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Mechanical Systems Subject to Holonomic Constraints: Differential-Algebraic Formulations and Conservative Integration

Oscar Gonzalez

Département de Mathématiques
École Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

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Author information: Phone: +41 21 693 2767; Fax: +41 21 693 5530;
E-mail: gonzalez@dma.epfl.ch

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Oscar Gonzalez[1]

Département de Mathématiques
École Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

Abstract

The numerical integration in time of the equations of motion for mechanical systems subject to holonomic constraints is considered. Schemes are introduced for the direct treatment of a differential-algebraic form of the equations that preserve the constraints, the total energy, and other integrals such as linear and angular momentum arising from affine symmetries. Moreover, the schemes can be shown to preserve the property of time-reversibility in an appropriate sense. An example is given to illustrate various aspects of the proposed methods.

1 Introduction

The equations of motion for a conservative mechanical system subject to holonomic constraints can often be written in the differential-algebraic [5] form

$$\left.\begin{array}{rcl} \dot{q} & = & D_2H(q,p) \\ \dot{p} & = & -D_1H(q,p) - Dg(q)^T\lambda \\ 0 & = & g(q) \end{array}\right\} \tag{1}$$

where $q \in \mathbb{R}^n$ are the configuration variables, $p \in \mathbb{R}^n$ are variables conjugate to the velocities $\dot{q}$ in an appropriate sense, $g : \mathbb{R}^n \to \mathbb{R}^m$ $(m < n)$ is a smooth constraint function, $\lambda \in \mathbb{R}^m$ is a vector of (Lagrange) multipliers, and $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a smooth function which represents the Hamiltonian function for the system in the absence of constraints.

Associated with the system (1) are the sets

$$\begin{aligned} \mathcal{Q} &= \{q \in \mathbb{R}^n \mid g(q) = 0\} \\ \mathcal{M} &= \{(q,p) \in \mathbb{R}^n \times \mathbb{R}^n \mid Dg(q)D_2H(q,p) = 0 \quad \text{and} \quad g(q) = 0\}. \end{aligned} \tag{2}$$

The set $\mathcal{Q}$ is called the configuration space for the system and, assuming $Dg(q) \in \mathbb{R}^{m\times n}$ has rank m for each $q \in \mathcal{Q}$, it is an $(n-m)$-dimensional manifold. The set $\mathcal{M}$ may be referred to as the intrinsic phase space for the system, and it has the property that if $(q,p,\lambda)(t)$ is a smooth solution of (1), then $(q,p)(t) \in \mathcal{M}$. Assuming $D_2^2H(q,p) \in \mathbb{R}^{n\times n}$ is invertible for any $(q,p) \in \mathcal{M}$, we find that $\mathcal{M}$ is actually a $(2n-2m)$-dimensional manifold, and that (1) implicitly defines a vector field on $\mathcal{M}$. Moreover, this vector field is Hamiltonian with a Hamiltonian function defined by the restriction $H|_{\mathcal{M}}$ and a symplectic structure defined by

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the restriction of the canonical structure of $\mathbb{R}^n \times \mathbb{R}^n$ to $\mathcal{M}$ [18]. More details on the general theory of differential-algebraic systems may be found in [5, 24], and details about Hamiltonian systems on manifolds may be found in [2, 20].

There has been much interest in the development of numerical schemes for the differential-algebraic system (1) that preserve some of its structure. The case in which $H(q,p)$ is separable

$$H(q,p) = p \cdot M^{-1}p + V(q), \quad M \in \mathbb{R}^{n\times n} \tag{3}$$

was studied in [19], where variants [1] of the time-reversible Verlet scheme that preserved $\mathcal{Q}$, and variants that preserved $\mathcal{M}$ together with its symplectic structure, were considered. Of these methods, it was reported that those which preserved $\mathcal{M}$ produced nearly identical results as those which preserved only $\mathcal{Q}$. The case of a general Hamiltonian was studied in [15, 22], where it was shown that there exist partitioned Runge-Kutta methods that preserve $\mathcal{M}$ along with its symplectic structure for arbitrary $H(q,p)$ (see also [23]). Rather than treat (1) directly, one may alternatively consider stabilized differential-algebraic formulations [5, 6, 7], or unconstrained formulations in which the constraints appear as invariants [4, 12, 18].

