

SYMPLECTIC INTEGRATORS FOR INDEX 1 CONSTRAINTS*

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Abstract. We show that symplectic Runge–Kutta methods provide effective symplectic integrators for Hamiltonian systems with index 1 constraints. These include the Hamiltonian description of variational problems subject to position and velocity constraints nondegenerate in the velocities, such as those arising in sub-Riemannian geometry and control theory.

Key words. symplectic integrators, differential-algebraic equations, index 1 systems, variational nonholonomic equations, vakonomic equations, optimal control problems

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1. Introduction: Constrained Hamiltonian systems. There are several different types of constrained dynamical systems. First, the constraints themselves can be *holonomic* (depending only on position) or *nonholonomic* (depending on position and velocity but not the derivative of a holonomic constraint). Nonholonomic constraints are associated with two main types of dynamical system (we adopt the terminology of [2]):

1. The *dynamic nonholonomic equations*, also known as the Lagrange–d’Alembert equations, that describe many mechanical systems in rolling and sliding contact. They have been the subject of several studies in geometric numerical integration (see, e.g., [4, 5, 11, 12] and references therein), but as the equations are not in general Hamiltonian or variational and their geometric properties are not fully understood, there is no consensus as to their best discrete version.

2. The *variational nonholonomic equations*, also known as the vakonomic equations, that are the subject of this paper. They arise in two main contexts in dynamics. The first is from the *Lagrange problem*, that of finding curves $q(t)$ in the configuration manifold M that make the action

$$\int_{t_0}^{t_1} L(q, \dot{q}) dt$$

stationary among all curves satisfying the fixed endpoint conditions $q(t_0) = q_0$, $q(t_1) = q_1$ and satisfying the nonholonomic constraints $g(q, \dot{q}) = 0$. If the action has the form

$$\int_{t_0}^{t_1} \langle \dot{q}, \dot{q} \rangle_q dt$$

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for some metric $\langle \cdot, \cdot \rangle_q$ on M and the constraint is that $q(t)$ is tangent to a maximally nonintegrable distribution on M , the Lagrange problem becomes the *sub-Riemannian geodesic problem* that defines the sub-Riemannian geometry of M [7, 13],¹ an active branch of geometry. Some Lie groups (the Carnot groups, of which the Heisenberg group is an example) have a natural sub-Riemannian structure.

The second is in optimal control problems. Under (quite weak) conditions, the Lagrange problem is equivalent to the optimal control problem $\min_u \int_{t_0}^{t_1} g(q, u) dt$ subject to $q(t_0) = q_0$, $q(t_1) = q_1$, and $\dot{q} = f(q, u)$ —the control u can be eliminated [2, Thm. 7.3.3]. Many applications of the variational nonholonomic equations—to kinematic sub-Riemannian optimal control problems, to control on semisimple Lie groups and symmetric spaces, to the motion of a particle in a magnetic field, and to optimal control on Riemannian manifolds and Lie groups—are discussed in detail in Chapter 7 of [2]. Many familiar situations—from parking a car (an example we model numerically in section 5), riding a bike, rolling a ball, to controlling a satellite or a falling cat controlling itself—are described using the variational nonholonomic equations.

A Hamiltonian formulation of the variational nonholonomic equations is to consider

$$(1.1) \quad J\dot{z} = \nabla H(z), \quad z \in C \subset \mathbb{R}^m,$$

where $z \in \mathbb{R}^m$, $\omega := \frac{1}{2}dz \wedge Jdz$ is a closed 2-form,² $H: \mathbb{R}^m \rightarrow \mathbb{R}$ is a Hamiltonian, and C is a constraint submanifold such that $i^*\omega$ (where $i: C \rightarrow \mathbb{R}^m$ is the inclusion of C in \mathbb{R}^m) is nondegenerate, i.e., such that $(C, i^*\omega)$ is a symplectic manifold. The dynamics on C depends only on the restricted Hamiltonian i^*H and restricted symplectic form $i^*\omega$. Indeed, systems with holonomic constraints also take this form, with $z = (q, p)$, $\omega = dq \wedge dp$, and $C = \{(q, p) : h_i(q) = 0, Dh_i(q)H_p(q, p) = 0, 1 \leq i \leq k\}$ consisting of primary and secondary constraints; a nondegeneracy assumption ensures that C is symplectic. The widely used RATTLE method [8, 10] provides a (class of) symplectic integrators for this case when J is constant: it integrates in coordinates z with Lagrange multipliers to enforce the constraints. However, it is striking that there are no known symplectic integrators for general constrained Hamiltonian systems of the form of (1.1).

