g}$ of the infinite dimensional Lie algebra of all vector fields on $\mathbb{R}^n$ [1]. Let us assume that there is a corresponding Lie subgroup G such that $\mathbf{g} = T_{id}G$ [23],[1]. An important aspect of those differential equations is that the corresponding flow X_t forms a one–parametric subgroup in G. For Hamiltonian differential equations on a symplectic manifold this is the subgroup of canonical mappings and for differential equations of type (4), the flow X_t is M–orthogonal.

Especially in the context of long term integrations, it is desirable to discretize differential equations of this type in such a way that the corresponding iteration map belongs to the same subgroup G as the flow X_t. We will call those integrators Lie algebraic integrators.

The following result concerning the backward error analysis of Lie algebraic integrators can be made:

LEMMA 6.1. *Let us assume that the vector field X in*

$$x' = X(x)$$

belongs to a Lie subalgebra $\mathbf{g}$ of the Lie algebra of all vector fields on $\mathbb{R}^n$. Let us assume furthermore that

$$x_{k+1} = \psi_h(x_k)$$

is a Lie algebraic integrator for this subalgebra $\mathbf{g}$, i.e. $\psi_h \in G$ for all h sufficiently small. Then, for a constant step-size h, there is a vector field $\tilde{X}(h)$ belonging to the same subalgebra $\mathbf{g}$ with corresponding flow $\tilde{X}_t(h)$ such that

$$\psi_h \approx \tilde{X}_h(h)$$

Thus the iteration map ψ_h can be considered as the time-h-flow of the perturbed vector field $\tilde{X}(h)$ which belongs to the same subalgebra $\mathbf{g}$ as X.

Proof: The Taylor expansion of ψ_h can be written as

$$\psi_h = \sum_{i=0}^{\infty} h^i \psi_{h=0}^{[i]}$$

Let $\tilde{X}(h)$ be some vector field such that the corresponding flow $\tilde{X}_t(h)$ satisfies

$$\tilde{X}_h(h) = \psi_h + O(h^{p+1})$$

(In the first place we simply take $\tilde{X}(h) = X$ and p equal to the order of the scheme.) Again we write the Taylor expansion of $\tilde{X}_h$ as

$$\tilde{X}_h(h) = \sum_{i=0}^{\infty} h^i \tilde{X}_{h=0}^{[i]}$$

Define the mapping $Y^{[p+1]} : \mathbb{R}^n \to \mathbb{R}^n$ by

$$Y^{[p+1]} + O(h) = \frac{\psi_h - \tilde{X}_h}{h^{p+1}}$$

Then, since $\tilde{X}_h(h), \psi_h \in G$ for all h sufficiently small and $\tilde{X}_{h=0}(h=0) = \psi_{h=0} = id$, $Y^{[p+1]} \in T_{id}G = \mathbf{g}$ and

$$Y^{[p+1]} = \psi^{[p+1]} - \tilde{X}^{[p+1]}$$

Next we define a new $\tilde{X}(h)$ by

$$\tilde{X}(h) := \tilde{X}(h) + h^p Y^{[p+1]}$$

with $\tilde{X}_h(h)$ now satisfying

$$\tilde{X}_h(h) = \psi_h + O(h^{p+2})$$

Thus, by increasing p, we finally obtain

$$\tilde{X}(h) \approx X + \sum_{i=1}^{\infty} h^i Y^{[i]}$$

and

$$\psi_h \approx \tilde{X}_h(h)$$

Since X and all the $Y^{[i]}$ belong to one and the same subalgebra, any linear combination and especially $\tilde{X}(h)$ belongs to this subalgebra too. □

For M-orthogonal integrators (flows, respectively) the corresponding Lie algebra $\mathbf{g}$ consists of all vector fields of the type

$$X(x) = J(x)\,Mx$$

with $J(x)$ skew-symmetric. Its Lie bracket $[\,,\,]$ is given by the Lie bracket of arbitrary vector fields on $\mathbb{R}^n$; i.e., the ith component of $Z = [X, Y]$ is defined by

$$[X,Y]_i = \sum_{i=1}^{n} Y_i \frac{\partial X_j}{\partial x_i} - X_i \frac{\partial Y_j}{\partial x_i}$$

In case $J(x) = J = const.$, this formula reduces to

$$J_3\,Mx = [J_1 Mx, J_2 Mx] = (J_1 M J_2 - J_2 M J_1)\,Mx$$

and J_3 is skew-symmetric as required. Furthermore, let $B_h(x)\,x$ be an arbitrary one-parametric family of M-orthogonal mappings with $B_{h=0}(x) = I$, then

$$\frac{\partial}{\partial h} B_h(x)\,x_{|h=0} =: X(x) \in T_{id}G$$

by definition but also $X \in \mathbf{g}$. Thus $\mathbf{g} = T_{id}G$.