In this article we consider variants of the time-reversible, integral-preserving schemes of [9, 10] for the direct treatment of (1). It will be shown that schemes can be constructed for (1) which preserve $\mathcal{Q}$, the restricted Hamiltonian $H|_{\mathcal{Q}}$ and other integrals such as linear and angular momentum arising from affine symmetries in the problem. The appeal of preserving an energy-like quantity such as $H|_{\mathcal{Q}}$ can be traced back to [25] and the concept of energy stability. For unconstrained problems, an analysis of the symmetry and stability properties of integral-preserving schemes may be found in [9, 10], and various applications of such methods may be found in [11, 26].

The presentation is structured as follows. Integrals and symmetry properties of (1) are discussed in Section 2, and a general integral-preserving scheme is outlined in Section 3. In Section 4 the general scheme is specialized to the case of a constrained four-particle model problem and a numerical example is given. A detailed numerical analysis of the schemes developed here will be given elsewhere.

2 Integrals and Symmetry

The differential-algebraic system (1) may possess various physically meaningful integrals that one would like to preserve under discretization. To bring these integrals into evidence, we rewrite (1) in the form

$$\left.\begin{array}{rcr} \dot{q} &=& D_2\mathcal{H}(q,p,\lambda) \\ \dot{p} &=& -D_1\mathcal{H}(q,p,\lambda) \\ 0 &=& D_3\mathcal{H}(q,p,\lambda) \end{array}\right\} \tag{4}$$

where $\mathcal{H} : \mathcal{P} \to \mathbb{R}$ is an augmented Hamiltonian function defined as

$$\mathcal{H}(q,p,\lambda) = H(q,p) + \lambda \cdot g(q) \tag{5}$$

and $\mathcal{P} = \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m$. Since we will be interested in integrals defined on the ambient space $P = \mathbb{R}^n \times \mathbb{R}^n$, we note that the rate of change of any smooth function $\phi : P \to \mathbb{R}$ along a solution of (4) is given by the expression

$$\frac{d}{dt}\phi(q,p) = \{\phi, \mathcal{H}_\lambda\}(q,p) \tag{6}$$

where $\mathcal{H}_\lambda = \mathcal{H}(\cdot,\lambda) : P \to \mathbb{R}$ and $\{\cdot,\cdot\}$ is the canonical Poisson bracket associated with P, namely

$$\{\phi,\psi\}(q,p) = D_1\phi(q,p)\cdot D_2\psi(q,p) - D_2\phi(q,p)\cdot D_1\psi(q,p). \tag{7}$$

2.1 Fundamental Integral

The differential-algebraic system (4) always possesses an integral due to the skew-symmetry of the bracket $\{\cdot,\cdot\}$. In particular, the augmented Hamiltonian function $\mathcal{H}$ is conserved along any solution $(q,p,\lambda)(t) \in \mathcal{P}$ in the sense that

$$\frac{d}{dt}\mathcal{H}(q,p,\lambda) = 0, \quad \text{which implies} \quad \frac{d}{dt}H(q,p) = 0 \tag{8}$$

because $(q,p)(t) \in \mathcal{M}$.

2.2 Symmetry-Related Integrals

The system (4) may possess various integrals associated with symmetry properties of $\mathcal{H}$ under the action of a Lie group on P. To see this, let $G \subset \mathbb{R}^k$ be a Lie group, with tangent space at the identity denoted by $T_eG \subset \mathbb{R}^k$, and let $\Phi : G \times P \to P$ denote a regular Poisson action of G on P [21]. Recall that the action of G is Poisson if, for any two smooth functions $\phi,\psi : P \to \mathbb{R}$, we have

$$\{\phi,\psi\}\circ\Phi_\gamma = \{\phi\circ\Phi_\gamma, \psi\circ\Phi_\gamma\} \quad \forall\gamma \in G, \tag{9}$$

where $\Phi_\gamma = \Phi(\gamma,\cdot) : P \to P$. To any $\xi \in T_eG$ we associate a vector field $\xi_P : P \to P$ defined by

$$\xi_P(q,p) = \frac{d}{ds}\Big|_{s=0}\Phi(\exp(s\xi),q,p) = (v_\xi(q,p), w_\xi(q,p)) \tag{10}$$

where $\exp : T_eG \to G$ is the exponential map on G, and we recall that a momentum map for the system $(P,\{\cdot,\cdot\},G,\Phi)$ is a map $J : P \to T_e^*G$ satisfying

$$\left.\begin{aligned} D_1J_\xi(q,p) &= -w_\xi(q,p) \\ D_2J_\xi(q,p) &= v_\xi(q,p) \end{aligned}\right\} \quad \forall\xi \in T_eG, \tag{11}$$

where $J_\xi : P \to \mathbb{R}$ is defined as $J_\xi(q,p) = J(q,p)\cdot\xi$.