In this paper we describe a class of symplectic integrators for a class of Hamiltonian systems of the form (1.1) containing constraints that can depend on both position and velocity. The systems are those of index 1 and the integrators are given in Propositions 2.2 and 3.1, which are our main results. The class includes the Hamiltonian description of the variational nonholonomic equations, including the sub-Riemannian geodesic equations, and we give this application first, in Propositions 1.1 and 1.2, as it motivates the consideration of index 1 Hamiltonian systems. The construction is generalized to include both holonomic and nonholonomic constraints in section 4. Sample applications are given to calculating the sub-Riemannian geodesics of a wheeled vehicle (the “parallel parking” problem) in section 5 and of the Heisenberg group in section 6.

In the following proposition, the linear independence assumption on the constraints is equivalent to constraining the velocities to lie in an $(n - k)$ -dimensional distribution of the tangent space of the positions.

¹Also known as Carnot geometry in France and nonholonomic Riemannian geometry in Russia [15]; the metric induced by sub-Riemannian geodesics is known as the Carnot–Carathéodory metric.

²We use vector notation in wedge products, writing $dq \wedge dp$ for $\sum_{i=1}^m dq_i \wedge dp_i$ and $dz \wedge Jdz$ for $\sum_{i,j=1}^m J_{ij} dz_i \wedge dz_j$, where the dimension m is determined from the context.

PROPOSITION 1.1. *Let M be a symmetric nonsingular $n \times n$ mass matrix, $V: \mathbb{R}^n \rightarrow \mathbb{R}$ be a smooth potential, $g_i: \mathbb{R}^n \rightarrow \mathbb{R}^n$, $i = 1, \dots, k$, be smooth functions whose values are linearly independent for all arguments, and q be a smooth extremal with fixed endpoints for the functional*

$$(1.2) \quad S(q) = \int_{t_0}^{t_1} L(t, q, \dot{q}) dt = \int_{t_0}^{t_1} \left(\frac{1}{2} \dot{q}^T M \dot{q} - V(q) \right) dt$$

subject to the constraints $g_i(q) \cdot \dot{q} = 0$, $i = 1, \dots, k$. Then

$$(1.3) \quad J\dot{z} = \nabla H(z),$$

where

$$J = \begin{pmatrix} 0 & -\mathbb{I}_{n \times n} & 0 \\ \mathbb{I}_{n \times n} & 0 & 0 \\ 0 & 0 & 0_{k \times k} \end{pmatrix}, \quad z = \begin{pmatrix} q \\ p \\ \lambda \end{pmatrix} \in \mathbb{R}^{2n+k},$$

$$p = M\dot{q} - \sum_{i=1}^k \lambda_i g_i(q),$$

$$H(z) = \frac{1}{2} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right)^T M^{-1} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right) + V(q),$$

and, furthermore, the Euler–Lagrange equations for (1.2) are equivalent to the generalized Hamiltonian system (1.3). Equation (1.3) forms a constrained Hamiltonian system of the type (1.1) with constraint submanifold C a graph over (q, p) , i.e., $C := \{(q, p, \lambda) : \lambda = \tilde{\lambda}(q, p)\}$ and restricted symplectic form $i^* \omega = dq \wedge dp$.

Proof. Introducing Lagrange multipliers $\lambda_1, \dots, \lambda_k$, the Euler–Lagrange equations for (1.2) are

$$(1.4) \quad \frac{d}{dt} (\nabla_{\dot{q}} F) - \nabla_q F = 0,$$

$$(1.5) \quad g_i(q) \cdot \dot{q} = 0, \quad i = 1, \dots, k,$$

where

$$F(q, \dot{q}, \lambda) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q) - \sum_{i=1}^k \lambda_i g_i(q) \cdot \dot{q}.$$

Expanding out (1.4) gives the Euler–Lagrange equations

$$(1.6) \quad \frac{d}{dt} \left(M\dot{q} - \sum_{i=1}^k \lambda_i g_i(q) \right) - \nabla_q F = 0,$$

$$\frac{d}{dt} \left(M\dot{q} - \sum_{i=1}^k \lambda_i g_i(q) \right) + \left(\nabla V(q) + \sum_{i=1}^k \lambda_i Dg_i(q) \dot{q} \right) = 0.$$

Define the conjugate momentum $p \in \mathbb{R}^n$ using the standard Legendre transform

$$(1.7) \quad p := \nabla_{\dot{q}} F = M\dot{q} - \sum_{i=1}^k \lambda_i g_i(q)$$

so that

$$(1.8) \quad \dot{q} = M^{-1} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right).$$

Using (1.7) and (1.8) in (1.4) gives

$$(1.9) \quad \dot{p} = -\nabla V(q) - \sum_{i=1}^k \lambda_i Dg_i(q) M^{-1} \left(p + \sum_{j=1}^k \lambda_j g_j(q) \right).$$

