Line Integral Solution of Hamiltonian Systems with Holonomic Constraints

Luigi Brugnano\textsuperscript{a}, Gianmarco Gurioli\textsuperscript{a}, Ewa B. Weinmüller\textsuperscript{b}

\textsuperscript{a} Dipartimento di Matematica e Informatica "U. Dini", Viale Morgagni 67/a, I-50134 Firenze, Italy.
\textsuperscript{b} Institute for Analysis and Scientific Computing, Vienna University of Technology, A-1040 Wien, Austria.

– Dedicated to John Butcher, on the occasion of his 84-th birthday –

Abstract

In this paper we extend the application of Hamiltonian Boundary Value Methods (HBVMs), a class of energy-conserving Runge-Kutta methods for Hamiltonian problems, to the numerical solution of Hamiltonian systems with holonomic constraints. The extension is obtained through a straightforward use of the so called line integral approach on which the methods rely, which is here used also for dealing with the constraints. As a result, the modified methods conserve both the Hamiltonian and the constraints, as is shown in their analysis. Some numerical tests are reported, to give evidence of the theoretical findings.

Keywords: constrained Hamiltonian systems; holonomic constraints; energy-conserving methods; line integral methods; Hamiltonian Boundary Value Methods; HBVMs.

MSC: 65P10, 65L80, 65L06.

1 Introduction

We shall here consider the numerical solution of a constrained Hamiltonian dynamics, described, for sake of simplicity, by the separable Hamiltonian

\[ H(q, p) = \frac{1}{2} p^\top M^{-1} p + U(q), \quad q, p \in \mathbb{R}^m. \tag{1} \]

However, the arguments can be extended to a general Hamiltonian in a straightforward way, as is sketched in the sequel. The problem is completed by \( \nu \) holonomic constraints,

\[ g(q) = 0 \in \mathbb{R}^\nu, \tag{2} \]

where we shall suppose \( \nu < m \) and, moreover, we shall also assume that all points are regular for the constraints, i.e., \( \nabla g(q) \in \mathbb{R}^{m \times \nu} \) has full column rank. Moreover, for sake of brevity, hereafter, both \( U \) and \( g \) will be assumed to be suitably regular (e.g., analytic).

It is well-known that the problem defined by (1)-(2) can be cast in Hamiltonian form by defining the augmented Hamiltonian

\[ \hat{H}(q, p, \lambda) = H(q, p) + \lambda^\top g(q), \tag{3} \]

\[ \lambda \in \mathbb{R}^\nu. \]
where $\lambda$ is the vector of Lagrange multipliers, leading to the constrained Hamiltonian system,

$$
\dot{q} = M^{-1}p, \quad \dot{p} = -\nabla U(q) - \nabla g(q)\lambda, \quad g(q) = 0, \quad t \geq 0,
$$

equipped with a set of consistent initial conditions,

$$
q(0) = q_0, \quad p(0) = p_0,
$$

such that

$$
g(q_0) = 0, \quad \nabla g(q_0)^\top M^{-1}p_0 = 0.
$$

We observe that the condition $g(q_0) = 0$ ensures that $q_0$ belongs to the manifold

$$
\mathcal{M} = \{ q \in \mathbb{R}^m : g(q) = 0 \},
$$

as required by the constraints, whereas the condition $\nabla g(q_0)^\top M^{-1}p_0$ means that the motion initially stays on the tangent space to $\mathcal{M}$ at $q_0$. At a continuous level, this condition is satisfied by all points on the trajectory solution, since, in order for the constraints to be conserved, one has:

$$
\dot{g}(q) = \nabla g(q)^\top \dot{q} = \nabla g(q)^\top M^{-1}p = 0.
$$

We observe that, for a general Hamiltonian, the requirement (7) is easily seen to become

$$
\nabla g(q)^\top H_p(q,p) = 0,
$$

where, hereafter, $H_q$ and $H_p$ will denote the partial derivatives of $H$ w.r.t. $q$ and $p$, respectively and, similarly, for second order derivatives, such as $H_{pp}$. A similar notation will be also used for the augmented Hamiltonian $\hat{H}$ defined at (3).

It must be stressed that the condition (7) can be conveniently relaxed, when dealing with a numerical approximation, only asking for $\nabla g(q)^\top M^{-1}p$ to be suitably small along the numerical solution. Consequently, when solving the problem on the interval $[0, h]$, we shall require that the obtained approximations,

$$
q_1 \approx q(h), \quad p_1 \approx p(h),
$$

do satisfy the conservation of both the Hamiltonian and the constraints,

$$
H(q_1, p_1) = H(q_0, p_0), \quad g(q_1) = g(q_0) = 0,
$$

and require that

$$
\nabla g(q_1)^\top M^{-1}p_1 = O(h^r), \quad r \geq 1.
$$

We notice that (10) is equivalent to require that

$$
\hat{H}(q_1, p_1, \lambda) = \hat{H}(q_0, p_0, \lambda), \quad g(q_1) = g(q_0) = 0,
$$

with the parameter $\lambda$ chosen in order to satisfy the constraints $g(q_1) = 0$. For sake of completeness and later use, we recall that in the continuous case a formal expression for the vector $\lambda$ is obtained by differentiating once more (7), i.e.,

$$
\ddot{g}(q) = \nabla^2 g(q)(M^{-1}p, M^{-1}p) - \nabla g(q)^\top M^{-1} [\nabla U(q) + \nabla g(q)\lambda],
$$

from which one derives, by imposing the vanishing of this derivative:

$$
[\nabla g(q)^\top M^{-1}\nabla g(q)] \lambda = \nabla^2 g(q)(M^{-1}p, M^{-1}p) - \nabla g(q)^\top M^{-1}\nabla U(q).
$$

Consequently, the following result is proved.
Theorem 1  The vector $\lambda$ exists and is uniquely determined, provided that matrix
\[ \nabla g(q)^\top M^{-1} \nabla g(q) \]
is nonsingular.

In a similar way, for a general Hamiltonian, one proves the following result.