Proposition 2.1 *Suppose the system $(P,\{\cdot,\cdot\},G,\Phi)$ possesses a momentum map $J : P \to T_e^*G$. If the unconstrained Hamiltonian $H : P \to \mathbb{R}$ and the constraint function $g : P \to \mathbb{R}^m$ are G-invariant, that is*

$$H\circ\Phi_\gamma = H \quad \textit{and} \quad g\circ\Phi_\gamma = g \quad \forall\gamma \in G, \tag{12}$$

then J is conserved along any solution $(q,p,\lambda)(t) \in \mathcal{P}$ of (4) in the sense that

$$\frac{d}{dt}J(q,p) = 0. \tag{13}$$

Proof. Let $\xi \in T_e G$ be arbitrary. Then the rate of change of J_ξ along a solution is

$$\begin{aligned}\frac{d}{dt} J_\xi(q,p) &= \ \{J_\xi, \mathcal{H}_\lambda\}(q,p) \\ &= -\{\mathcal{H}_\lambda, J_\xi\}(q,p) \\ &= -\frac{d}{ds}\Big|_{s=0} \mathcal{H}_\lambda(\Phi_{\exp(s\xi)}(q,p)) \\ &= \ 0\end{aligned} \tag{14}$$

where the last line follows from the G-invariance of $\mathcal{H}_\lambda$, which is implied by that of H and g. Since $J_\xi = J \cdot \xi$, the result follows by the arbitrariness of ξ. ■

3 Conserving Integration Schemes

We next generalize the schemes developed in [9] to differential-algebraic systems of the form (1). We suppose that $H(q,p)$ and $g(q)$ are invariant under the action Φ of a Lie group G on P, and that this action has a momentum map $J(q,p)$. For each $\gamma \in G$, we assume that Φ_γ is an affine map on P and that $J(q,p)$ is at most quadratic in (q,p). Under these assumptions, schemes can be developed for (1) which preserve $\mathcal{Q}$, H and J.

The schemes developed in [9] are based on the notion of a *discrete derivative* of a smooth function $f : P \to \mathbb{R}$, which is defined to be a mapping $\mathsf{D}f : P \times P \to P$ satisfying the *directionality* property

$$\mathsf{D}f(x,y) \cdot (y - x) = f(y) - f(x) \tag{15}$$

for all $x = (x_q, x_p) \in P$ and $y = (y_q, y_p) \in P$, and the *consistency* property

$$\mathsf{D}f(x,y) = Df\left(\tfrac{x+y}{2}\right) + \mathcal{O}(|y-x|^r) \tag{16}$$

for some $r \geq 1$ and all $x, y \in P$ with $|y - x|$ sufficiently small. Moreover, for the case when $f : P \to \mathbb{R}$ is invariant under the action of G on P, the discrete derivative of f is said to be G-equivariant if it satisfies the additional *orthogonality* property

$$\mathsf{D}f(x,y) \cdot (v_\xi(z), w_\xi(z)) = 0 \tag{17}$$

for all $x, y \in P$ and $\xi \in T_e G$ where $z = (x+y)/2$. In [9] various formulae are given for constructing equivariant discrete derivatives with $r = 2$.