Defining $H(q, p, \lambda) := \dot{q} \cdot p - F(q, \dot{q}, \lambda)$ gives

$$\begin{aligned} H &= \dot{q} \cdot p - F(q, \dot{q}, \lambda) \\ &= \dot{q} \cdot p - \frac{1}{2} \dot{q}^T M \dot{q} + V(q) + \sum_{i=1}^k \lambda_i g_i(q) \cdot \dot{q} \\ &= \dot{q} \cdot \left(p - \frac{1}{2} M \dot{q} + \sum_{i=1}^k \lambda_i g_i(q) \right) + V(q) \\ &= \dot{q} \cdot \left(M \dot{q} - \sum_{i=1}^k \lambda_i g_i(q) - \frac{1}{2} M \dot{q} + \sum_{i=1}^k \lambda_i g_i(q) \right) + V(q) \\ &= \dot{q} \cdot \left(\frac{1}{2} M \dot{q} \right) + V(q) \\ &= \frac{1}{2} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right)^T M^{-1} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right) + V(q). \end{aligned}$$

A calculation shows the equivalence of the right-hand side of (1.8) and $\nabla_p H$, of the right-hand side of (1.9) and $-\nabla_q H(q, p, \lambda)$, and of constraints $g_i(q) \cdot \dot{q} = 0$ and $0 = \nabla_\lambda H(q, p, \lambda)$.

The constraints $0 = \nabla_\lambda H(q, p, \lambda)$ are the set of equations linear in λ ,

$$(1.10) \quad \begin{pmatrix} g_1 \cdot M^{-1} g_1 & \cdots & g_1 \cdot M^{-1} g_k \\ \vdots & \ddots & \vdots \\ g_k \cdot M^{-1} g_1 & \cdots & g_k \cdot M^{-1} g_k \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_k \end{pmatrix} = - \begin{pmatrix} g_1 \cdot M^{-1} p \\ \vdots \\ g_k \cdot M^{-1} p \end{pmatrix},$$

which has a unique solution for λ for all q, p because the matrix is $GM^{-1}G^T$, where G is the $k \times n$ matrix whose i th row is g_i^T . The assumption that the g_i are linearly independent means that G has full rank k and hence that $GM^{-1}G^T$ is nonsingular. The constraints therefore have a unique solution for λ that we write as $\lambda = \tilde{\lambda}(q, p)$, that is, the constraint submanifold is a graph over (q, p) . Differentiating these constraints with respect to t then yields ODEs for $\dot{\lambda}$, that is, the system (1.3) has (differentiation) index 1. The symplectic form on C is $\frac{1}{2} dz \wedge J dz = dq \wedge dp$. \square

We emphasize that although Proposition 1.1 is not original, the usual treatment is to go one step further and eliminate the Lagrange multipliers λ to get a canonical Hamiltonian system in (q, p) [2, Thm. 7.3.1]. This step may not be desirable either analytically or numerically.

Under certain conditions, namely, that the Legendre transform that defines the conjugate momenta is invertible to give \dot{q} , Proposition 1.1 can be generalized to allow

a general Lagrangian and general constraints. A very thorough geometric treatment of this type of constraint, applying the Gotay–Nestor geometric version of the Dirac–Bergmann constraint algorithm, can be found in [9]. The proof of the following proposition follows the same lines as that of Proposition 1.1 and is omitted.

PROPOSITION 1.2. *If the Legendre transform mapping $(\dot{q}, q, \lambda) \rightarrow (p, q, \lambda)$ given in (1.12) is invertible, then the Euler–Lagrange equations for the action*

$$S(q) = \int_{t_0}^{t_1} L(t, q, \dot{q}) dt$$

subject to the constraints $g_i(q, \dot{q}) = 0, i = 1, \dots, k$, are equivalent to the generalized Hamiltonian system

$$(1.11) \quad J\dot{z} = \nabla H(z),$$

where

$$(1.12) \quad J = \begin{pmatrix} 0 & -\mathbb{I}_{n \times n} & 0 \\ \mathbb{I}_{n \times n} & 0 & 0 \\ 0 & 0 & 0_{k \times k} \end{pmatrix}, \quad z = \begin{pmatrix} q \\ p \\ \lambda \end{pmatrix}, \quad p = \nabla_{\dot{q}} F(q, \dot{q}, \lambda),$$

$$H(z) = \dot{q} \cdot p - F(q, \dot{q}, \lambda), \quad F(q, \dot{q}, \lambda) = L(t, q, \dot{q}) - \sum_{i=1}^k \lambda_i g_i(q, \dot{q}).$$

If, in addition, the matrix $G(q, \dot{q})$ given by $G_{ij} = \partial g_i(q, \dot{q}) / \partial \dot{q}_j$ has full rank k for all q, \dot{q} , then the system of (1.11) has index 1, i.e., can be solved for $\lambda = \tilde{\lambda}(q, p)$.

Proposition 1.2 can be generalized further, to any singular Lagrangian $L(q, \dot{q}, \lambda)$, and still further to Lagrangians $L(z, \dot{z})$, where $|L_{\dot{z}\dot{z}}| = 0$, but the required nondegeneracy assumptions are not as geometrically transparent as those in Proposition 1.2.