Theorem 2  The vector $\lambda$ exists and is uniquely determined, provided that matrix
\[ \nabla g(q)^\top H_{pp}(q,p) \nabla g(q) \]
is nonsingular.

The numerical solution of Hamiltonian problems with holonomic constraints has been the subject of many researches, resulting into methods using different approaches: starting from the basic Shake-Rattle method [36, 3], which has been proved to be symplectic [30], higher order methods have been obtained through symplectic PRK methods [24], composition methods [32, 33], symmetric LMFs [23], together with further different approaches based, e.g., on local parametrizations of the manifold containing the solution [4], or relying on projection techniques [34, 37]. Additional references are [28, 35, 25, 31] and the monographs [5, 29, 26, 27].

In this paper we pursue a different approach, based on the use of the so called line integrals, which has already been used for deriving the class of energy-conserving Runge-Kutta methods, for unconstrained Hamiltonian systems, called Hamiltonian Boundary Value Methods (HBVMs) [11, 12, 13, 16, 17] (see also the recent monograph [10]). Such methods have already been extended in a number of directions (see, e.g., [6, 9, 14, 15, 2, 8, 1]), and are here extended to cope with the constrained problem (1)-(2). Roughly speaking, the conservation of the invariant will be obtained by requiring the vanishing of a suitable line integral, representing a discrete-time version of (7) (or (8), in the general case). In fact, if we fix a stepsize $h > 0$, then the conservation of the constraints (2) at $h$, starting from the point $q_0$ defined in (5), can be recast as the vanishing of the line integral

\[ g(q(h)) - g(q(0)) = \int_0^h \nabla g(q(t))^\top \dot{q}(t) dt. \]

For the continuous solution, in fact, this integral vanishes since the integrand is identically zero, by virtue of (4) and (7). Nevertheless, we can relax this requirement, if we consider a numerical method, providing a discrete-time dynamics. In fact, in such a case, the conservation properties have to be satisfied only at a set of discrete times which are multiples of the stepsize $h$. Consequently, one can consider an approximation $\sigma_1(t)$, locally approximating $q(t)$, such that:

\[ \sigma_1(0) = q_0, \quad \sigma_1(h) =: q_1 \approx q(h), \]

and

\[ g(q_1) - g(q_0) = g(\sigma_1(h)) - g(\sigma_1(0)) = \int_0^h \nabla g(\sigma_1(t))^\top \dot{\sigma}_1(t) dt = 0, \]

but without requiring the integrand be identically zero. This, in turn, will provide us with a proper choice of the vector of the multiplier $\lambda$. As a result, one eventually obtains a suitable modification of the basic HBVMs which, in this new setting, are able to conserve both the Hamiltonian and the
constraints, while retaining their original order. In so doing, all the available machinery for efficiently implementing the original methods (see, e.g., [13, 7, 10]), which make them very reliable and robust for numerically solving unconstrained Hamiltonian problems, can be adapted for efficiently dealing with the holonomic constraints.

With this premise, in Section 2 we start providing the framework for devising the methods via a suitable choice of the vector $\lambda$ of the Lagrange multipliers. Then, in Section 3 we obtain fully discrete methods, resulting in a suitable modification of the original HBVMs. Section 4 then provides some numerical tests on a number of constrained Hamiltonian problems and, at last, Section 5 contains a few conclusions and future directions of investigations.

## 2 Polynomial approximation

Since we shall speak about a one-step method, it will be sufficient to study its application on the interval $[0,h]$, since the same arguments apply to the subsequent integration steps. In order to obtain the approximations (9), let us consider the orthonormal basis on $[0,1]$ given by the shifted and scaled Legendre polynomials $\{P_j\}$,

$$P_j \in \Pi_j,$$

$$\int_0^1 P_i(c)P_j(c) = \delta_{ij}, \quad \forall i, j = 0, 1, \ldots,$$  \hspace{1cm} (15)

along with the expansions, along this basis,

$$M^{-1}p(ch) = \sum_{j \geq 0} P_j(c)\gamma_j(p), \quad \nabla U(q(ch)) = \sum_{j \geq 0} P_j(c)\psi_j(q),$$

$$\nabla g(q(ch)) = \sum_{j \geq 0} P_j(c)\rho_j(q), \quad c \in [0, 1],$$  \hspace{1cm} (16)

with

$$\gamma_j(p) = M^{-1}\int_0^1 P_j(c)p(ch)dc,$$

$$\psi_j(q) = \int_0^1 P_j(c)\nabla U(q(ch))dc,$$

$$\rho_j(q) = \int_0^1 P_j(c)\nabla g(q(ch))dc, \quad j \geq 0.$$  \hspace{1cm} (17)

Consequently, the differential equations in (4), over the interval $[0,h]$, can be rewritten, respectively, as:

$$\dot{q}(ch) = \sum_{j \geq 0} P_j(c)\gamma_j(p), \quad \dot{p}(ch) = -\sum_{j \geq 0} P_j(c)[\psi_j(q) + \rho_j(q)\lambda], \quad c \in [0, 1].$$  \hspace{1cm} (18)

Moreover, by imposing the initial conditions (5), one formally obtains that:

$$q(ch) = q_0 + h\sum_{j \geq 0}\int_0^c P_j(x)dx \gamma_j(p), \quad p(ch) = p_0 - h\sum_{j \geq 0}\int_0^c P_j(x)dx[\psi_j(q) + \rho_j(q)\lambda], \quad c \in [0, 1].$$  \hspace{1cm} (19)

The following result is known [16, Lemma 1].

**Lemma 1** Let $G: [0,h] \to V$, with $V$ a vector space, admit a Taylor expansion at 0. Then

$$\int_0^1 P_j(c)G(ch)dc = O(h^j), \quad j \geq 0.$$
As a straightforward consequence, one has the following result.