REMARK 6.1. *The above lemma can be used to show that, based on a first order Lie algebraic integrator, Lie algebraic integrators of any order can be constructed by the method given in* [25] *for Hamiltonian systems.*

7. Concluding Remark. The results of this paper can be generalized on the one side to Hamiltonian differential equations

$$x' = J(x)\nabla T(x) \tag{17}$$

where $J(x)$ is the structure matrix of some Poisson bracket and T is a quadratic Hamiltonian, and on the other side to Hamiltonian systems

$$x' = \{x, H\}$$

with a Lie–Poisson bracket $\{\,,\,\}$ and a Hamiltonian of the type

$$H(x) = \sum_{i=1}^{n} H_i(x_i)$$

An example of such a Hamiltonian system is given in [6] where a finite dimensional approximation of the Vlasov–Poisson equations is discussed.

REFERENCES

[1] Adams, M, Ratiu, T., Schmid, R., The Lie Group Structure of Diffeomorphism Groups and Invertible Fourier Integral Operators with Applications, in: *Infinite Dimensional Groups with Applications*, Kac, V. (editor), Springer Verlag, 1985.

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

[3] Austin, M., Krishnaprasad, P.S., Wang, L.S., Almost Poisson Integration of Rigid Body Systems, Technical Research Report TR 91–45r1, University of Maryland, 1991.

[4] Benzel, S., Ge, Z., Scovel, C., Elementary Construction of Higher Order Lie–Poisson Integrators, *Physics Letters A*, 174(1993), 229–232.

[5] Brenan, K.E., Campbell, S.L., and Petzold, L.R., *Numerical Solution of Intial-Value Problems in DAEs*, North Holland, 1989.

[6] Channell, P.J., Scovel, J.C., Integrators for Lie–Poisson Dynamical Systems, *Physica D*, 50(1991), 80–91.

[7] Cooper, G.J., Stability of Runge–Kutta Methods for Trajectory Problems, *IMA J. Numer. Anal.*, 7(1987), 1–13.

[8] Chorin, A.J., Hughes, T.J.R., Marsden, J.E., McCracken, M, Product Formulas and Numerical Algorithms, *Comm. Pure and Appl. Math.*, 31(1978), 205–256.

[9] Dieci, L., Russell, R.D., Van Vleck, E., Unitary Integrators and Applications to Continuous Orthonormalization Techniques, Research Report 92–11, Simon Fraser University, 1992.

[10] Forest, E., Ruth, R.D., Fourth–Order Symplectic Integration, *Physica D*, 43(1990), 105–117.

[11] Ge, Z., Marsden, J., Lie–Poisson Hamilton–Jacobi Theory and Lie–Poisson Integrators, *Phys. Letters A*, 33(1988)3, 134–139.

[12] Hairer, E., Backward Analysis of Numerical Integrators and Symplectic Methods, Techn. Report, Universitè of Genv̀e, 1993.

[13] Hairer, E., Norsett, S.P., Wanner, G., *Solving Ordinary Differential Equations, I*, Springer Verlag, 1987.

[14] Hairer, E., Wanner, G., *Solving Ordinary Differential Equations, II*, Springer Verlag, 1991.

[15] Neri, F., Lie Algebras and Canonical Integration, Department of Physics, University of Maryland, preprint, 1988.

[16] Okunbor, D. and Skeel, R.D., Explicit canonical methods for Hamiltonian Systems, *Math. Comp.*, 59(1992), 439–455.

[17] Olver, P.J., *Applications of Lie Groups to Differential Equations*, Springer Verlag, New York, 1986.

[18] Ruth, R.D., A Canonical Integration Technique, *IEEE Trans. Nucl. Sci.*, 30(1983), 2669–2671.

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

[20] Scovel, C., Symplectic Integration of Hamiltonian Systems, in *The Geometry of Hamiltonian Systems*, Ratiu, T. (editor), Springer Verlag, 1991.

[21] Simo, J., Wong, K.K., Unconditionally Stable Algorithms for Rigid Body Dynamics that Exactly Preserve Energy and Momentum, *International Journal for Numerical Methods in Engineering*, 31(1991), 19–52.

[22] Stuart, A.M., Humphries, A.R., Model Problems in Numerical Stability Theory for Initial Value Problems, Technical Report NA–92–16, Stanford University, 1992.

[23] Varadarajan, V.S., *Lie Groups, Lie Algebras, and Their Representation*, Prentice–Hall, Englewood Cliffs, 1974.

[24] Wojciechowski, S., Hamiltonian Structure and Complete Integrability in Analytical Mechanics, in *Soliton Theory: A Survey of Results*, Fordy, A.P. (ed.), Manchester University Press, 1990.

[25] Yoshida, H., Construction of Higher Order Symplectic Integrators, *Phys. Lett. A*, 150(1990), 262–268.

[26] Zeitlin, V., Finite–Mode Analysis of 2D Ideal Hydrodynamics, *Physica D*, 49(1991), 353–369.