2. Symplectic integrators for generalized Hamiltonian systems. The Hamiltonian form (1.3) suggests considering generalized Hamiltonian systems of the form

$$(2.1) \quad J\dot{z} = \nabla H(z), \quad z \in \mathbb{R}^m,$$

where J is a constant antisymmetric matrix, and we do not specify the constraints. Note that many kinds of constrained Hamiltonian systems (including those with holonomic constraints) can be written in this form; the constraint manifold C is constructed as the subset of initial conditions for which the equations have a solution. In general, these equations may not have solutions for all initial conditions; in the extreme case $J = 0$, the equations are purely algebraic. However, it is easily seen that any solutions that do exist do preserve the (“presymplectic”) 2-form $\frac{1}{2} dz \wedge J dz$, which is degenerate when J is singular—this does not require the invertibility of J .

LEMMA 2.1. *Any solutions to (2.1) preserve the 2-form $\frac{1}{2} dz \wedge J dz$.*

Proof. We have

$$\begin{aligned} \frac{1}{2}(dz \wedge J dz)_t &= \frac{1}{2}(dz \wedge J dz_t + dz_t \wedge J dz) \\ &= dz \wedge J dz_t \\ &= dz \wedge H_{zz}(z) dz \\ &= 0. \quad \square \end{aligned}$$

In the particular case of Proposition 1.1, the generalized Hamiltonian system that is obtained is equivalent to a canonical Hamiltonian system obtained by eliminating the Lagrange multipliers λ . Let $\lambda = \tilde{\lambda}(q, p)$ be the solution to (1.10). Then Hamilton's equations for $\tilde{H}(q, p) := H(q, p, \tilde{\lambda}(q, p))$ are

$$\begin{aligned} \dot{q}_i &= \frac{\partial \tilde{H}}{\partial p_i}(q, p) \\ &= \frac{\partial H}{\partial p_i}(q, p, \tilde{\lambda}(q, p)) + \sum_{j=1}^k \frac{\partial H}{\partial \lambda_j}(q, p, \tilde{\lambda}(q, p)) \frac{\partial \tilde{\lambda}_j}{\partial p_i}(q, p) \\ &= \frac{\partial H}{\partial p_i}(q, p, \tilde{\lambda}(q, p)) \end{aligned}$$

(and similarly for \dot{p}), which, together with $\frac{\partial H}{\partial \lambda}(q, p, \tilde{\lambda}(q, p)) = 0$, are equivalent to (1.3). That is, the two operations of eliminating the Lagrange multipliers and mapping the Hamiltonian to its Hamiltonian vector field commute; this can also be seen abstractly by considering the symplectic manifold C with canonical coordinates (q, p) , symplectic form $dq \wedge dp$, and Hamiltonian i^*H .

Certain Runge–Kutta methods, e.g., the midpoint rule, are known to be symplectic when the structure matrix J is invertible [8]. However, as for the continuous time case, J need not be invertible.

PROPOSITION 2.2. *Any solutions of any symplectic Runge–Kutta method applied to $J\dot{z} = \nabla H$ preserve the 2-form $\frac{1}{2}dz \wedge Jdz$, where J is any constant antisymmetric matrix.*

Proof. The s stage symplectic Runge–Kutta method is

$$(2.2) \quad JZ_i = Jz_0 + \Delta t \sum_{j=1}^s a_{ij} JF_j,$$

$$(2.3) \quad Jz_1 = Jz_0 + \Delta t \sum_{j=1}^s b_j JF_j,$$

where

$$(2.4) \quad JF_j = \nabla H(Z_j).$$

Here Δt is the time step and the method maps z_0 to z_1 . The coefficients of a symplectic Runge–Kutta method obey

$$(2.5) \quad b_i b_j - b_j a_{ji} - b_i a_{ij} = 0.$$

Taking the exterior derivative of (2.2), (2.3), and (2.4) gives

$$(2.6) \quad Jdz_0 = JdZ_i - \Delta t \sum_{j=1}^s a_{ij} JdF_j,$$

$$(2.7) \quad Jdz_1 = Jdz_0 - \Delta t \sum_{j=1}^s b_j JdF_j,$$

$$(2.8) \quad JdF_j = H_{zz}(Z_j)dZ_j.$$

From (2.8),

$$(2.9) \quad dZ_j \wedge JdF_j = dZ_j \wedge H_{zz}(Z_j)dZ_j = 0.$$

Substitution now gives, in the same way as in the original study of B-stability by Burrage and Butcher [3],

