SYMPLECTIC INTEGRATION OF CONSTRAINED HAMILTONIAN SYSTEMS BY COMPOSITION METHODS

SEBASTIAN REICH
INSTITUT FÜR ANGEWANDTE ANALYSIS UND STOCHASTIK
MOHRENSTRAßE 39
BERLIN, 10117, GERMANY
E–MAIL: NA.REICH@NA-NET.ORNL.GOV *

Abstract. Recent work reported in the literature suggests that for the long-term integration of Hamiltonian dynamical systems one should use methods that preserve the symplectic structure of the flow. In this paper we investigate the symplecticity of numerical integrators for constrained Hamiltonian systems with holonomic constraints. We will derive the following two results:

(i) We show that any first or second order symplectic integrator for unconstrained problems can be generalized to constrained systems such that the resulting scheme is symplectic and preserves the constraints. Based on this, higher order methods can be derived by the same composition methods as used for unconstrained problems.

(ii) Leimkuhler and Reich [17] derived symplectic integrators based on Dirac's reformulation of the constrained problem as an unconstrained Hamiltonian system. However, although the unconstrained reformulation can be handled by direct application of any symplectic implicit Runge-Kutta method, the resulting schemes do not preserve the constraints. In this paper we show that these schemes can be modified such that they also preserve the constraints.

Key words. Hamiltonian systems, differential-algebraic equations, canonical discretization schemes, Lie groups

AMS(MOS) subject classifications. 65L05, 65L20

* This work was partially supported under NSERC Canada Grant OGP0004306 and by the German Science Foundation.

1. Introduction. There has been much recent interest in the numerical integration of Hamiltonian systems

$$q' = +\nabla_p H(q,p) \\ p' = -\nabla_q H(q,p) \tag{1}$$

where $q, p \in \mathbf{R}^n$, and $H : \mathbf{R}^{2n} \to \mathbf{R}$ is sufficiently smooth. In applications, typically arising in the context of mechanics [3], astronomy [3], and molecular dynamics [1], the Hamiltonian H is of the form

$$H(q,p) = \frac{p^t M^{-1} p}{2} + V(q) \tag{2}$$

where M is the positive definite mass matrix of the system. This results in the Hamiltonian system

$$q' = M^{-1}p \\ p' = -\nabla V(q) \tag{3}$$

The flow of a Hamiltonian system (1), (3) respectively, is known to be symplectic, i.e., the differential 2-form

$$dq \wedge dp = \sum_{i=1}^{n} dq^i \wedge dp^i \tag{4}$$

is preserved [3]. Another preserved quantity is the Hamiltonian H which is a first integral of (1), (3) respectively, i.e.

$$H(q(t), p(t)) = \text{const.} \tag{5}$$

along solutions.

Much recent research has gone into developing numerical discretization schemes that inherit the symplectic structure of the original system (see, e.g., Sanz-Serna's overview [25] on this subject). It has been observed [10], [21] 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 preserve the Hamiltonian H to high accuracy over long periods of time [6].

A natural question is what happens when (1) is constrained by algebraic equations on q and/or p. In this paper, we restrict ourselves to the case of holonomic constraints

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

$g : \mathbf{R}^n \to \mathbf{R}^m$. One way to derive the corresponding equations of motion is to replace the constraints by a potential which grows large when the system deviates from the locus of the constraints [4], [23]. This can, e.g., be achieved by using the following modified Hamiltonian H_C

$$H_C(q,p) = H(q,p) + \frac{1}{2\epsilon} g(q)^t g(q)$$

$0 < \epsilon << 1$, with the corresponding equations of motion

$$\begin{aligned} q' &= +\nabla_p H(q,p) \\ p' &= -\nabla_q H(q,p) - \tfrac{1}{\epsilon} G(q)^t\, g(q) \end{aligned} \tag{7}$$

where $G(q)^t = \nabla_q g(q) = g_q(q)^t \in \mathbf{R}^{n\times m}$. By introducing the new variable $\lambda \in \mathbf{R}^m$

$$\lambda = \frac{1}{\epsilon} g(q)$$

these equations can be rewritten as

$$\begin{aligned} q' &= +\nabla_p H(q,p) \\ p' &= -\nabla_q H(q,p) - G(q)^t\, \lambda \\ \lambda &= \frac{1}{\epsilon} g(q) \end{aligned}$$

which in the limit $\epsilon \to 0$ gives rise to the constrained Hamiltonian system

$$\begin{aligned} q' &= +\nabla_p H(q,p) \\ p' &= -\nabla_q H(q,p) - G(q)^t\, \lambda \\ 0 &= g(q) \end{aligned} \tag{8}$$

Note that the same equations could be derived directly from a constrained Lagrange-type variational principle [4].

In addition to the explicit constraint (6), there is a hidden constraint

$$0 = G(q)\, \nabla_p H(q,p)$$

$G(q) = g_q(q) \in \mathbf{R}^{m\times n}$, which is obtained by differentiating (6) once with respect to time and substituting $q' = \nabla_p H(q,p)$. A further differentiation of (6) with respect to time yields an equation solvable for λ if

$$G(q) H_{pp}(q,p) G(q)^t \tag{9}$$

is invertible, which we will assume from now on. Thus (8) defines implicitly a Hamiltonian vector field on the $(2n-2m)$-dimensional manifold

$$\mathcal{M} = \{(q,p) : g(q) = 0,\, G(q)\nabla_p H(q,p) = 0\} \tag{10}$$

with the symplectic structure on $\mathcal{M}$ defined by the restriction of the 2-form (4) to $\mathcal{M}$. (See Section 2 for more details.)

In the literature on the numerical integration of differential equations (see, e.g., [9]), constrained systems (8) are called differential-algebraic equations (DAEs) of index three. Discretization schemes suitable for such problems have been derived (see, e.g., [5], [11]). However, none of these schemes can automatically be expected to preserve the symplectic structure on $\mathcal{M}$.