To a discrete derivative $\mathsf{D}f(x,y) \in P$ one associates partial discrete derivatives $\mathsf{D}_1 f(x,y) \in \mathbb{R}^n$ and $\mathsf{D}_2 f(x,y) \in \mathbb{R}^n$ according to the relation

$$\mathsf{D}f(x,y) \cdot (u_q, u_p) = \mathsf{D}_1 f(x,y) \cdot u_q + \mathsf{D}_2 f(x,y) \cdot u_p \tag{18}$$

for all $u = (u_q, u_p) \in P$. From (18) we see that a discrete derivative operator D on P induces a discrete derivative operator d on $\mathbb{R}^n$. To see this, let $h(x_q)$ be a given function of $x_q \in \mathbb{R}^n$ and let $\bar{h}(x)$ be that function on P defined as

$$\bar{h}(x) = h(x_q), \qquad \forall x = (x_q, x_p) \in P. \tag{19}$$

Then d is defined as

$$\mathsf{d}h(x_q, y_q) = \mathsf{D}_1\bar{h}(x, y). \tag{20}$$

Finally, discrete derivatives are defined for vector-valued functions, such as the constraint function $g : \mathbb{R}^n \to \mathbb{R}^m$, in the obvious way at the component level.

An integral-preserving scheme for the differential-algebraic system (1) can now be stated. Let D denote an equivariant discrete derivative operator for functions of $(q, p) \in \mathbb{R}^n \times \mathbb{R}^n$, and let d denote the induced equivariant discrete derivative operator for functions of $q \in \mathbb{R}^n$. Then an integral-preserving scheme for (1) is

$$\left.\begin{aligned} q_{n+1} - q_n &= \Delta t\ \mathsf{D}_2 H(x_n, x_{n+1}) \\ p_{n+1} - p_n &= -\Delta t\ \mathsf{D}_1 H(x_n, x_{n+1}) - \Delta t\ \mathsf{d}g(q_n, q_{n+1})^T \lambda_{n+1} \\ 0 &= g(q_{n+1}) \end{aligned}\right\} \tag{21}$$

where $x = (q, p) \in P$ and $\Delta t > 0$ is the time step.

Proposition 3.1 *The constraint g, Hamiltonian H and momentum map J (at most quadratic) are preserved along any solution sequence $(q_n, p_n, \lambda_n) \in \mathcal{P}$ of (21) in the sense that*

$$\left.\begin{aligned} g(q_n) &= 0 \\ H(q_n, p_n) &= H(q_0, p_0) \\ J(q_n, p_n) &= J(q_0, p_0) \end{aligned}\right\} \qquad n = 0, 1, 2, \ldots . \tag{22}$$

Proof. Preservation of the constraint is obvious in view of $(21)_3$. To establish that the integral $H(q, p)$ is preserved, we take the inner product of $(21)_1$ with $(p_{n+1} - p_n)$, the inner product of $(21)_2$ with $(q_{n+1} - q_n)$ and subtract to get

$$\begin{aligned} \mathsf{D}_1 H(x_n, x_{n+1}) \cdot (q_{n+1} - q_n) + \mathsf{D}_2 H(x_n, x_{n+1}) \cdot (p_{n+1} - p_n) \\ + \lambda_{n+1} \cdot [\mathsf{d}g(q_n, q_{n+1})](q_{n+1} - q_n) = 0 \end{aligned} \tag{23}$$

which, in view of the directionality property of the discrete derivative, yields

$$H(x_{n+1}) - H(x_n) + \lambda_{n+1} \cdot [g(q_{n+1}) - g(q_n)] = 0. \tag{24}$$

The result for H then follows from the fact that $g(q_{n+1}) = g(q_n) = 0$. To establish the result for J, let $\xi \in T_e G$ be arbitrary. Then, since the function $J_\xi : P \to \mathbb{R}$ is at most quadratic, we have

$$\begin{aligned} J_\xi(x_{n+1}) - J_\xi(x_n) = D_1 J_\xi(q_{n+\frac{1}{2}}, p_{n+\frac{1}{2}}) \cdot (q_{n+1} - q_n) \\ + D_2 J_\xi(q_{n+\frac{1}{2}}, p_{n+\frac{1}{2}}) \cdot (p_{n+1} - p_n) \end{aligned} \tag{25}$$

where $(\cdot)_{n+\frac{1}{2}} = \frac{1}{2}[(\cdot)_n + (\cdot)_{n+1}]$ and D_i are the exact partial derivatives. Using (11) we obtain

$$\begin{aligned} &J_\xi(x_{n+1}) - J_\xi(x_n) \\ &\quad = v_\xi(x_{n+\frac{1}{2}}) \cdot (p_{n+1} - p_n) - w_\xi(x_{n+\frac{1}{2}}) \cdot (q_{n+1} - q_n). \end{aligned} \tag{26}$$