$$\begin{aligned} dz_1 \wedge Jdz_1 &= dz_0 \wedge Jdz_0 + 2\Delta t \sum_{j=1}^s dZ_j \wedge JdF_j \\ &\quad + (\Delta t)^2 \sum_{i,j=1}^s (b_i b_j - b_j a_{ji} - b_i a_{ij}) dF_i \wedge JdF_j \\ &= dz_0 \wedge Jdz_0 \end{aligned}$$

using (2.5) and (2.9). This establishes the proposition. \square

Note that the underlying structure can be seen very clearly in the case of the midpoint rule

$$(2.10) \quad \frac{Jz_1 - Jz_0}{\Delta t} = \nabla H \left(\frac{z_0 + z_1}{2} \right) := \nabla H(\bar{z}),$$

for which

$$\begin{aligned} dz_1 \wedge Jdz_1 - dz_0 \wedge Jdz_0 &= (dz_0 + dz_1) \wedge J(dz_1 - dz_0) \\ &= (dz_0 + dz_1) \wedge \frac{1}{2} \Delta t H_{zz}(\bar{z})(dz_0 + dz_1) \\ &= 0. \end{aligned}$$

A full study of the geometry of the relations (z_0, z_1) generated in Proposition 2.2 remains to be undertaken.³ Unfortunately, the relations (z_0, z_1) in Proposition 2.2 do not yield good integrators for arbitrary J and H . For example, holonomic constraints can be specified as generalized Hamiltonian systems with $H = \tilde{H}(q, p) + \sum_{i=1}^k \lambda_i h_i(q)$. In this case the midpoint rule, say, generates maps from *all* (q_0, p_0) to (q_1, p_1) with the constraints satisfied at the midpoint. Not only is the phase space “wrong,” this method is known to be not convergent in general [6]. The situation is much better for index 1 constraints.

3. Symplectic integrators for index 1 constraints.

PROPOSITION 3.1. *Let J be any constant antisymmetric matrix and let H be a Hamiltonian such that the generalized Hamiltonian system*

$$(3.1) \quad J\dot{z} = \nabla H(z)$$

has index 1, i.e., such that when the system is written in Darboux coordinates (q, p, λ) , the constraint $H_\lambda = 0$ has a unique solution for λ for all q and p . Then any symplectic Runge–Kutta method (2.2)–(2.5) applied to (3.1) is well defined for sufficiently small

³The relations generated in Proposition 2.2 are a generalization of the Viterbo generating functions used in symplectic topology [16]. These take the form $S: Q \times \mathbb{R}^k \rightarrow \mathbb{R}$; the submanifold $p = S_q(q, \lambda)$, $0 = S_\lambda(q, \lambda)$ is Lagrangian in T^*Q . The parameters λ allow the representation of larger classes of Lagrangian submanifolds than the standard generating function $S(q)$ which generates $p = S_q(q)$ which is necessarily a graph over Q .

Δt , convergent of the same order as the Runge–Kutta method, preserves the constraint submanifold, and preserves the symplectic form on the constraint submanifold.

Proof. By linear covariance of Runge–Kutta methods we can assume that J is in Darboux form (although the theorem holds in any basis). Then the constraint part of the Runge–Kutta equations read

$$0 = \nabla_\lambda H(Q_i, P_i, \Lambda_i), \quad i = 1, \dots, k,$$

$$0 \frac{\lambda_1 - \lambda_0}{\Delta t} = \sum_{i=1}^s b_i \nabla_\lambda H(Q_i, P_i, \Lambda_i).$$

Therefore the Lagrange multipliers Λ_i at each stage are given by the *exact* Lagrange multipliers evaluated at (Q_i, P_i) , i.e., $\Lambda_i = \tilde{\lambda}(Q_i, P_i)$, and λ_1 is arbitrary. For convenience, we add the extra equations $\lambda_0 = \tilde{\lambda}(q_0, p_0)$, $\lambda_1 = \tilde{\lambda}(q_1, p_1)$, which do not affect the method at all. The resulting method is equivalent to that obtained by eliminating the Lagrange multipliers in the Hamiltonian, applying a symplectic Runge–Kutta method, and lifting back to the constraint manifold by $\lambda = \tilde{\lambda}(q, p)$. It is therefore well defined for sufficiently small Δt and convergent of the same order as the Runge–Kutta method. Because $\frac{1}{2} dz \wedge J dz = dq \wedge dp$, the symplectic form $dq \wedge dp$ is preserved on the constraint manifold. \square

Note that the assumptions are satisfied if $|H_{\lambda\lambda}| \neq 0$. The constraints may be nonlinear in λ and need not be solved analytically; the entire Runge–Kutta system for (Q_i, P_i, Λ_i) can be numerically solved simultaneously.