Few results have been published so far on the symplectic integration of constrained systems of type (8): In [17], Leimkuhler and Reich suggested to treat the constrained equations (8) via symplectic parametrization of the constraint manifold and by methods based on Dirac's theory on weak invariants. These methods lead to unconstrained Hamiltonian systems of type (1) which can be handled by direct application of symplectic implicit Runge-Kutta methods. However, numerical experiments [17] indicate that those methods suffer some drawbacks concerning the stability and preservation of the constraints and/or the Hamiltonian. In [18], Leimkuhler and Skeel showed that the constrained system (8) with the particular Hamiltonian (2) can be integrated directly by proper modifications [2] of the second order Verlet scheme. The resulting scheme is symplectic and preserves the constraints. More recently it has been shown by Jay [15] and Reich [22] that partitioned Runge-Kutta methods which are symplectic for unconstrained systems (1) also preserve the 2-form (4) when applied directly to the constrained system (8). However, except for the couples of s-stage Lobatto IIIA and Lobatto IIIB methods [15], none of these methods preserves the constraint manifold $\mathcal{M}$. Furthermore, all known symplectic constraint-preserving integrators suffer from step-size restrictions due to stability bounds, i.e., none of the existing methods is algebraically stable [14].

In this paper we suggest a projection technique that allows to apply symplectic integrators, suitable for the integration of unconstrained systems (1), to the integration of constrained systems as well. The resulting schemes preserve the constrained manifold $\mathcal{M}$ and are symplectic on $\mathcal{M}$. As a main consequence of this approach we are able to derive schemes that are A-stable and/or are especially suited for systems with an Hamiltonian of type (2). In particular, we show in Section 3 that any first or second order symplectic integrator can be modified such that the resulting scheme for the constrained formulation (8) is constraint-preserving and symplectic. Higher order methods can then be obtained by a proper composition of these first and second order schemes as discussed, e.g., by McLachlan in [19] for unconstrained systems. While these schemes are based on the direct numerical integration of the constrained formulation (8), in Section 4 we make use of the reformulations of (8) as an unconstrained problem as suggested by Leimkuhler and Reich in [17]. Based on this and the projection technique introduced in Section 3, we show that it is possible to modify any symplectic implicit Runge-Kutta method such that the resulting modified scheme is constraint-preserving and symplectic.

We also give a backward error analysis of the schemes derived in this paper. Similar to the unconstrained case (see, e.g., Auerbach and Friedman [6] or Hairer [13]), we show that the numerical solutions can be formally interpreted as the exact solution of a certain perturbed Hamiltonian system evaluated at discrete time points.

2. Mathematical Background. In this section we summarize a few results on Hamiltonian systems and symplectic integrators as needed throughout this paper. We start with the unconstrained formulation (1). Upon introducing the (generalized) Poisson bracket

$$\{F, G\} \;=\; F_q\, G_p^t - F_p\, G_q^t \tag{11}$$

where $F : \mathbf{R}^{2n} \to \mathbf{R}^l$ and $G : \mathbf{R}^{2n} \to \mathbf{R}^k$, $k, l \geq 1$, are sufficiently smooth functions, we can rewrite (1) as

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

with $x = (q^t, p^t)^t$. More generally, the time evolution of any function $f : \mathbf{R}^{2n} \to \mathbf{R}^m$, $m \geq 1$, is given by

$$f' \;=\; \{f, H\}$$

If we introduce furthermore the differential operator D_G, $G : \mathbf{R}^{2n} \to \mathbf{R}$, by

$$D_G\, F \;=\; \{F, G\}$$

then we can rewrite (1) also in the form

$$x' \;=\; D_H\, x$$

with the formal solution given by

$$x(t) \;=\; [\exp{(t D_H)}]\, (x(0))$$

i.e., we denote the flow generated by the differential operator D_H by $\exp{(t D_H)}$. For each t, $|t|$ small enough, the mapping $\exp{(t D_H)}$ is a diffeomorphism in $\mathbf{R}^{2n}$ [3]. The diffeomorphism in $\mathbf{R}^{2n}$ form a group. If ϕ and ψ are two elements in the group, then their composition is denoted by $\phi \cdot \psi$, i.e., $\phi \cdot \psi\, (x) = \phi(\psi(x))$.

The flow of a Hamiltonian vector field (1) has the important property that $\exp{(t D_H)}$ is a canonical map for all t [3], i.e., $\exp{(t D_H)}$ preserves the differential 2-form (4). Furthermore, a mapping $f : \mathbf{R}^{2n} \to \mathbf{R}^m$ satisfies

$$[f \cdot \exp{(t D_H)}]\, (x) \;=\; \text{const.}$$

for all $x \in \mathbf{R}^{2n}$, i.e., is a first integral of (1), if and only if

$$0 \;=\; f' \;=\; \{f, H\}$$

Assume now that the discretization of (1) results in the one-step method

$$x_{k+1} = \Psi_h(x_k) \tag{12}$$

Then Ψ_h is called a symplectic integrator, if it preserves the 2-form (4), i.e., Ψ_h is a canonical mapping for all $h > 0$. In [13], Hairer has proven the following backward error result for symplectic integrators:

For fixed step-size h, there exists a perturbed Hamiltonian function $\tilde{H}$, given in terms of an asymptotic expansion, such that

$$\Psi_h = \exp(hD_{\tilde{H}})$$

i.e., formally, the map Ψ_h can be considered as the time-h-map of the flow corresponding to a perturbed Hamiltonian vector field

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

If Ψ_h is a scheme of order ν, then

$$H = \tilde{H} + O(h^\nu)$$

Yoshida [31] first noticed that for unconstrained systems (1) higher order methods can be constructed by a proper composition of second order symmetric methods such as the implicit midpoint [14] or Verlet [30] method. The idea is the following one: Let Ψ_h denote the time-h-flow defined by a symmetric second order method. Then the composed mapping

$$\Psi_{c_1 h} \cdot \Psi_{c_2 h} \cdot \Psi_{c_1 h} \tag{13}$$

with $2c_1 + c_2 = 1$ and $2c_1^3 + c_2^3 = 0$ is of fourth order. More generally, if Ψ_h is symmetric and of order $\nu = 2l$, $l > 1$, then the composed method (13) with $2c_1 + c_2 = 1$ and $2c_1^{\nu+1} + c_2^{\nu+1} = 0$ is of order $\nu + 2$. The proof of this result is based on the fact that for symmetric methods the corresponding perturbed Hamiltonian $\tilde{H}$ satisfies

$$\tilde{H} = H_0 + h^2 H_2 + h^4 H_4 + \ldots$$

i.e., the odd terms in the Taylor expansion of $\tilde{H}$ with respect to h disappear. Upon rewriting (13) as

$$\exp(c_1 h D_{\tilde{H}}) \cdot \exp(c_2 h D_{\tilde{H}}) \cdot \exp(c_1 h D_{\tilde{H}}) \tag{14}$$

the analysis of (13) can be easily carried out in terms of the Baker-Campbell-Hausdorff (BCH) formula [29] which states that for any two differential operators D_A and D_B, the product of the exponential functions $\exp(hD_A)$ and $\exp(hD_B)$ can be expressed formally as a single exponential function $\exp(hD_C)$ where

$$\begin{aligned} C \;:=\; & A + B + \tfrac{h}{2}\{B, A\} + \\ & + \tfrac{h^2}{12}(\{\{A, B\}, B\} + \{\{B, A\}, A\}) + \tfrac{h^3}{24}\{\{\{A, B\}, B\}, A\} + \\ & + \;\ldots \end{aligned} \tag{15}$$