**Corollary 1** All the coefficients defined at (17) are $O(h^3)$.

In order to obtain a polynomial approximation $\sigma_1 \approx q$ and $\sigma_2 \approx p$ of degree $s$, let us truncate the series at the right-hand sides in (18) to finite sums,

$$
\dot{\sigma}_1(ch) = \sum_{j=0}^{s-1} P_j(c)\gamma_j(\sigma_2), \quad \dot{\sigma}_2(ch) = -\sum_{j=0}^{s-1} P_j(c)[\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda], \quad c \in [0, 1],
$$

(20)

where the coefficients are defined according to (17) by formally replacing $q$ and $p$ with $\sigma_1$ and $\sigma_2$, respectively. Consequently, in place of (19), one has

$$
\sigma_1(ch) = q_0 + h \sum_{j=0}^{s-1} \int_0^c P_j(x)dx \gamma_j(\sigma_2), \quad \sigma_2(ch) = p_0 - h \sum_{j=0}^{s-1} \int_0^c P_j(x)dx[\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda],
$$

(21)

with the new approximations given, by virtue of (15), by:

$$
q_1 := \sigma_1(h) \equiv q_0 + h\gamma_0(\sigma_2), \quad p_1 := \sigma_2(h) \equiv p_0 - h[\psi_0(\sigma_1) + \rho_0(\sigma_1)\lambda].
$$

(22)

Concerning the conservation properties of the obtained approximations, the following result holds true.

**Theorem 3** With reference to the approximations (20)–(22), for all $\lambda \in \mathbb{R}^\nu$ one has:

$$
\dot{H}(q_1, p_1, \lambda) = \dot{H}(q_0, p_0, \lambda).
$$

**Proof** For a given $\lambda \in \mathbb{R}^\nu$, from (3), (20), and (22), one obtains:

$$
\dot{H}(q_1, p_1, \lambda) - \dot{H}(q_0, p_0, \lambda) = \dot{H}(\sigma_1(h), \sigma_2(h), \lambda) - \dot{H}(\sigma_1(0), \sigma_2(0), \lambda)
$$

$$
= \int_0^h \frac{d}{dt} \dot{H}(\sigma_1(t), \sigma_2(t))dt = \int_0^h \left\{ \dot{H}_q(\sigma_1(t), \sigma_2(t))\dot{\sigma}_1(t) + \dot{H}_p(\sigma_1(t), \sigma_2(t))\dot{\sigma}_2(t) \right\} dt
$$

$$
= h \int_0^1 \left\{ [\nabla U(\sigma_1(ch)) + \nabla g(\sigma_1(ch))\lambda]^{\top} \dot{\sigma}_1(ch) + [M^{-1}\sigma_2(ch)]^{\top} \dot{\sigma}_2(ch) \right\} dc
$$

$$
= h \int_0^1 \left\{ [\nabla U(\sigma_1(ch)) + \nabla g(\sigma_1(ch))\lambda]^{\top} \sum_{j=0}^{s-1} P_j(c)\gamma_j(\sigma_2) - [M^{-1}\sigma_2(ch)]^{\top} \sum_{j=0}^{s-1} P_j(c)[\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda] \right\} dc
$$

$$
= h \sum_{j=0}^{s-1} \left\{ \left( \int_0^1 P_j(c)[\nabla U(\sigma_1(ch)) + \nabla g(\sigma_1(ch))\lambda] dc \right)^{\top} \gamma_j(\sigma_2) - \left( M^{-1} \int_0^1 P_j(c)\sigma_2(ch) dc \right)^{\top} [\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda] \right\}
$$

$$
= h \sum_{j=0}^{s-1} \left\{ [\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda]^{\top} \gamma_j(\sigma_2) - \gamma_j(\sigma_2)^{\top} [\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda] \right\} = 0. \square
$$
Consequently, as observed above, the conservation of the Hamiltonian (1) is granted, once the constraints are also satisfied, i.e., \( g(q_1) = 0 \). As sketched in Section 1, for this purpose, we shall resort to a line integral argument to determine the vector \( \lambda \), thus proving the following theorem.

**Theorem 4** Let us assume \( \nabla g(q_0)^{\top} M^{-1} \nabla g(q_0) \in \mathbb{R}^{\nu \times \nu} \) be nonsingular. Then, for all sufficiently small \( h > 0 \), there exists \( \lambda \in \mathbb{R}^\nu \) such that \( g(q_1) = 0 \).

For a general Hamiltonian function \( H(q,p) \), the previous result modifies as follows, the proof being similar as that of Theorem 4, though slightly more technical.

**Theorem 5** Let us assume \( \nabla g(q_0)^{\top} H_{qp}(q_0,p_0) \nabla g(q_0) \in \mathbb{R}^{\nu \times \nu} \) be nonsingular. Then, for all sufficiently small \( h > 0 \), there exists \( \lambda \in \mathbb{R}^\nu \) such that \( g(q_1) = 0 \).

**Remark 1** Clearly, Theorems 4 and 5 are the discrete counterparts of Theorems 1 and 2, respectively.

Before proving Theorem 4, we need to state the following preliminary results.

**Lemma 2** With reference to the polynomial basis (15), one has:

\[
\int_0^1 P_j(c) \int_0^c P_i(x)dx = (X_s)_{j+1,i+1}, \quad i,j = 0, \ldots, s-1, \tag{23}
\]

i.e., the \((j+1,i+1)\)-st entry of the matrix

\[
X_s := \begin{pmatrix}
\xi_0 & \xi_1 & \cdots & \xi_s-1 \\
\xi_1 & 0 & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots \\
\xi_s-1 & 0 & \cdots & 0
\end{pmatrix}, \quad \xi_j = \frac{1}{2\sqrt{|4j^2-1|}}, \quad j = 0, \ldots, s-1. \tag{24}
\]