COROLLARY 3.2. *Symplectic Runge–Kutta methods yield convergent constraint-preserving symplectic integrators for the Hamiltonian formulation of the Lagrange and sub-Riemannian problems given in Propositions 1.1 and 1.2. When velocities are calculated using the Legendre transform, the constraints $g_i(q) \cdot \dot{q} = 0$ (resp., $g(q, \dot{q}) = 0$) are satisfied exactly at the stages, and if the endpoint Lagrange multipliers are defined by $H_\lambda(q_n, p_n, \lambda_n) = 0$, then the constraints are satisfied exactly at the endpoints.*

4. Variational problems with holonomic and nonholonomic constraints.

Proposition 1.1 allowed a nonholonomic variational problem to be converted into an index 1 constrained Hamiltonian system that can be integrated using the symplectic midpoint rule. In this section we show that if *holonomic* constraints are added to the original variational problem, then the resulting Hamiltonian system is a simple *holonomically* constrained system. This system can be solved by a symplectic method such as RATTLE [10, 14].

PROPOSITION 4.1. *Let M be a symmetric nonsingular $n \times n$ mass matrix, $V: \mathbb{R}^n \rightarrow \mathbb{R}$ a smooth potential, $g_i: \mathbb{R}^n \rightarrow \mathbb{R}^n$, $i = 1, \dots, k$, be k smooth functions, and q be a smooth extremal with fixed endpoints for the functional*

$$(4.1) \quad S(q) = \int_{t_0}^{t_1} L(t, q, \dot{q}) dt = \int_{t_0}^{t_1} \left(\frac{1}{2} \dot{q}^T M \dot{q} - V(q) \right) dt$$

subject to the velocity constraints $g_i(q) \cdot \dot{q} = 0, i = 1, \dots, k$, and the holonomic constraints $h_i(q) = 0, i = 1, \dots, l$. Then

$$(4.2) \quad J\dot{z} = \nabla H(z),$$

where

$$J = \begin{pmatrix} 0 & -\mathbb{I}_{n \times n} & 0 & 0 \\ \mathbb{I}_{n \times n} & 0 & 0 & 0 \\ 0 & 0 & 0_{k \times k} & 0 \\ 0 & 0 & 0 & 0_{l \times l} \end{pmatrix}, \quad z = \begin{pmatrix} q \\ p \\ \lambda \\ \lambda^h \end{pmatrix},$$

$$p = M\dot{q} - \sum_{i=1}^k \lambda_i g_i(q),$$

$$H(z) = \frac{1}{2} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right)^T M^{-1} \left(p + \sum_{i=1}^k \lambda_i g_i(q) \right) + V(q) + \sum_{i=1}^l \lambda_i^h h_i(q),$$

and, furthermore, the Euler–Lagrange equations for (4.1) are equivalent to the generalized Hamiltonian system (4.2). If, in addition, the velocity constraints are linearly independent for all q , then (4.2) is equivalent to a canonical holonomically constrained Hamiltonian system.

Proof. As in Proposition 1.1 the extended Lagrangian F , the conjugate momenta p , and the Hamiltonian $H(q, p, \lambda, \lambda^h)$ are defined by

$$F := \frac{1}{2} \dot{q}^T M \dot{q} - V(q) - \sum_{i=1}^k \lambda_i g_i(q) \cdot \dot{q} - \sum_{i=1}^l \lambda_i^h h_i(q),$$

$$p := \nabla_{\dot{q}} F = M \dot{q} - \sum_{i=1}^k \lambda_i g_i(q),$$

$$H := \dot{q} \cdot p - F.$$

The rest of the proof is a calculation along the same lines as for Proposition 1.1. □

PROPOSITION 4.2. *Subject to standard nondegeneracy assumptions on the Hamiltonian, the following algorithm yields a convergent, second-order integrator that is symplectic on the constraint manifold defined by the (primary) holonomic constraints and the secondary constraints induced by them: (i) apply RATTLE using the holonomic constraints; (ii) in the inner step of RATTLE, when a time step of the unconstrained system is required, apply the midpoint rule to the generalized Hamiltonian system with Hamiltonian $H(q, p, \lambda, 0)$.*

Proof. Eliminating the velocity constraints by solving for the Lagrange multipliers λ_i yields a standard holonomically constrained system. Applying RATTLE (with the midpoint rule in the inner step) to this system yields a convergent second-order integrator on the constraint surface. Applying the midpoint rule in the inner step is equivalent to applying the midpoint rule to the generalized Hamiltonian system with Hamiltonian $H(q, p, \lambda, 0)$. □

5. Example: Sub-Riemannian geodesics. Trajectories of a two-wheeled vehicle with a front steering wheel and a nonsteering back wheel, moving on a smooth surface, will be modeled. We consider the two-wheeled vehicle shown in Figure 5.1 with length L , back wheel at (z, w) , and front wheel at (x, y) . The front wheel is at an angle ϕ and the vehicle is at an angle θ .