Since $hD_A = D_{hA}$ for arbitrary functions $A : \mathbf{R}^{2n} \to \mathbf{R}$, the BCH formula (15) can be applied to (14) and after repeated application of (15) we obtain a differential operator $D_{\tilde{H}_Y}$ with

$$\tilde{H}_Y = (2c_1 + c_2)H_0 + h^2(2c_1^3 + c_2^3)H_2 + O(h^4)$$

Thus, as stated before, (13) is of fourth order if $2c_1 + c_2 = 1$ and $2c_1^3 + c_2^3 = 0$.

Let us turn now to constrained Hamiltonian systems (8). Upon using the Poisson bracket (11), we can rewrite (8) as

$$x' = \{x, H\} + \{x, g\}\lambda \tag{16}$$
$$0 = g \tag{17}$$

Now, since

$$\begin{aligned} 0 &= g' \\ &= \{g, H\} + \{g, g\}\lambda \\ &= \{g, H\} \end{aligned}$$

we obtain the hidden constraint function

$$f := \{g, H\} = G\nabla_p H$$

where $G = g_q$. The constraint manifold (10) becomes

$$\mathcal{M} = \{(q, p) : g(q) = 0,\ f(q, p) = 0\}$$

and the symplectic structure on $\mathcal{M}$ is given by the restriction of (4) to $\mathcal{M}$ [4].

The hidden constraint function f has again to satisfy

$$\begin{aligned} 0 &= f' \\ &= \{f, H\} + \{f, g\}\lambda \end{aligned}$$

Now, since we assumed

$$\{f, g\}(x) = G(q)\, H_{pp}(q, p)\, G(q)^t$$

to be invertible, the algebraic variable λ is determined by

$$\lambda = -\{f, g\}^{-1}\{f, H\} \tag{18}$$

By substituting this expression for λ in (16), we obtain the unconstrained formulation

$$x' = \{x, H\} - \{x, g\}\{f, g\}^{-1}\{f, H\} \tag{19}$$

Since the algebraic variable λ in (8) is obtained by differentiating the constraint function g twice, the constraint formulation (8) is a particular example of a differential-algebraic equation (DAE) of index three [9].

The equation (19) is not Hamiltonian under the Poisson bracket $\{\,,\,\}$. A Hamiltonian formulation can be obtained upon introducing the modified Hamiltonian

$$H_{\mathcal{M}} = H + g^t\lambda$$

where λ as a function of x is again given by (18). This gives rise to the unconstrained Hamiltonian system

$$
\begin{aligned}
x' &= \{x, H_{\mathcal{M}}\} \\
&= \{x, H\} + \{x, g\}\lambda + \{x, \lambda\}g
\end{aligned}
\tag{20}
$$

which, since $g = 0$ on $\mathcal{M}$, coincides with (19) on $\mathcal{M}$.

As suggested by Leimkuhler and Reich, the unconstrained formulation (20) can now be integrated by any symplectic integrator suitable for the integration of systems of type (1). However, the resulting schemes will, in general, not preserve the constraint manifold $\mathcal{M}$. The same is true for the direct numerical integration of the constrained formulation (8) by symplectic implicit Runge-Kutta methods [22]. To overcome this problem, we will introduce in the following section a projection technique that allows to modify most of these schemes in such a way that they are not only symplectic but also preserve the constraint manifold $\mathcal{M}$.

3. Symplectic Integration of the Constrained Formulation.

3.1. First and Second Order Methods. In this section, we derive first and second order symplectic, constraint-preserving integrators for constrained systems (8). These schemes are based on the composition of a first or second order symplectic integrator for unconstrained systems and the mapping

$$
\begin{aligned}
\bar{q} &= q \\
\bar{p} &= p - h\, G(q)^t\, \Lambda(q, p)
\end{aligned}
\tag{21}
$$

where the function Λ has to be chosen in a proper way such that the overall scheme satisfies the constraints. For the analysis of theses schemes we need the following:

LEMMA 3.1. *Let $\Lambda : \mathbf{R}^{2n} \to \mathbf{R}^m$ be an arbitrary function of $x = (q^t, p^t)^t$ and let q satisfy $g(q) = 0$. Then the mapping* (21) *is a canonical map, i.e., preserves the 2-form* (4).

Proof: The discretization of the unconstrained Hamiltonian system (1) with Hamiltonian $H = g^t \Lambda$ by the first order symplectic Euler method [31] results in the symplectic map

$$
\begin{aligned}
\bar{q} &= q + h\Lambda_p(\bar{q}, p)^t g(\bar{q}) \\
\bar{p} &= p - h[\Lambda_q(\bar{q}, p)^t g(\bar{q}) + G(\bar{q})^t \Lambda(\bar{q}, p)]
\end{aligned}
\tag{22}
$$

This map reduces to (21) under the assumption that $g(q) = g(\bar{q}) = 0$. This proves the symplecticity of (21). □

According to the backward error result due to Hairer [19], there exists, in terms of an asymptotic expansion, a perturbed Hamiltonian function $\tilde{H}$ such that (22) is the exact time-h-flow of the Hamiltonian system (1) with Hamiltonian $H = \tilde{H}$. Under the assumption that $g(q) = 0$, the perturbed Hamiltonian $\tilde{H}$ can be written as $\tilde{H} = g^t \tilde{\Lambda}$ with $\tilde{\Lambda}$ being now a perturbation of the function Λ. Thus, with a slight abuse of notation, we can rewrite the mapping (21) as $\exp(hD_{g^t\tilde{\Lambda}})$. For notational simplicity, we will not distinguish between $\tilde{\Lambda}$ and Λ and will simply write $\exp(hD_{g^t\Lambda})$ instead of $\exp(hD_{g^t\tilde{\Lambda}})$.