**Proof** Since the integrand at the left-hand side in (23) is a polynomial of degree at most \( 2s-1 \), the integral can be exactly computed via the Gauss-Legendre formula of order \( 2s \). Let then \( c_1, \ldots, c_s \) be the zeros of \( P_s \) and \( b_1, \ldots, b_s \) be the corresponding weights. Consequently, by defining the matrices

\[
P_s = (P_{j-1}(c_i)), \quad I_s = \left( \int_0^{c_i} P_{j-1}(x)dx \right), \quad \Omega = \text{diag}(b_1, \ldots, b_s) \in \mathbb{R}^{s \times s}, \tag{25}
\]

one obtains, by setting \( e_i \in \mathbb{R}^s \) the \( i \)-th unit vector,

\[
\int_0^1 P_j(c) \int_0^c P_i(x)dx = \sum_{\ell=1}^s b_\ell P_j(c_\ell) \int_0^{c_\ell} P_i(x)dx \equiv e_{j+1}^\top P_s^\top \Omega I_s e_{i+1}.
\]

The thesis then follows by observing that, because of the properties of Legendre polynomials (see, e.g., [10, Section 1.4.3]), one has,

\[
I_s = P_s X_s, \quad P_s^\top \Omega P_s = I_s,
\]

where \( X_s \) is the matrix defined at (24), and \( I_s \in \mathbb{R}^{s \times s} \) is the identity matrix. □
Lemma 3  With reference to (17) and (20), one has:

\[
\rho_0(\sigma_1) = \nabla g(q_0) + \frac{h}{2} \nabla^2 g(q_0) M^{-1} p_0 + O(h^2),
\]

\[
\rho_0(\sigma_1)^T M^{-1} p_0 = \nabla g(q_0)^T M^{-1} p_0 + \frac{h}{2} \nabla^2 g(q_0)(M^{-1} p_0, M^{-1} p_0) + O(h^2).
\]

Proof  Concerning the first equality, from Lemma 1 and Corollary 1 one has:

\[
\rho_0(\sigma_1) = \int_0^1 \nabla g(\sigma_1(ch)) dc = \int_0^1 [\nabla g(\sigma_1(0)) + ch \nabla^2 g(\sigma_1(0)) \dot{\sigma}_1(0) + O((ch)^2)] dc
\]

\[
= \nabla g(\sigma_1(0)) + \frac{h}{2} \nabla^2 g(\sigma_1(0)) \dot{\sigma}_1(0) + O(h^2)
\]

\[
= \nabla g(q_0) + \frac{h}{2} \nabla^2 g(q_0) \sum_{j=0}^{s-1} P_j(0) \gamma_j(\sigma_2) + O(h^2)
\]

\[
= \nabla g(q_0) + \frac{h}{2} \nabla^2 g(q_0) M^{-1} [p_0 + O(h)] + O(h^2)
\]

\[
= \nabla g(q_0) + \frac{h}{2} \nabla^2 g(q_0) M^{-1} p_0 + O(h^2).
\]

The second point then follows by transposition and right-multiplication by \( M^{-1} p_0 \). □

We are now able to prove Theorem 4.

Proof (of Theorem 4).  From (20)–(22), and assuming \( g(q_0) = 0 \), one has:

\[
g(q_1) = g(q_1) - g(q_0) = g(\sigma_1(h)) - g(\sigma_1(0)) = \int_0^h \frac{d}{dt} g(\sigma_1(t)) dt
\]

\[
= \int_0^h \nabla g(\sigma_1(t))^T \dot{\sigma}_1(t) dt = h \int_0^1 \nabla g(\sigma_1(ch))^T \dot{\sigma}_1(ch) dc = h \int_0^1 \nabla g(\sigma_1(ch))^T \sum_{j=0}^{s-1} P_j(c) \gamma_j(\sigma_2) dc
\]

\[
= h \sum_{j=0}^{s-1} \rho_j(\sigma_1)^T \gamma_j(\sigma_2) = h \sum_{j=0}^{s-1} \rho_j(\sigma_1)^T M^{-1} \int_0^1 P_j(c) \sigma_2(ch) dc
\]

\[
= h \sum_{j=0}^{s-1} \rho_j(\sigma_1)^T M^{-1} \int_0^1 P_j(c) \left\{ p_0 - h \sum_{i=0}^{s-1} \int_0^c P_i(x) dx [\psi_i(\sigma_1) + \rho_i(\sigma_1) \lambda] \right\} dc
\]

\[
= h \sum_{j=0}^{s-1} \rho_j(\sigma_1)^T M^{-1} p_0 \int_0^1 P_j(c) dc
\]

\[
- h^2 \sum_{i,j=0}^{s-1} \rho_j(\sigma_1)^T M^{-1} [\psi_i(\sigma_1) + \rho_i(\sigma_1) \lambda] \int_0^1 P_j(c) \int_0^c P_i(x) dx dc.
\]
Upon observing that, because of (15),
\[ \int_0^1 P_j(c) dc = \delta_{j0}, \]
and considering (23)-(24), one then obtains:

\[
g(\sigma_1(h)) - g(\sigma_1(0)) = h\rho_0(\sigma_1)^\top M^{-1} \{ p_0 - h[\xi_0(\psi_0(\sigma_1) + \rho_0(\sigma_1)\lambda) - \xi_1(\psi_1(\sigma_1) + \rho_1(\sigma_1)\lambda)] \}
- h^2 \sum_{j=1}^{s-2} \rho_j(\sigma_1)^\top M^{-1} \{ [\xi_j(\psi_j(\sigma_1) + \rho_j(\sigma_1)\lambda) - \xi_{j+1}(\psi_{j+1}(\sigma_1) + \rho_{j+1}(\sigma_1)\lambda)] \}
- h^2 \rho_{s-1}(\sigma_1)^\top M^{-1} [\xi_{s-1}(\psi_{s-1}(\sigma_1) + \rho_{s-1}(\sigma_1)\lambda)] =: \tilde{\Gamma}(\sigma_1, \sigma_2, \lambda, h). \tag{26} \]

By virtue of (17) and Corollary 1, one then obtains:
\[
\frac{g(\sigma_1(h)) - g(\sigma_1(0)) - h\rho_0(\sigma_1)^\top M^{-1} p_0}{h^2} = -\frac{1}{2} \left\{ \left[ \rho_0(\sigma_1)^\top M^{-1} \rho_0(\sigma_1) + O(h) \right] \lambda + \rho_0(\sigma_1)^\top M^{-1} \psi_0(\sigma_1) + O(h) \right\}. \tag{27} \]