Combining the above equation with $(21)_{1,2}$ gives

$$
\begin{aligned}
J_\xi(x_{n+1}) - J_\xi(x_n) \\
&= -\Delta t \ \mathsf{D}_2 H(x_n, x_{n+1}) \cdot w_\xi(x_{n+\frac{1}{2}}) \\
&\qquad - \Delta t \ \mathsf{D}_1 H(x_n, x_{n+1}) \cdot v_\xi(x_{n+\frac{1}{2}}) \\
&\qquad - \Delta t \ \lambda_{n+1} \cdot [\mathsf{d}g(q_n, q_{n+1})] v_\xi(x_{n+\frac{1}{2}}) \\
&= -\Delta t \ \mathsf{D}\mathcal{H}_{\lambda_{n+1}}(x_n, x_{n+1}) \cdot (v_\xi(x_{n+\frac{1}{2}}), w_\xi(x_{n+\frac{1}{2}}))
\end{aligned}
\tag{27}
$$

which vanishes in view of the orthogonality condition of the equivariant discrete derivative D applied to the function $\mathcal{H}_\lambda : P \to \mathbb{R}$. Since $J_\xi = J \cdot \xi$, the result follows from the arbitrariness of ξ. ■

It is important to note that while $q_n \in \mathcal{Q}$, one may have $(q_n, p_n) \notin \mathcal{M}$, and so the scheme does not generally preserve the intrinsic phase space $\mathcal{M}$. Thus, along a solution sequence of (21), the conserved Hamiltonian $H(q_n, p_n)$ is generally only an approximation to the physical energy of the system. The problem lies in the fact that the velocity vector corresponding to p_n may not be tangent to the configuration space $\mathcal{Q}$. However, schemes that preserve only $\mathcal{Q}$ may have some merit. For example, in [19] it was reported that variants of the Verlet scheme that preserved only $\mathcal{Q}$ produced nearly identical results as variants that preserved $\mathcal{M}$.

4 Example

Consider four particles in $\mathbb{R}^3$ as shown in Figure 1 with masses $m_i > 0$ and positions $q_i \in \mathbb{R}^3$, and let $q = (q_1, \ldots, q_4)$. Assume the particles are under the influence of a potential

$$
V(q) = \tilde{V}_1(\pi_1(q)) + \tilde{V}_2(\pi_2(q))
\tag{28}
$$

where $\pi_1(q) = |q_1 - q_3|^2$ and $\pi_2(q) = |q_2 - q_4|^2$. Furthermore, assume the system is subject to configuration constraints of the form

$$
\left.
\begin{aligned}
g_1(q) &= \sqrt{\zeta_1(q)} - L_1 = 0 \\
g_2(q) &= \sqrt{\zeta_2(q)} - L_2 = 0
\end{aligned}
\right\}
\tag{29}
$$

where $\zeta_1(q) = |q_1 - q_2|^2$, $\zeta_2(q) = |q_3 - q_4|^2$, and $L_1, L_2 > 0$ are given constants. Introducing momentum variables $p = (p_1, \ldots, p_4)$, we find that the equations of motion for the current system can be written in the form (1) with $n = 12$, $m = 2$ and Hamiltonian

$$
H(q,p) = \sum_{i=1}^{4} \frac{1}{2m_i} |p_i|^2 + V(q).
\tag{30}
$$

The constraint $g = (g_1, g_2)$ and the Hamiltonian H are invariant under the group $G_1 = \mathbb{R}^3$ acting by translations on q, and the group $G_2 = SO(3)$ acting by rotations on (q,p). The momentum map associated with the action of G_1 is the total linear momentum

$$
L(q,p) = \sum_{i=1}^{4} p_i,
\tag{31}
$$

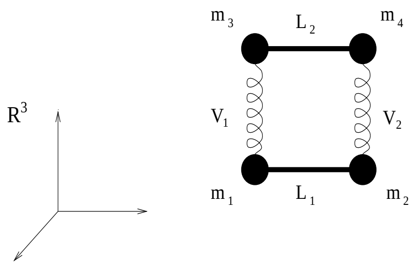


Figure 1: Constrained four particle system.

and that associated with G_2 is the total angular momentum (about the origin)

$$J(q,p) = \sum_{i=1}^{4} q_i \times p_i. \tag{32}$$

The system defined by H and g thus preserves the fundamental integral H, and the momentum maps L and J.