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

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

associated to the constrained problem

$$\begin{aligned} x' &= \{x,H\} + \{x,g\}\lambda \\ 0 &= g \end{aligned} \tag{23}$$

Then we suggest the following scheme for the integration of the constrained problem (23):
Step 1.

$$\begin{aligned} \bar{q}_k &= q_k \\ \bar{p}_k &= p_k - \frac{h}{2} G(q_k)^t \Lambda_k \end{aligned}$$

Step 2.

$$\begin{pmatrix} \bar{q}_{k+1} \\ \bar{p}_{k+1} \end{pmatrix} = \Psi_h \begin{pmatrix} \bar{q}_k \\ \bar{p}_k \end{pmatrix}$$

Step 3.

$$\begin{aligned} q_{k+1} &= \bar{q}_{k+1} \\ p_{k+1} &= \bar{p}_{k+1} - \frac{h}{2} G(\bar{q}_{k+1})^t \Lambda_{k+1} \end{aligned}$$

with Λ_k chosen such that

$$0 = g(q_{k+1})$$

and Λ_{k+1} chosen such that

$$0 = f(q_{k+1}, p_{k+1})$$

For the analysis of this scheme it is convenient to use the following backward error result for the mapping Ψ_h due to Hairer [13] (see also Section 2): There exists, in terms of an asymptotic expansion, a perturbed Hamiltonian function $\tilde{H}$ such that

$$\Psi_h = \exp(hD_{\tilde{H}})$$

and $\tilde{H} = H + O(h^\nu)$, $\nu = 1, 2$ depending on whether Ψ_h is of first or second order. Thus, using also the fact that the mapping (21) is equivalent to $\exp(hD_{g^t\Lambda})$, the above scheme can be rewritten as $\Phi_h : \mathcal{M} \to \mathcal{M}$ with Φ_h defined by

$$\Phi_h := \exp\left(\frac{h}{2} D_{g^t\Lambda_{k+1}}\right) \cdot \exp(hD_{\tilde{H}}) \cdot \exp\left(\frac{h}{2} D_{g^t\Lambda_k}\right) \tag{24}$$

subject to

$$0 \;=\; g \cdot \Phi_h \;=\; f \cdot \Phi_h$$

THEOREM 3.2. *The scheme (24) is symplectic, constraint-preserving, and of the same order as Ψ_h, i.e., of first or second order depending on whether Ψ_h is of first or second order.*

Proof: The first two properties are obvious. To prove the order result we make use of the Baker-Campbell-Hausdorff formula (15) which, applied twice to (24), yields

$$\Phi_h \;=\; \exp\left(hD_{\tilde{H}_{\mathcal{M}}}\right)$$

where $\tilde{H}_{\mathcal{M}}$ is given by

$$\begin{aligned} \tilde{H}_{\mathcal{M}} \;&=\; \tilde{H} + \tfrac{1}{2}g^t(\Lambda_k + \Lambda_{k+1}) + \\ &\quad + \tfrac{h}{4}(\{g, \tilde{H}\}(\Lambda_k - \Lambda_{k+1})) + O(h^2) \end{aligned} \tag{25}$$

Note that the mapping Φ_h can be formally extented to a neighborhood of $\mathcal{M}$ in $\mathbf{R}^{2n}$ by replacing the map (21) in Step1 and 3 of the above scheme by the map (22) as done before in the proof of Lemma 3.1. Thus all the necessary differentiations can be carried out in $\mathbf{R}^{2n}$. However, the results restricted to $\mathcal{M}$ do not depend on such an extension.

Now, since

$$\begin{aligned} 0 \;&=\; f \cdot \Phi_h \\ &=\; f \cdot \exp\left(hD_{\tilde{H}_{\mathcal{M}}}\right) \end{aligned}$$

we obtain (see Section 2)

$$\begin{aligned} 0 \;&=\; \{f, \tilde{H}_{\mathcal{M}}\} \\ &=\; \{f, \tilde{H}\} + \frac{1}{2}\{f, g\}(\Lambda_k + \Lambda_{k+1}) + O(h) \end{aligned}$$

which, together with $\tilde{H} = H + O(h)$, implies that

$$\frac{1}{2}(\Lambda_k + \Lambda_{k+1}) \;=\; \lambda + O(h)$$

with λ given by (18). Thus, if Ψ_h is of first order, then

$$\tilde{H}_{\mathcal{M}} = H_{\mathcal{M}} + O(h)$$

with $H_{\mathcal{M}} = H + g^t\lambda$ as in Section 2. In case that Ψ_h is of second order, $g \cdot \Phi_h = 0$ implies that

$$\begin{aligned} 0 \;&=\; \{g, \tilde{H}_{\mathcal{M}}\} \\ &=\; \{g, \tilde{H}\} + \frac{h}{4}\{g, \{g, \tilde{H}\}\}(\Lambda_k - \Lambda_{k+1}) + O(h^2) \\ &=\; f + \frac{h}{4}\{g, f\}(\Lambda_k - \Lambda_{k+1}) + O(h^2) \end{aligned}$$

and therefore

$$\Lambda_k - \Lambda_{k+1} \;=\; O(h)$$

Since now also

$$\Lambda_k + \Lambda_{k+1} \;=\; \lambda + O(h^2)$$

we finally obtain

$$\tilde{H}_{\mathcal{M}} \;=\; H_{\mathcal{M}} + O(h^2)$$

which proves the second order convergence of the scheme. □

Remark: The parameters Λ_k and Λ_{k+1} are determined in the k-th integration step by the nonlinear equations $g \cdot \Phi_h\,(q_k, p_k) = 0$, $f \cdot \Phi_h\,(q_k, p_k) = 0$ respectively. Since we assumed that $G(q)H_{pp}(q,p)G(q)^t$ is invertible, these equations have a locally unique solution for h small enough and the nonlinear equations ca be solved conveniently by Newton's method. If necessary, an excellent initial guess for Λ_k and Λ_{k+1} can be obtained from $\lambda(q_k, p_k$ and using the above error analysis. □