By considering that from (17) and the result of Lemma 3 one has:

\[
\frac{g(\sigma_1(h)) - g(\sigma_1(0)) - h\rho_0(\sigma_1)^\top M^{-1} p_0}{h^2} = \frac{1}{2} \left\{ \tilde{g}(q_0) - \nabla^2 g(q_0)(M^{-1} p_0, M^{-1} p_0) + O(h) \right\},
\]

\[
\rho_0(\sigma_1)^\top M^{-1} \rho_0(\sigma_1) = \nabla g(q_0)^\top M^{-1} \nabla g(q_0) + O(h),
\]

\[
\rho_0(\sigma_1)^\top M^{-1} \psi_0(\sigma_1) = \nabla g(q_0)^\top M^{-1} \nabla U(q_0) + O(h),
\]

it follows that (27) tends to (13), as \( h \to 0 \). Consequently, \( \lambda \) exists for all sufficiently small stepsizes \( h > 0 \). On the other hand, one obtains that \( g(q_1) - g(q_0) = g(q_1) = 0 \), provided that (see (26))

\[ \tilde{\Gamma}(\sigma_1, \sigma_2, \lambda, h) = 0, \]

i.e.,

\[
\rho_0(\sigma_1)^\top M^{-1} p_0 \tag{28}
= h \sum_{j=0}^{s-2} \rho_j(\sigma_1)^\top M^{-1} \{ \xi_j[\psi_{j+1}(\sigma_1) + \rho_{j+1}(\sigma_1)\lambda] - \xi_j[\psi_{j+1}(\sigma_1) + \rho_{j+1}(\sigma_1)\lambda] \}
+ h \xi_{s-1}(\sigma_1)^\top M^{-1} [\psi_{s-2}(\sigma_1) + \rho_{s-2}(\sigma_1)\lambda]
= h \left\{ \left[ \xi_0 \rho_0(\sigma_1)^\top M^{-1} \rho_0(\sigma_1) + \sum_{j=1}^{s-1} \xi_j \left[ \rho_j(\sigma_1)^\top M^{-1} \rho_{j-1}(\sigma_1) - \rho_{j-1}(\sigma_1)^\top M^{-1} \rho_j(\sigma_1) \right] \right] \lambda
+ \xi_0 \rho_0(\sigma_1)^\top M^{-1} \psi_0(\sigma_1) + \sum_{j=1}^{s-1} \xi_j \left[ \rho_j(\sigma_1)^\top M^{-1} \psi_{j-1}(\sigma_1) - \rho_{j-1}(\sigma_1)^\top M^{-1} \psi_j(\sigma_1) \right] \right\},
\]
which can be formally recasted as the linear system

\[ A(h)\lambda = b(h), \]  

(29)

with the coefficient matrix and the left-hand side given, by virtue of (17) and Corollary 1, by

\[ A(h) = h\xi_0\rho_0(\sigma_1)^\top M^{-1}\rho_0(\sigma_1) + O(h^2) = \frac{h}{2}\nabla g(q_0)^\top M^{-1}\nabla g(q_0) + O(h^2), \]  

(30)

and

\[ b(h) = \rho_0(\sigma_1)^\top M^{-1}p_0 - \xi_0h\rho_0(\sigma_1)^\top M^{-1}\psi_0(\sigma_1) + O(h^2) = \nabla g(q_0)^\top M^{-1}p_0 + \frac{h}{2}\left[\nabla^2 g(q_0)(M^{-1}p_0, M^{-1}p_0) - \nabla g(q_0)^\top M^{-1}\nabla U(q_0)\right] + O(h^2). \]  

(31)

Consequently, (29) is consistent with (14), since \( \nabla g(q_0)^\top M^{-1}p_0 = 0. \) □

**Remark 2** With reference to the vector \( \lambda \) defined at (29)-(31), one has that \( \lambda = O(1) \). In fact, \( A(h) = O(h) \) and, due to the fact that \( \nabla g(q_0)^\top M^{-1}p_0 = 0 \), also \( b(h) = O(h) \). One would arrive to the same conclusion, provided that \( \nabla g(q_0)^\top M^{-1}p_0 = O(h^r) \), \( r \geq 1 \), as we require for the numerical approximation (see (11)). This, in turn, is sufficient to establish the order of the obtained approximations (9)-(22), according to the next theorem.

**Theorem 6** Assume that the vector \( \lambda = O(1) \). Then, \( q_1 - q(h) = O(h^{2s+1}) = p_1 - p(h) \). Consequently, the method has order \( 2s \).

**Proof** Let us set

\[ y = \begin{pmatrix} q \\ p \end{pmatrix}, \quad \sigma = \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}, \quad \Psi_j(\sigma; \lambda) = \begin{pmatrix} \gamma_j(\sigma_2) \\ -\psi_j(\sigma_1) - \rho_j(\sigma_1)\lambda \end{pmatrix}, \]

and \( y(t; \tau, \eta) \) be the solution of the problem (4), whose right-hand side will be denoted by \( f_\lambda(y) \), satisfying the initial condition \( y(\tau) = \eta \). Moreover, let us set \( \Phi(t, \tau) \) the fundamental matrix solution, solving the associated variational problem

\[ \dot{\Phi}(t, \tau) = f'_\lambda(y(t; \tau, \eta))\Phi(t, \tau), \quad t \geq \tau, \quad \Phi(\tau, \tau) = I, \]

and

\[ \Gamma_j := \int_0^1 P_j(c)\Phi(h, ch)dc, \quad j \geq 0. \]

We observe that, by virtue of Lemma 1 and of the hypothesis on \( \lambda \), both \( \Psi_j(\sigma; \lambda) \) and \( \Gamma_j \) are \( O(h^j) \). Then, one has:
Corollary 2 Under the hypotheses of the previous Theorem 6, one obtains:

\[
\nabla g(q_1)^\top M^{-1}p_1 = \nabla g(q(h))^\top M^{-1}p(h) + O(h^{2s+1}).
\]

(32)

Remark 3 It is worth noticing that, according to what seen in Remark 2, (32) allows to satisfy the requirement \( \lambda = O(1) \) in Theorem 6, for \( N = O(h^{-2s}) \) integration steps, at least.