If the speed of the front wheel is v , the velocity of the front wheel must obey

$$\dot{x} = v \cos \phi, \quad \dot{y} = v \sin \phi.$$

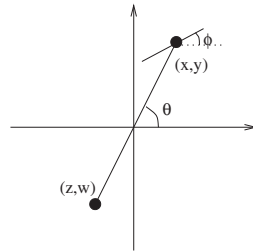


FIG. 5.1. A two-wheeled vehicle showing the front wheel angle ϕ and the vehicle angle θ .

Eliminating v , the velocity of the front wheel obeys the constraint

$$(5.1) \quad \dot{x} \sin \phi - \dot{y} \cos \phi = 0.$$

Similarly, the velocity of the back wheel obeys the constraint

$$(5.2) \quad \dot{z} \sin \theta - \dot{w} \cos \theta = 0.$$

We can eliminate (5.2), and thus the variables z and w , using the distance between the two wheels, which relates the four variables. Notice that

$$x - z = L \cos \theta, \quad y - w = L \sin \theta,$$

so that

$$\dot{z} = \dot{x} + L\dot{\theta} \sin \theta, \quad \dot{w} = \dot{y} - L\dot{\theta} \cos \theta,$$

which substituted into (5.2) gives

$$(5.3) \quad \dot{x} \sin \theta - \dot{y} \cos \theta + L\dot{\theta} = 0.$$

We take the Lagrangian to be

$$(5.4) \quad L = \frac{1}{2} (\dot{x}^2 + \dot{y}^2 + \alpha \dot{\theta}^2 + \beta \dot{\phi}^2) - V(x, y),$$

where the potential $V(x, y)$ is the (scaled) height of the surface, which together with the constraints (5.1) and (5.3) gives an index 1 system as in Proposition 1.1. That is, when $V = 0$ we are calculating geodesics of the sub-Riemannian metric defined by (5.4), (5.1), and (5.3). To put it another way, we are seeking shortest paths that move the vehicle from one configuration to another subject to the constraints of its geometry—the “parallel parking” problem. In the numerics, we use the midpoint rule.

We first used the potential $V(x, y) = -\cos r$, where r is the midpoint of the vehicle, and numerically checked the second-order convergence of the method to a reference solution computed by MATLAB’s `ode15s`, numerical conservation of the symplectic form, exact conservation of the original constraints (up to round-off error), and behavior of the energy error. A sample result is shown in Figure 5.2, in which the energy errors appear to be bounded, as expected for a symplectic integrator.

We then studied special solutions of the free motion case $V = 0$, which has two simple solutions that are relative equilibria for the translation and rotation symmetries of the problem, namely, straight line and circular motion. If the vehicle starts with

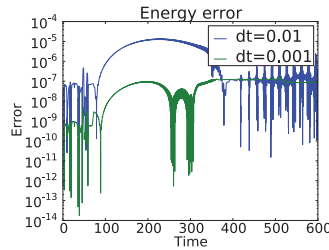


FIG. 5.2. The energy error over time. This is the energy at each step minus the initial energy. The vehicle is trapped in the potential bowl $V(x,y)$, and the energy error does not show a linear growth in time.

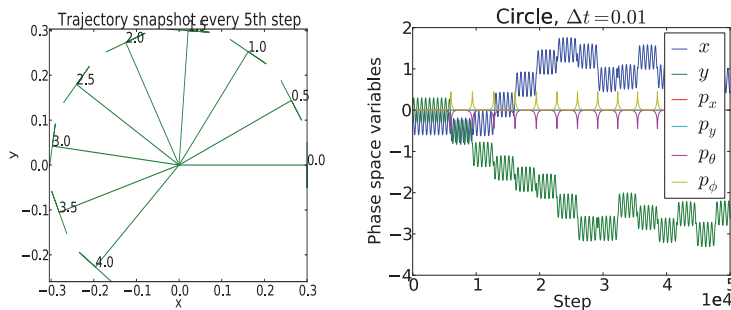


FIG. 5.3. Snapshots every fifth step of the two-wheeled vehicle starting at $(x,y,\theta,\phi,p_x,p_y,p_\theta,p_\phi) = (0.3,0,0,\pi,0,1.09,1)$, with $\Delta t = 0.1$, and zero potential. The vehicle stays in a circle for many revolutions (not shown for clarity), but this geodesic is not stable, so the vehicle eventually wanders, as shown in the longer orbit on the right. The solutions for p_θ and p_ϕ suggest a relative homoclinic orbit.

$\theta = \phi = 0$, the exact solution is a straight line motion. Let $\theta = \phi = 0$, $\dot{x} = 1$, and $\dot{y} = 0$. The constraints in (5.1) and (5.3) are satisfied. Equation (1.8) gives the initial generalized momenta values: all are zero except $p_x = 1$. The discretization gives the exact solution; however, as the solution is unstable, round-off errors eventually cause the vehicle to wander.