Remark: The proof of Theorem 3.2 also provides a backward error analysis similar to that given by Hairer in [13] for unconstrained systems, i.e., there exists, in terms of an asymptotic expansion, a perturbed Hamiltonian function $\tilde{H}_{\mathcal{M}}$ with

$$0 \;=\; \{g, \tilde{H}_{\mathcal{M}}\} \;=\; \{f, \tilde{H}_{\mathcal{M}}\}$$

on $\mathcal{M}$ (meaning that $\mathcal{M}$ is an invariant manifold) and

$$\tilde{H}_{\mathcal{M}} \;=\; H_{\mathcal{M}} + O(h^\nu)$$

with $\nu = 1, 2$ depending on the order of the scheme (24) such that

$$\Phi_h \;=\; \exp\left(hD_{\tilde{H}_{\mathcal{M}}}\right)$$

□

Let us discuss now the scheme (24) for different choices of the integrator Ψ_h and for Hamiltonian functions of the form

$$H(q,p) \;=\; \frac{p^t M^{-1} p}{2} + V(q)$$

We start with the first order symplectic Euler method [24]. In this case the iteration for the q-variable becomes:

$$q_{k+1} \;=\; q_k + hM^{-1}p_k - h^2 M^{-1}\nabla V(q_k) - \frac{h^2}{2} M^{-1} G(q_k)^t \Lambda_k$$

subject to

$$0 \;=\; g(q_{k+1})$$

The p-variable is updated by

$$p_{k+1} = p_k - h\nabla V(q_k) - \frac{h}{2}(G(q_k)^t\Lambda_k + G(q_{k+1})^t\Lambda_{k+1})$$

where Λ_{k+1} is now determined by the constraint

$$0 \;=\; G(q_{k+1})\, M^{-1} p_{k+1}$$

A second order algorithm can be obtained by applying the popular Verlet scheme [30] to (24). We obtain

$$\begin{aligned} q_{k+1} &= q_k + hM^{-1}p_{k+1/2} \\ p_{k+1/2} &= p_k - \frac{h}{2}(\nabla V(q_k) + G(q_k)^t\Lambda_k) \\ 0 &= g(q_{k+1}) \end{aligned}$$

and

$$\begin{aligned} p_{k+1} &= p_{k+1/2} - \frac{h}{2}(\nabla V(q_{k+1}) + G(q_{k+1})^t\Lambda_{k+1}) \\ 0 &= G(q_{k+1})\, M^{-1} p_{k+1} \end{aligned}$$

This scheme is identical to the one derived by Anderson in [2]. It was first shown to be symplectic by Leimkuhler and Skeel in [18].

While these two schemes suffer from severe step-size restrictions due to the stability bounds of the method (which in the linear case are identical to the stability bounds for the corresponding unconstrained scheme), application of the implicit midpoint rule to (24) results in an algebraically stable method [14]. Now the iteration in the q-variable becomes

$$\begin{aligned} q_{k+1} &= q_k + hM^{-1}p_k - \frac{h^2}{2}M^{-1}\nabla V(\frac{q_k + q_{k+1}}{2}) - \frac{h^2}{2}M^{-1}G(q_k)\Lambda_k \\ 0 &= g(q_{k+1}) \end{aligned}$$

and the p-variable is updated by

$$\begin{aligned} p_{k+1} &= p_k - h\nabla V(\frac{q_k + q_{k+1}}{2}) - \frac{h}{2}(G(q_k)^t\Lambda_k + G(q_{k+1})^t\Lambda_{k+1}) \\ 0 &= G(q_{k+1})\, M^{-1} p_{k+1} \end{aligned}$$

This scheme is computationally far more expensive than the modified Verlet scheme. However, it can be applied to problems with an Hamiltonian

$$H(q,p) \;=\; \frac{p^t M^{-1} p}{2} + V_1(q) + \frac{1}{\epsilon}V_2(q)$$

where $\epsilon > 0$ is a small number. This type of Hamiltonian systems arise, for example, in molecular dynamics simulations [1],[27].

Any other symplectic, second order method for unconstrained problems, such as the multiple-time-step methods [8] etc., can now be generalized to the constrained case along the same lines. This is especially useful whenever one wishes to exploit the special structure of the Hamiltonian H. Based on these second order schemes, methods of higher order can be constructed, e.g., by Yoshida's method [31], or, more generally, by composition methods as discussed, e.g., by McLachlan in [19]. This is the subject of the following subsection.

3.2. Higher Order Methods. As mentioned in Section 2, Yoshida [31] noticed that for unconstrained systems higher order methods can be constructed by a proper composition of second order symmetric methods such as the midpoint or Verlet method.

Let us now generalize this result to constrained systems (23). As in Section 3.1, let Ψ_h be a symmetric second order discretization of the corresponding unconstrained problem. Then we use the mapping

$$\Phi_h \quad := \quad \Psi_h \cdot \exp\left(\frac{h}{2} D_{g^t\Lambda}\right) \tag{26}$$

with Λ chosen such that $g \cdot \Phi_h = 0$, as the basic method in the construction of higher order methods. Note that (26) is the same as (24) except that we do not project down onto $f = 0$. Let us consider now the following composition

$$\exp\left(\frac{h}{2} D_{g^t\Lambda}\right) \cdot \Phi_{c_1 h} \cdot \Phi_{c_2 h} \cdot \Phi_{c_1 h} \tag{27}$$

with Λ such that $f = 0$. This scheme is clearly symplectic and constraint-preserving. Furthermore:

THEOREM 3.3. *The scheme* (27) *with* $2c_1 + c_2 = 1$ *and* $2c_1^3 + c_2^3 = 0$ *is of fourth order. If* Φ_h *is already of order* $\nu = 2l$, $l > 1$ *and symmetric, then the composed method* (27) *with* $2c_1 + c_2 = 1$ *and* $2c_1^{\nu+1} + c_2^{\nu+1} = 0$ *is of order* $\nu + 2$.