3 Full discretization

We observe that, in order to obtain a computational method, the integrals defining the coefficients

\[
\gamma_j(\sigma_2), \quad \psi_j(\sigma_1), \quad \rho_j(\sigma_1), \quad j = 0, \ldots, s - 1,
\]

obtained from (17) with \( \sigma_1 \) and \( \sigma_2 \) in place of \( q \) and \( p \), respectively, need to be conveniently approximated. For this purpose, following the streamline of HBVM(\( k, s \)) methods [12, 16, 10], one can use a Gauss-Legendre quadrature of order 2\( k \) (that is, the interpolatory quadrature formula based at the zeros of \( P_k(c) \)), with nodes and weights \( (\hat{c}_i, \hat{b}_i) \), where \( k \geq s \). Consequently, one obtains the following approximations:

\[
\gamma_j(\sigma_2) \approx \hat{\gamma}_j := M^{-1} \sum_{\ell=1}^k \hat{b}_\ell P_j(\hat{c}_\ell)\sigma_2(\hat{c}_\ell h), \quad \psi_j(\sigma_1) \approx \hat{\psi}_j := \sum_{\ell=1}^k \hat{b}_\ell P_j(\hat{c}_\ell)\nabla U(\sigma_1(\hat{c}_\ell h)),
\]

\[
\rho_j(\sigma_1) \approx \hat{\rho}_j := \sum_{\ell=1}^k \hat{b}_\ell P_j(\hat{c}_\ell)\nabla g(\sigma_1(\hat{c}_\ell h)), \quad j = 0, \ldots, s - 1.
\]

(33)

In so doing, one formally obtains a \( k \)-stage Runge-Kutta method, whose computational cost, however, depends on \( s \) rather than on \( k \),\(^1\) since the actual unknowns are the 3\( s \) coefficients (33) and

\(^1\)We refer, e.g., to [13, 10] for full details.
the vector $\lambda$. As matter of fact, let us formulate the discrete problem to be solved at each integration step, consisting into a vector formulation of (33). For this purpose, let us define the matrices (compare with (25)),

$$
\hat{P}_s = (P_{j-1}(\hat{e}_1)), \quad \hat{I}_s = \left( \int_0^{\hat{e}_i} P_{j-1}(x) \, dx \right) \in \mathbb{R}^{k \times s}, \quad \hat{\Omega} = \text{diag}(\hat{b}_1, \ldots, \hat{b}_k) \in \mathbb{R}^{k \times k},
$$

and the vectors and matrices

$$
e = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^k, \quad \hat{\gamma} = \begin{pmatrix} \hat{\gamma}_0 \\ \vdots \\ \hat{\gamma}_{s-1} \end{pmatrix}, \quad \hat{\psi} = \begin{pmatrix} \hat{\psi}_0 \\ \vdots \\ \hat{\psi}_{s-1} \end{pmatrix} \in \mathbb{R}^{s m}, \quad \hat{\rho} = \begin{pmatrix} \hat{\rho}_0 \\ \vdots \\ \hat{\rho}_{s-1} \end{pmatrix} \in \mathbb{R}^{s m \times \nu},
$$

where we recall that $m$ is the dimension of the continuous problem and $\nu$ is the number of constraints. Then, the $3s$ equations in (33), defining the discrete problem to be solved, amount to the system of equations, of (block) dimension $s$,

$$
\hat{\gamma} = \hat{P}_s^T \hat{\Omega} \otimes M^{-1} \left[ e \otimes p_0 - h\hat{I}_s \otimes I_m \left( \hat{\psi} + \hat{\rho} \lambda \right) \right], \\
\hat{\psi} = \hat{P}_s^T \hat{\Omega} \otimes I_m \nabla U \left( e \otimes q_0 + h\hat{I}_s \otimes I_m \hat{\gamma} \right), \\
\hat{\rho} = \hat{P}_s^T \hat{\Omega} \otimes I_m \nabla g \left( e \otimes q_0 + h\hat{I}_s \otimes I_m \hat{\gamma} \right),
$$

(34)

together with the equation (28)-(29) for $\lambda$ which, by taking into account the formal substitutions due to the approximations in (33), can be rewritten as

$$
h \left[ \xi_0 \hat{\rho}_0^T M^{-1} \hat{\rho}_0 + \sum_{j=1}^{s-1} \xi_j \left( \hat{\rho}_j^T M^{-1} \hat{\rho}_{j-1} - \hat{\rho}_{j-1}^T M^{-1} \hat{\rho}_j \right) \right] \lambda \\
= \hat{\rho}_0^T M^{-1} \left( p_0 - h\xi_0 \hat{\psi}_0 \right) - h \sum_{j=1}^{s-1} \xi_j \left( \hat{\rho}_j^T M^{-1} \hat{\psi}_{j-1} - \hat{\rho}_{j-1}^T M^{-1} \hat{\psi}_j \right).
$$

(35)

In the equations (34), $\nabla U$, when evaluated in a block vector of (block) dimension $k$, stands for the block vector made up of the $k$ vectors resulting from the corresponding application of the function. The same straightforward notational convention has been used for $\nabla g$. The new approximation is then given, according to (22) and taking into account (33), by

$$
q_1 = q_0 + h\hat{\gamma}_0, \quad p_1 = p_0 - h[\hat{\psi}_0 + \hat{\rho}_0 \lambda].
$$

(36)

We observe that the three equations in (34), together with (36), formally coincide with those provided by a HBVM($k$, $s$) method\(^2\) for solving the problem defined by the Hamiltonian (3), where the vector of the multiplier $\lambda$ is considered as a parameter:\(^3\)

$$
\dot{q} = M^{-1} p, \quad \dot{p} = -\nabla U(q) - \nabla g(q) \lambda, \quad t \geq 0, \quad q(0) = q_0, \ p(0) = p_0.
$$

(37)

\(^2\)Here, $s$ concerns the degree of the polynomial approximation (as it has been explained in Section 2), and $k$ defines the order (2$k$, indeed) of the quadrature in the approximations (33).