A conserving scheme of the form (21) for the present system requires a discrete derivative operator D for $H(q,p)$ and $g(q)$ satisfying the orthogonality conditions associated with G_1 and G_2. Using the results in [9] we obtain the implicit, one-step scheme

$$\left.\begin{aligned} q_i^{n+1} - q_i^n &= \quad \Delta t\, m_i^{-1} p_i^{n+\frac{1}{2}} \\ p_i^{n+1} - p_i^n &= -\Delta t\, \mathsf{D}_i V(q^n, q^{n+1}) - \Delta t\, \lambda_1^{n+1} \mathsf{D}_i g_1(q^n, q^{n+1}) \\ &\quad - \Delta t\, \lambda_2^{n+1} \mathsf{D}_i g_2(q^n, q^{n+1}) \\ 0 &= \quad g_1(q^{n+1}) \\ 0 &= \quad g_2(q^{n+1}) \end{aligned}\right\} \tag{33}$$

where $(\cdot)^{n+\frac{1}{2}} = \frac{1}{2}[(\cdot)^n + (\cdot)^{n+1}]$ and

$$\left.\begin{aligned} \mathsf{D}_i V(q^n, q^{n+1}) &= \left[\frac{\tilde{V}_1(\pi_1^{n+1}) - \tilde{V}_1(\pi_1^n)}{\pi_1^{n+1} - \pi_1^n}\right] \frac{\partial \pi_1}{\partial q_i}(q^{n+\frac{1}{2}}) \\ &\quad + \left[\frac{\tilde{V}_2(\pi_2^{n+1}) - \tilde{V}_2(\pi_2^n)}{\pi_2^{n+1} - \pi_2^n}\right] \frac{\partial \pi_2}{\partial q_i}(q^{n+\frac{1}{2}}) \\ \mathsf{D}_i g_1(q^n, q^{n+1}) &= \left[\frac{\tilde{g}_1(\zeta_1^{n+1}) - \tilde{g}_1(\zeta_1^n)}{\zeta_1^{n+1} - \zeta_1^n}\right] \frac{\partial \zeta_1}{\partial q_i}(q^{n+\frac{1}{2}}) \\ \mathsf{D}_i g_2(q^n, q^{n+1}) &= \left[\frac{\tilde{g}_2(\zeta_2^{n+1}) - \tilde{g}_2(\zeta_2^n)}{\zeta_2^{n+1} - \zeta_2^n}\right] \frac{\partial \zeta_2}{\partial q_i}(q^{n+\frac{1}{2}}). \end{aligned}\right\} \tag{34}$$

The above scheme conserves the configuration space $\mathcal{Q}$, the total energy $H(q,p)$, and the linear and angular momentum maps $L(q,p)$ and $J(q,p)$. Moreover, it is straightforward to show that the scheme is time-reversible in the sense of [22].

Remarks 4.1

1. For unconstrained systems, the idea of approximating the derivative of a potential with a finite-difference quotient in order to achieve energy and momentum conservation can be traced back to [13, 14, 16, 17]. In the present example, these difference quotients are a special case of the equivariant discrete derivative formulae presented in [9].

2. The integral-preserving properties of the above scheme are automatic; in particular, the integrals are not enforced through the introduction of extra multipliers and projection steps [3, 8]. In contrast with the scheme presented here, methods based on the use of extra multipliers to preserve integrals are generally not time-reversible.

To illustrate the performance of the scheme a simulation was done using the following parameters and initial data:

$$m_1 = 1.0, \quad m_2 = 3.0, \quad m_3 = 2.3, \quad m_4 = 1.7, \quad L_1 = 1.0, \quad L_2 = 1.0$$

$$\begin{aligned} V_1(q) &= \tfrac{1}{4}K_1(|q_1 - q_3|^2 - 1)^2, \qquad K_1 = 100 \\ V_2(q) &= \tfrac{1}{4}K_2(|q_2 - q_4|^2 - 1)^2, \qquad K_2 = 1000 \end{aligned}$$

$$\begin{aligned} q_1^0 &= (0,0,0), \quad q_2^0 = (1,0,0), \quad q_3^0 = (0,1,0), \quad q_4^0 = (1,1,0) \\ p_1^0 &= (0,0,0), \quad p_2^0 = (0,0,0), \quad p_3^0 = (0,0,0), \quad p_4^0 = (0,0,2). \end{aligned}$$

Figure 2 shows the motion computed over the time interval $[0, 10s]$ with a time step of $\Delta t = 0.01s$. The dotted lines in the figure show the initial positions of the "rigid bars" to which the points masses are attached.