Proof: Let us consider first the composition

$$\Phi_{c_1 h} \cdot \Phi_{c_2 h} \cdot \Phi_{c_1 h} \tag{28}$$

with

$$\Phi_h \quad = \quad \exp\left(\frac{h}{2} D_{g^t\Lambda}\right) \cdot \Psi_h \cdot \exp\left(\frac{h}{2} D_{g^t\Lambda}\right) \tag{29}$$

and Λ chosen such that $g \cdot \Phi_h = 0$. Since (29) is now symmetric, the corresponding perturbed Hamiltonian $\tilde{H}$ of (29) satisfies

$$\tilde{H} \quad = \quad H_0 + h^2 H_2 + h^4 H_4 + \ldots$$

and application of the Baker-Campbell-Hausdorff formula to the composition (28) immediately yields the same order conditions as found by Yoshida for unconstrained systems. The method (28) preserves $g = 0$ but not $f = 0$. However, since the method (28) satisfies $f = O(h^{\nu+1})$, an additional projection step $\exp\left(\frac{h}{2} D_{g^t\Lambda}\right)$ onto the constraint $f = 0$ will not destroy the overall order of the scheme. Moreover, the effect of

$\exp(c_i \frac{h}{2} D_{g^t\Lambda})$ at the end of each application of (29) gets canceled by the subsequent application of the same map (but different internal step-size c_i) onto that result. Thus (29) can be replaced by (26) and we obtain the composition (27). Along the same lines all of Yoshida's higher order methods can now be generalized to constrained systems. $\Box$

There exist other, sometimes even more efficient, composition methods. A careful discussion of such methods for unconstrained systems (1) has been given by McLachlan in [19]. Since all these methods are based on a proper application of the Baker-Campbell-Hausdorff formula, one can generalize them to constrained problems as outlined above for Yoshida's method.

4. Symplectic Integrators for the Unconstrained Formulation. In this section, we use the reformulation of (8) as an unconstrained problem

$$
\begin{aligned}
x' &= \{x, H_{\mathcal{M}}\} \\
&= \{x, H\} + \{x, g\}\,\lambda + \{x, \lambda\}\,g
\end{aligned}
\tag{30}
$$

with λ as a function of x given by (18), to derive higher order symplectic and constraint-preserving schemes.

As suggested by Leimkuhler and Reich [17], (30) can be discretized by any symplectic integrator suited for the discretization of general Hamiltonian systems of type (1). However, those schemes, although symplectic, will not, in general, preserve the constraint manifold $\mathcal{M}$. In fact, for some formulations an exponential instability with respect to the constraints was observed [17]. Here we suggest instead to remove these instabilities by applying the same projection technique as used throughout Section 3. Specifically:

Let Ψ_h be any symplectic integrator for the unconstrained Hamiltonian system (30). Let $\tilde{H}$ be the corresponding perturbed Hamiltonian function, i.e., $\Psi_h = \exp(hD_{\tilde{H}})$ and $\tilde{H} = H_{\mathcal{M}} + O(h^\nu)$ where ν is the order of the scheme Ψ_h. Then we suggest the following constraint preserving integrator $\Phi_h : \mathcal{M} \to \mathcal{M}$:

$$
\Phi_h \;:=\; \exp(\frac{h}{2} D_{g^t\Lambda_{k+1}}) \cdot \exp(hD_{\tilde{H}}) \cdot \exp(\frac{h}{2} D_{g^t\Lambda_k})
\tag{31}
$$

with Λ_k and Λ_{k+1} chosen such that

$$
0 \;=\; g \cdot \Phi_h \;=\; f \cdot \Phi_h
$$

THEOREM 4.1. *The scheme* (31) *is symplectic, constraint-preserving, and of the same order as* $\Psi_h = \exp(hD_{\tilde{H}})$.

Proof: The first two properties are again obvious. To prove the order result, note that

$$
g \cdot \Psi_h \;=\; O(h^{\nu+1})
$$

and

$$
f \cdot \Psi_h \;=\; O(h^{\nu+1})
$$

where ν is the order of the scheme Ψ_h. Upon rewriting Ψ_h as

$$\begin{aligned} q_{k+1} &= q_k + h\,F_q(q_k, p_k) \\ p_{k+1} &= p_k + h\,F_p(q_k, p_k) \end{aligned}$$

it follows easily that Λ_k and Λ_{k+1} satisfy

$$\Lambda_k \;=\; O(h^{\nu-1}) \tag{32}$$

and, since $G(q_{k+1})^t = G(q_k)^t + O(h)$,

$$\Lambda_k + \Lambda_{k+1} \;=\; O(h^{\nu}) \tag{33}$$

Furthermore, as in the proof of Theorem 3.2, there exists a perturbed Hamiltonian function $\tilde{H}_{\mathcal{M}}$ such that

$$\Phi_h \;=\; \exp\left(hD_{\tilde{H}_{\mathcal{M}}}\right)$$

the asymptotic expansion of $\tilde{H}_{\mathcal{M}}$ is again given by (25) plus terms of higher order that either contain Λ_k and/or Λ_{k+1}. Since Λ_k and Λ_{k+1} satisfy (32), (33) respectively, (25) yields

$$\tilde{H}_{\mathcal{M}} \;=\; H_{\mathcal{M}} + O(h^{\nu})$$

with $H_{\mathcal{M}} = H + g^t\lambda$ as in Section 2. □

Let us assume that the system (30) is discretized by a symplectic Runge-Kutta method with Butcher's tableau [14]

$$\begin{array}{c|c} c & A \\ \hline & b^t \end{array}$$

Upon using tensor product notation [16], the scheme (31) becomes

$$\begin{aligned} q_{k+1} &= q_k + h(b^t \otimes I)\nabla_p H_{\mathcal{M}} \\ \bar{p}_{k+1} &= p_k - h(b^t \otimes I)\nabla_q H_{\mathcal{M}} - \tfrac{h}{2}G(q_k)^t\Lambda_k \\ \\ Q &= e \otimes q_k + h(A \otimes I)\nabla_p H_{\mathcal{M}} \\ P &= e \otimes p_k - h(A \otimes I)\nabla_q H_{\mathcal{M}} - \tfrac{h}{2}\, e \otimes G(q_k)^t\Lambda_k \\ \\ 0 &= g(q_{k+1}) \end{aligned} \tag{34}$$

and

$$\begin{aligned} p_{k+1} &= \bar{p}_{k+1} - \frac{h}{2}G(q_{k+1})^t\Lambda_{k+1} \\ 0 &= f(q_{k+1}, p_{k+1}) \end{aligned}$$

where $e^t = [1, 1, \ldots, 1]$, I is the identity matrix, and

$$Q = \begin{bmatrix} Q^1 \\ Q^2 \\ \cdot \\ \cdot \\ \cdot \\ Q^s \end{bmatrix}, \qquad \nabla_p H_{\mathcal{M}} = \begin{bmatrix} \nabla_p H_{\mathcal{M}}(Q^1, P^1) \\ \nabla_p H_{\mathcal{M}}(Q^2, P^2) \\ \cdot \\ \cdot \\ \cdot \\ \nabla_p H_{\mathcal{M}}(Q^s, P^s) \end{bmatrix}$$

etc. Provided that A is invertible and h is sufficiently small, the existence and local uniqueness of the solution $(q_{k+1}, \bar{p}_{k+1}, \Lambda_k)$ in (34) can be shown. Furthermore, the nonlinear system of equations (34) can be solved by simplified Newton iterations with the approximate Jacobian

$$\begin{pmatrix} I_{sn} & -h\, A \otimes H_{pp}(q_k, p_k) & 0 \\ 0 & I_{sn} & \frac{h}{2}\, e \otimes G(q_k)^t \\ 0 & h\, b^t \otimes G(q_k)^t H_{pp}(q_k, p_k) & 0 \end{pmatrix}$$