\(^3\)Clearly, the problem (37) represents the “unconstrained” version of (4).
We refer, e.g., to [13, 10] for full details. Consequently, the additional equation (35) defines the proper extension of such a method for handling the constrained Hamiltonian problem (1)-(2). For this reason, we shall continue to refer to the numerical method defined by (34), (35), and (36) as to HBVM($k, s$). Clearly, it is a ready to use numerical method.

The discrete problem (34)-(35) can be solved via a straightforward fixed-point iteration, which clearly converges, under regularity assumptions, for all sufficiently small stepizes $h > 0$.\(^4\) Moreover, for separable Hamiltonians, as is the case of problem (1), one has that the last two equations in (34) can be substituted into the first one, thus obtaining a single vector equation in the unknown $\hat{\gamma}$. In fact, by setting

$$\Theta_\lambda(q) := \nabla U(q) + \nabla g(q)\lambda,$$

one obtains:

$$\hat{\gamma} = \hat{P}_s^T\hat{\Omega} \otimes M^{-1} \left[ e \otimes p_0 - h\hat{I}_s\hat{P}_s^T\hat{\Omega} \otimes I_m \Theta_\lambda \left( e \otimes q_0 + h\hat{I}_s \otimes I_m \hat{\gamma} \right) \right],$$

plus the equation (35) for $\lambda$. We skip here further details, since they are exactly the same as for the original HBVMs, when applied to separable (unconstrained) Hamiltonian problems [13, 10].

The following result can be proved, by using Theorem 6 along with standard arguments in the analysis of HBVMs [16, 10].

**Theorem 7** For all $k \geq s$, the HBVM($k, s$) method (34)–(36):

- has order $2s$, and the result of Corollary 2 continues to hold;
- is symmetric;
- exactly conserves the Hamiltonian and the constraints, if both $H$ and $g$ are polynomials of degree not larger than $2k/s$. Differently,
- in the non polynomial case, it has an error in the Hamiltonian and/or in the constraints which is $O(h^{2k+1})$.

**Remark 4** It must be stressed that, from the last two points of Theorem 7, an exact or a (at least) practical conservation of both the constraints and the Hamiltonian can always be gained, by choosing $k$ large enough so that either the quadrature is exact, in the polynomial case, or the quadrature error is within round-off, in the non polynomial case. This feature will be always exploited in the numerical tests contained in Section 4.

It is worth mentioning that, when $k = s$, the HBVM($s, s$) method reduces to the $s$-stage Gauss collocation method. According to Theorem 7, it is able to conserve quadratic Hamiltonians and constraints. Consequently, a HBVM($k, s$) method, for $k > s$, can be regarded as a conserving variant of such Runge-Kutta method, suitable for non quadratic Hamiltonians and/or constraints.

We conclude this section by observing that, in the limit $k \to \infty$, one obviously retrieves the formulae studied in Section 2.

---

\(^4\) We refer to [13, 7, 10] for further details about different procedures for solving the discrete problem, which are based on suitable Newton-splitting procedures, already successfully implemented in other computational codes [18, 19, 20].

\(^5\) We shall omit the proof, for sake of brevity.
4 Numerical Tests

In this section, we provide a few numerical tests, aimed at confirming the theoretical properties of HBVM\((k, s)\) applied for numerically solving Hamiltonian problems with holonomic constraints in the form (1)-(2) (i.e., the properties described by Theorem 7).

Conical pendulum

We start considering the so called conical pendulum, a particular case of the spherical pendulum, namely a pendulum of mass \(m\), which is connected to a fixed point (i.e., the origin) by a massless rod of length \(L\). For the conical pendulum, the initial condition is such that the motion is periodic of period \(T\) and lies on the horizontal plane \(q_3 = z_0\).\(^6\) Assuming unit mass and length of the pendulum, and normalizing for the acceleration of gravity, the Hamiltonian is then given by:

\[
H(q, p) := \frac{1}{2} p^\top p + e_3^\top q, \quad q, p \in \mathbb{R}^3,
\]

where \(e_3 = (0, 0, 1)^\top\), with the constraint

\[
g(q) := q^\top q - 1 = 0.
\]

We shall use the consistent initial conditions

\[
q(0) = \begin{pmatrix} 2^{-\frac{1}{2}} \\ 0 \\ -2^{-\frac{1}{2}} \end{pmatrix}, \quad p(0) = \begin{pmatrix} 0 \\ 2^{-\frac{1}{2}} \\ 0 \end{pmatrix},
\]

generating a periodic motion with

\[
T = 2^{\frac{3}{4}} \pi, \quad z_0 = -2^{-\frac{1}{2}}.
\]

Moreover, in such a case, the multiplier \(\lambda\), which has the physical meaning of the tension on the rod, has to be constant, and turns out to be equal to

\[
\lambda_0 = 2^{-\frac{1}{2}}.
\]

We notice that both the Hamiltonian and the constraint are quadratic so that, according to Theorem 7, any HBVM\((s, s)\) method conserves both of them and has order \(2s\). In Table 1 we report the measured errors on both the solution \(e_y\) and the multiplier \(e_\lambda\), by solving the problem over 10 periods, with a stepsize \(h = T/n\). The estimated rates of convergence are also reported, for HBVM\((s, s)\), \(s = 2, 3, 4\), thus confirming the order of convergence \(2s\) of the methods. Both the Hamiltonian and the constraint are conserved up to round-off. It is remarkable that the error on the multiplier appears to be negligible, whichever is the stepsize used.