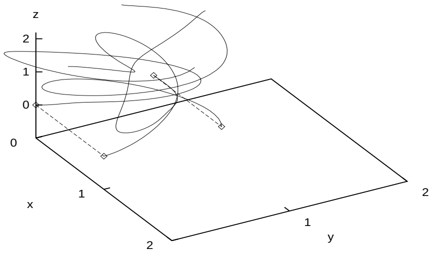
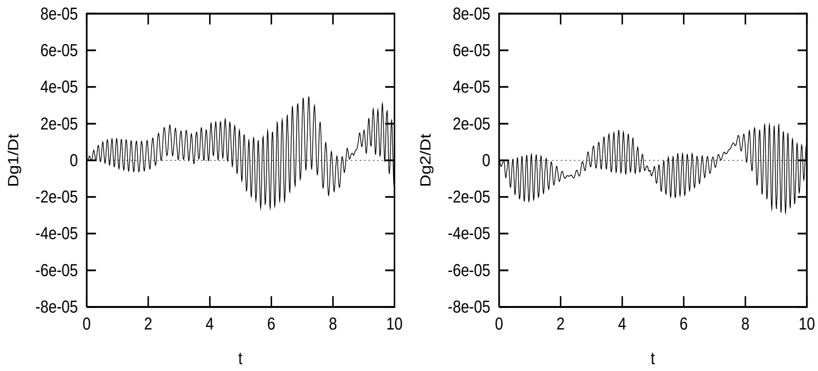


Figure 2: Motion of constrained four particle system.

By design, the constraints $g_1 = 0$, $g_2 = 0$, the total energy H, the three components of total linear momentum L and the three components of the total angular momentum J are conserved at each time step to the tolerance of the numerical computations. Ideally, one would also like the quantities

$$\dot{g}_1 = \sum_{i=1}^{4} \frac{\partial g_1}{\partial q_i}(q) \cdot m_i^{-1} p_i \quad \text{and} \quad \dot{g}_2 = \sum_{i=1}^{4} \frac{\partial g_2}{\partial q_i}(q) \cdot m_i^{-1} p_i$$

to vanish along the computed solution. However, as shown in Figure 3, these quantities exhibit bounded oscillations about zero. Thus, while the scheme preserves the configuration space $\mathcal{Q}$, it does not generally preserve the intrinsic phase space $\mathcal{M}$.



(a) (b)

Figure 3: Time history of velocity constraints.

Some of the convergence properties of the scheme are illustrated in Figure 4, which contains a plot of the relative error in the position q_4 at time $T = 0.1s$ versus the time step Δt. Denoting by $q_{4,\Delta t}(T)$ the value of q_4 at time T computed with time step Δt, the relative error is defined as

$$\text{relative error} = \frac{|q_{4,\Delta t}(T) - q_{4,e}(T)|}{|q_{4,e}(T)|}$$

where $q_{4,e}(T)$ represents the "exact" solution at time T computed with a time step $\Delta t = 10^{-5}s$. Figure 4 implies the scheme is second-order accurate in the positions. However, this level of accuracy is not necessarily achieved in the momenta and Lagrange multipliers since schemes may exhibit the phenomena of order reduction when applied to systems of differential-algebraic equations [5]. For the present scheme such issues will be discussed elsewhere.

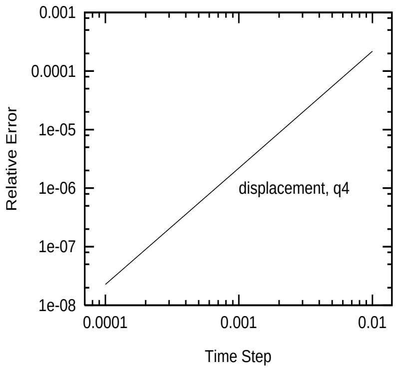


Figure 4: Relative error in q_4 versus time step.

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