Theorem 4.1 provides an easy way to derive higher order symplectic and constraint-preserving integrators. Any method suitable for general, non-separable Hamiltonians can be applied. However, even if H is separable, the corresponding Hamiltonian $H_{\mathcal{M}} = H + g^t \lambda$ will, in general, not be separable. In those cases, the methods derived in Section 3 can be computationally far less expensive than those considered in this section.

5. Numerical Example. A typical example of a constrained Hamiltonian system is given by the planar mathematical pendulum [7]. Using cartesian coordinates $q = (q_x, q_y)^t$ for the description of the position of the pendulum, the holonomic constraint on the length L of the rod is given by

$$0 = \sqrt{q_x^2 + q_y^2} - L$$

The Hamiltonian H in (23) can be expressed by

$$H(q, p) = \frac{p_x^2 + p_y^2}{2m} + mgq_y \tag{35}$$

and the equations of motion (23) become

$$\begin{aligned} q_x' &= \tfrac{p_x}{m} \\ q_y' &= \tfrac{p_y}{m} \\ p_x' &= -\tfrac{q_x}{L}\lambda \\ p_y' &= -mg - \tfrac{q_y}{L}\lambda \\ 0 &= \sqrt{q_x^2 + q_y^2} - L \end{aligned} \tag{36}$$

Here g denotes the gravitational constant. The hidden constraint is given by

$$0 = q_x\, p_x + q_y\, p_y$$

and equation (18) results in

$$\lambda = \frac{1}{L}(\frac{p_x^2 + p_y^2}{m} - mgq_y)$$

If the pendulum is started from rest with an initial angle of displacement ϕ_0, then the analytic solution of the corresponding initial value problem has period [7]

$$T = 4\sqrt{\frac{L}{g}} \int_0^{\frac{1}{2}\pi} \frac{du}{\sqrt{1 - \sin^2 u \, \sin^2 \frac{1}{2}\phi_0}}$$

which for our choice of the initial conditions ($\phi_0 = \pi/2$) becomes

$$T \approx 7.416298709\ldots$$

We have applied three different fourth order symplectic, constraint-preserving integrators with step-size $h = 0.04T$. We put $m = 1$, $g = 1$, $L = 1$, and chose consistent initial values $q_y = p_x = p_y = 0$, $q_x = 1$.

Since (35) is separable, we can integrate (36) with the second order modified Verlet scheme (see Section 3.1). Based on this, a fourth order integrator was obtained by applying Yoshida's idea (13). We also integrated (36) by applying the stabilized fourth order 2-stage Gauss-Legendre Runge-Kutta method [14] to the unconstrained reformulation of (36). For comparison we applied the fourth order 3-stage Lobatto IIIA-IIIB pair of Jay [15] to the constrained formulation (36) and also integrated the Hamiltonian state-space form

$$\phi'' = -\sin(\phi)$$

by the fourth order 2-stage Gauss-Legendre Runge-Kutta method.

In Table 1 we have plotted the phase error in the computed p_y at $t_k = l\,T$, $l = 1, 2, 4$, which is linear in l. (The exact solution would be $p_y(t_k) = 0$.) Note that this error behavior corresponds to the linear growth in the phase error for the symplectic integration of the Kepler problem [3] as rigorously proved by Calvo and Sanz-Serna in [10]. A non-symplectic integration of this mechanical system, as suggested, e.g., by Ascher, Chin and Reich in [5], results in a strongly damped oscillation with its equilibrium at $q_y = -1$. This was observed by applying the fourth order BDF-method [14].

We found that for all symplectic discretizations of (36) the numerical Hamiltonian remained bounded and did not grow with time. This corresponds to the behavior of symplectic integrators for unconstrained problems (1) [25]. In Table 2 we have plotted the maximum error in the numerical Hamiltonian for each method and step-size $h = 0.04T$ and $h = 0.004T$.

Among the symplectic methods, the quantitatively best results were obtained for the Gauss-Legendre and the Lobatto IIIA-IIIB Runge-Kutta methods. However, as we will discuss in more detail in the Conclusions, these methods are computational far more expensive than the fourth order method based on the modified Verlet scheme.

discretization scheme	h	$\lvert p_y(T)\rvert$	$\lvert p_y(2T)\rvert$	$\lvert p_y(4T)\rvert$
Yoshida	$0.04T$	.77e-1	.15	.31
Gauss-Legendre	$0.04T$	.71e-3	.14e-2	.28e-2
Lobatto	$0.04T$	.34e-3	.68e-3	.14e-2
SSF	$0.04T$	.26e-4	.52e-4	.10e-3

TABLE 1

Phase error in the variable p_y

discretization scheme	h	error	h	error
Yoshida	$0.04T$	.15e-1	$0.004T$	.86e-6
Gauss-Legendre	$0.04T$	.97e-4	$0.004T$	.10e-7
Lobatto	$0.04T$	.47e-4	$0.004T$	.47e-8
SSF	$0.04T$	.11e-4	$0.004T$	.11e-8

TABLE 2

Maximum error in the numerical Hamiltonian

6. Conclusions. In many applications, such as molecular dynamics and rigid bodies, the Hamiltonian is of the form (2) where the computation of $\nabla V(q)$ is rather expensive. The most popular second order scheme for the numerical integration of the corresponding constrained system is the modified Verlet scheme of Section 3.1 [28]. Although it requires the solution of a nonlinear system of equations, only one evaluation of $\nabla V(q)$ is needed per integration step. As pointed out in Section 3.2, based on the second order Verlet scheme, higher order methods can be obtained, e.g., by Yoshida's method. For example, the resulting fourth order scheme requires now 3 evaluations of $\nabla V(q)$ per integration step and the solution of three m-dimensional nonlinear systems of equations in the parameter Λ. However, the local truncation error of these methods is rather large (see also McLachlan's discussion on this subject for unconstrained problems in [19]). A far better local truncation error can be achieved with Jay's higher order Lobatto IIIA-IIIB pairs. In fact, the numerical results of Section 5 indicate that one has to use an about three times smaller step-size for the fourth order Yoshida method to obtain the same local discretization error as for the fourth order Lobatto method. But the 3-stage method requires $2l$ evaluations of $\nabla V(q)$ where l is the number of Newton iterations needed for solving the corresponding, in general, $2(n+m)$ dimensional nonlinear system of equations [18]. Thus, whenever $n \gg m$, the computation of $\nabla V(q)$ is expensive, and no extremely high-accuracy in the solutions is required, it seems preferable to use composition methods as discussed in this paper. Such problems arise, for example, in the context of molecular dynamics simulations [1].