For the circular motion, let $\theta = at$, $\phi = at + \frac{\pi}{2}$, $\dot{x} = -c \sin(\theta)$, and $\dot{y} = c \cos(\theta)$. There are two constants, a and c , to be determined. Equation (5.1) gives $\lambda = (1, -c)$, and (5.3) gives $aL = c$. Using these values in (1.7) gives the initial generalized momenta values: $(p_x, p_y, p_\theta, p_\phi) = (0, 0, a(1 + L^2), a)$. For this simple trajectory a is chosen to be 1. In Figure 5.3 the circle trajectory of the vehicle is confirmed. If the trajectory is computed for larger times the vehicle leaves the circle; the solution appears to be unstable but, interestingly, appears to repeatedly return to the circular orbit, indicating a possible relative homoclinic structure in this problem.

6. Example: The Heisenberg problem. A previous study of geometric integrators for sub-Riemannian variational problems used a discrete variational approach to obtain constrained symplectic integrators [1]. Our approach, applying symplectic integrators to the Hamiltonian formulation, yields geometric integrators with the same geometric properties but uses standard integrators that allow any order with standard implementations and does not require an approximation of \dot{q} , that is, it naturally yields first-order trajectories in (q,p) instead of second-order trajectories in q .

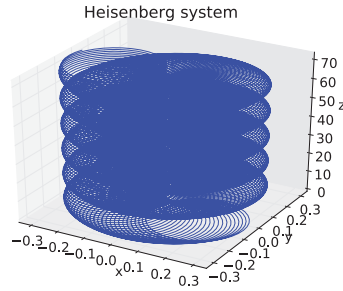


FIG. 6.1. The Heisenberg example starting at $(x, y, z, \dot{x}, \dot{y}, \dot{z}) = (0, 0, 0, 0.1, 0.3, 0)$ or $(x, y, z, p_x, p_y, p_z, \lambda) = (0, 0, 0, 0.1, 0.3, 1, 1)$. Qualitatively the results look like [1, p. 14].

We repeat the numerical illustration of [1, p. 12], the Heisenberg problem, using our approach. This is to find the extremal $q(t) = (x(t), y(t), z(t))$ of

$$S(q) = \int_{t_0}^{t_1} L(t, q, \dot{q}) dt = \int_{t_0}^{t_1} \left(\frac{1}{2} \dot{q}^T \dot{q} - V(q) \right) dt$$

subject to the constraint $g(q) \cdot \dot{q} = 0$, where $g(q) = (-y, x, 1)$.

Equation (1.8) gives \dot{q} :

$$(6.1) \quad \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} + \lambda \begin{pmatrix} -y \\ x \\ 1 \end{pmatrix}.$$

Using (1.9), \dot{p} can be written

$$(6.2) \quad \begin{pmatrix} \dot{p}_x \\ \dot{p}_y \\ \dot{p}_z \end{pmatrix} = -\nabla V(q) - \lambda \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \left[\begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} + \lambda \begin{pmatrix} -y \\ x \\ 1 \end{pmatrix} \right]$$

and we have the constraint $g \cdot (p + \lambda g) = 0$, which gives

$$\lambda = -\frac{g \cdot p}{g \cdot g}.$$

A simple trajectory starting with the same initial conditions as in [1, p. 15] is shown in Figure 6.1. Their initial conditions are $(x, y, z, \dot{x}, \dot{y}, \dot{z}, \lambda) = (0, 0, 0, 0.1, 0.3, 0, 1)$, which when converted to generalized momenta variables are $(x, y, z, p_x, p_y, p_z, \lambda) = (0, 0, 0, 0.1, 0.3, 1, 1)$. The results are consistent with [1, p. 14].

7. Discussion. We have constructed symplectic integrators for a different class of constrained Hamiltonian systems than the holonomic constraints most commonly considered in the literature. The class includes important practical problems arising in sub-Riemannian geometry. We have restricted our attention to symplectic Runge–Kutta methods; a generalization to partitioned methods in which different Runge–Kutta coefficients are used for q , for p , and for λ is straightforward. In other work [10], we reinterpret these methods as an instance of RATTLE in an extended phase space; that point of view also suggests different generalizations.

We note that the nondegeneracy conditions in Propositions 1.1, 1.2, and 4.1 are essential for the integrators in Proposition 3.1, indeed, for the entire approach,

to work. It is not clear to what extent the approach can be extended to handle more general constraints, for example, to the system $J\dot{z} = \nabla H + \lambda \nabla g$, where the constraint submanifold $g(z) = 0$ is symplectic. No symplectic, constraint-preserving method is known for this problem. As remarked before Proposition 3.1, a full study of the geometry of the relations (z_0, z_1) generated in Proposition 2.2 remains to be undertaken. Any solutions are symplectic, so this gives access to a much larger class of symplectic maps than do traditional generating functions. Note that new variables (analogous to λ) can be added as needed to generate larger classes of maps.

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