Next, in Figure 1 we plot the solution error over 100 periods, by using HBVM\((2, 2)\) with stepsize \(h = T/100 \approx 0.053\), whereas in Figure 2 is the plot of the multiplier, Hamiltonian, and constraint errors. One may see that a linear growth of the solution error is observed, whereas the errors of the multiplier, the constraint, and the Hamiltonian are negligible.

\(^6\)Clearly, \(0 > z_0 > -L\).
Figure 1: conical pendulum (38)–(42). Linear growth of the solution error for HBVM(2,2), over 100 periods and stepsize $h = T/100 \approx 0.053$.

Figure 2: conical pendulum (38)–(42). Multiplier error (dashed line), Hamiltonian error (solid line), and constraint error (dotted line), by using HBVM(2,2) with stepsize $h = T/100 \approx 0.053$. 

\[ \times 10^{-5} \]
Figure 3: modified pendulum (43)–(44) solved by using HBVM(2,2) with stepsize $h = 0.1 \times 10^4$ steps. Upper plot: Hamiltonian error. Lower plot: constraint error.

Figure 4: modified pendulum (43)–(44) solved by using HBVM(6,2) with stepsize $h = 0.1 \times 10^4$ steps. Upper plot: Hamiltonian error. Lower plot: constraint error.
Table 1: conical pendulum (38)–(42). $e_y$ and $e_\lambda$ are the solution and multiplier errors, respectively, when solving the problem over 10 periods with stepsize $h = T/n$, with the HBVM(s, s) method.

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Modified pendulum

We now consider a modified version of the previous problem, aimed at exploiting the possibility of getting energy and constraints conservation by using a suitable high-order quadrature (33). In more detail, we consider the following non quadratic polynomial Hamiltonian,

$$H(q, p) := \frac{1}{2} p^\top p + (e_3^\top q)^4, \quad q, p \in \mathbb{R}^3,$$

with the non quadratic polynomial constraint

$$g(q) := 3 \sum_{i=1}^{3} (e_i^\top q)^2(4-i) - 0.625 = 0.$$  (44)

In such a case, by using the same initial condition as in (40), we perform $10^4$ steps, by using the stepsize $h = 0.1$, with the HBVM(2,2) method. Due to the fact that both the Hamiltonian and the constraint are no more quadratic, we expect that both of them are not exactly conserved. This is indeed confirmed by the plots in Figure 3. On the other hand, according to Theorem 7, the HBVM(6,2) method is expected to exactly conserve both the Hamiltonian and the constraint, as is confirmed by the two plots in Figure 4.

Tethered satellites system

We now consider a closed-loop rotating triangular tethered satellites system,\(^7\) formed by three satellites (considered as mass-points) of mass $m_i$, $i = 1, 2, 3$, joined by inextensible, tight, and massless tethers, of length $L_i$, $i = 1, 2, 3$, orbitating around a massive body.\(^8\) As before, for sake of simplicity we shall assume unit masses and lengths, also normalizing for the gravity constant.

Consequently, if $q_i = (x_i, y_i, z_i)^\top \in \mathbb{R}^3$, $i = 1, 2, 3$, are the positions of the three satellites, the constraints are given by:

$$g(q) := \begin{pmatrix} (q_1 - q_2)^\top (q_1 - q_2) - 1 \\ (q_2 - q_3)^\top (q_2 - q_3) - 1 \\ (q_3 - q_1)^\top (q_3 - q_1) - 1 \end{pmatrix} = 0 \in \mathbb{R}^3,$$  (45)

\(^7\)This example has been adapted from [22, 37].

\(^8\)The Earth, in the original example.
whereas the Hamiltonian is given by

\[ H(q,p) = \sum_{i=1}^{3} \left( \frac{1}{2} p_i^\top p_i - \frac{1}{\sqrt{q_i^\top q_i}} \right). \]  \hspace{1cm} (46)

As a set of consistent initial conditions, we consider

\[ q_1(0) = \begin{pmatrix} 0 \\ \frac{1}{2} \\ z_0 \end{pmatrix}, \quad q_2(0) = \begin{pmatrix} 0 \\ -\frac{1}{2} \\ z_0 \end{pmatrix}, \quad q_3(0) = \begin{pmatrix} 0 \\ 0 \\ z_0 - \frac{\sqrt{3}}{2} \end{pmatrix}, \]  \hspace{1cm} (47)

and

\[ p_1(0) = p_2(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad p_3(0) = \begin{pmatrix} v_0 \\ 0 \\ 0 \end{pmatrix}, \]  \hspace{1cm} (48)

where we set \( z_0 = 20 \) and \( v_0 \) such that the initial Hamiltonian is 0. This provides a configuration in which the first two satellites remain parallel, moving in the planes \( y = \frac{1}{2} \) and \( y = -\frac{1}{2} \), respectively, and the third one moves around the tether joining the first two, in the plane \( y = 0 \). In such a case, the Hamiltonian is non polynomial. Nevertheless, by using the HBVM(6,2) method with stepsize \( h = 0.1 \) over \( 10^4 \) steps, we obtain a qualitatively correct solution, satisfying the conservation of both the Hamiltonian and the constraints within round-off, as one may see in Figures 5 and 6, respectively.

5 Conclusions

In this paper we have considered the numerical solution of Hamiltonian problems with holonomic constraints, by resorting to a line-integral formulation of the conservation of the constraints. This, in turn, has allowed us to derive an expression of the Lagrange multipliers which, remarkably, doesn’t use second derivatives. Upon discretization of the resulting formulae, we have obtained a suitable variant of Hamiltonian Boundary Value Methods (HBVMs), formerly devised as energy-conserving Runge-Kutta methods for unconstrained Hamiltonian problems. Numerical experiments duly confirm the theoretical achievements.

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References


Figure 5: Tethered satellites system (45)–(48) solved by using HBVM(6,2) with stepsize $h = 0.1$ over $10^4$ steps. Hamiltonian error.

Figure 6: Tethered satellites system (45)–(48) solved by using HBVM(6,2) with stepsize $h = 0.1$ over $10^4$ steps. Constraints error.