All the methods discussed so far have in common that they are not suited for the integration of Hamiltonians (2) with

$$V(q) \;=\; V_1(q) + \frac{1}{\epsilon} V_2(q)$$

where $\epsilon > 0$ is a small parameter. Such problems arise, for example, in the context of molecular dynamics simulations [27]. In this case one could either use multiple-time-step methods [8] or the implicit midpoint rule as the basic integrator in (24). Another possibility would be to use the following combination of the midpoint and Verlet scheme: Discretize the Hamiltonian

$$H_s(q,p) \;=\; \frac{p^t M^{-1} p}{2} + \frac{1}{\epsilon} V_2(q)$$

by the implicit midpoint rule and call the resulting scheme Ψ_h^s. Then

$$\Psi_h \;=\; \exp\left(\frac{h}{2} D_{V_1}\right) \cdot \Psi_h^s \cdot \exp\left(\frac{h}{2} D_{V_1}\right)$$

is a second order discretization of the Hamiltonian system corresponding to the Hamiltonian (2). Based on Ψ_h, a second order integrator for the corresponding constrained problem can be found as suggested in Section 3.1. This scheme should be useful for problems where the computation of $\nabla V_1(q)$ is rather expensive compared to the computation of $\nabla V_2(q)$.

Disregarding computational costs, very accurate and robust methods are obtained by using the schemes derived in Section 4. However, these schemes require the explicit computation of λ and its derivatives with respect to q and p. Thus, they should be applied only if a very high accuracy of the solution is needed.

7. Acknowledgement. The current work was done while the author was visiting the University of British Columbia. The author would also like to thank Uri Ascher and Ben Leimkuhler for many fruitful discussions.

REFERENCES

[1] Allen, M.P. and Tildesley, D.J., *Computer Simulations of Liquids*, Clarendon Press, Oxford, 1987.
[2] Anderson, H.C., RATTLE: A 'Velocity' Version of the SHAKE Algorithm for Molecular Dynamics Calculations, *J. Comp. Phys.*, 52(1983), 24–34.
[3] Arnold, V.I., *Mathematical Methods of Classical Mechanics*, Springer–Verlag, NY, 1975.
[4] Arnold, V.I., *Dynamical Systems III*, Springer–Verlag, NY, 1988.
[5] Ascher, U.M., Chin, H., and Reich, S., Stabilization of DAEs and Invariant Manifolds, to appear, *Num. Math.*, 67(1994), 131–149.
[6] Auerbach, S.P. and Friedman, A., Long-Term Behavior of Numerically Computed Orbits: Small and Intermediate Timestep Analysis of One-Dimensional Systems, *J. Comput. Phys.*, 93(1991), 189–223.
[7] Banach, S., *Mechanics*, Monografie Matematyczne, Tom XXIV, Warsawa, 1951.
[8] Biesiadecki, J.J. and Skeel, R.D., Danger of Multiple-Time-Step Methods, *J. Comput. Phys.*, 109(1993), 318–328.
[9] Brenan, K.E., Campbell, S.L., and Petzold, L.R., *Numerical Solution of Initial–Value Problems in DAEs*, North Holland, 1989.
[10] Calvo, M.P. and Sanz-Serna, J.M., The Development of Variable-Step Symplectic Integrators, With Application to the Two-Body Problem, *SIAM J. Sci. Comput.*, 14(1993)4, 936–952.
[11] Gear, C.W., Gupta, G.K., and Leimkuhler, B, Automatic Integration of Euler-Lagrange Equations with Constraints, *J. Comp. Appl. Math.*, 12&13(1985), 77–90.
[12] Griffiths, D.F. and Sanz-Serna, J.M., On the Scope of the Method of Modified Equations, *SIAM J. Sci. Comput.*, 7(1986), 994–1008.

[13] Hairer, E., Backward Analysis of Numerical Integrators and Symplectic Methods, *Annals of Numerical Mathematics*, 1(1994), 107–132.

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

[15] Jay, L., Symplectic Partitioned Runge-Kutta methods for Constrained Hamiltonian Systems, to appear, *SIAM J. Num. Anal.*, 1993.

[16] Lancester, P., *Theory of Matrices*, New York, Academic Press, 1969.

[17] Leimkuhler, B. and Reich, S., Symplectic Integration of Constrained Hamiltonian Systems, to appear, *Math. Comp.*, 63(1994), 589–605.

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

[19] McLachlan, R.I., On the Numerical Integration of Ordinary Differential Equations by Symmetric Composition Methods, to appear, *SIAM J. Sci. Comput.*, 1993.

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

[21] Okunbor, D. and Skeel, R.D., Explicit Canonical Methods for Hamiltonian Systems, *Math. Comp.*, 59(1992), 439–455.

[22] Reich, S., Symplectic Integration of Constrained Hamiltonian Systems by Runge-Kutta Methods, Techn. Report, Univ. of British Columbia, 1993.

[23] Rubin, H. and Ungar, P., Motion under a Strong Constraining Force, *Comm. Pure Appl. Math.*, 10(1957), 65–87.

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

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

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

[27] Skeel, R.D., Biesiadecki, J.J., and Okunbor, D., Symplectic Integration for Macromolecular Dynamics, to appear, *Proc. of the International Conference Computation of Differential Equations and Dynamical Systems*, World Scientific Publishing Co., 1992.

[28] Tobias, D.J., Brooks, C.L., Molecular Dynamics with Internal Coordinate Constraints. *J. Chem. Phys.*, 89(1988), 5115–5127.

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

[30] Verlet, L., Computer 'experiments' on classical fluids, *Phys. Rev.*, 159(1967), 98–103.

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