ARBITRARILY HIGH-ORDER ENERGY-CONSERVING METHODS FOR HAMILTONIAN PROBLEMS WITH QUADRATIC HOLONOMIC CONSTRAINTS

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Abstract

In this paper, we define arbitrarily high-order energy-conserving methods for Hamiltonian systems with quadratic holonomic constraints. The derivation of the methods is made within the so-called line integral framework. Numerical tests to illustrate the theoretical findings are presented.

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Key words: Constrained Hamiltonian systems, Quadratic holonomic constraints, Energy-conserving methods, Line integral methods, Hamiltonian Boundary Value Methods, HB-VMs.

1. Introduction

In recent years, much interest has been given to the modeling and/or simulation of tethered systems, where the dynamics of interconnected bodies is studied (see, e.g. [2, 25–27, 33, 34, 40, 42–45]). It turns out that the underlying dynamics is often described by a Hamiltonian system, for which the total energy is conserved.

Motivated by this fact, we here investigate the numerical approximation of a constrained Hamiltonian dynamics, described by the separable Hamiltonian

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

where \( M \) is a symmetric and positive-definite (SPD) matrix, subject to \( \nu \) quadratic holonomic constraints,

\[ g(q) = 0 \in \mathbb{R}^\nu, \quad \nu \leq m, \]

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i.e. the entries of \( g \) are quadratic polynomials. Hereafter, we shall assume all points be regular for the constraints, i.e. \( \nabla g(q) \in \mathbb{R}^{m \times \nu} \) has full column rank or, equivalently,  
\[
\nabla g(q)^\top M^{-1} \nabla g(q) \in \mathbb{R}^{\nu \times \nu} \quad \text{is SPD.}
\]  
(1.3)
Moreover, we shall assume that its smallest eigenvalue is bounded away from 0, in the domain of interest. Also, for sake of simplicity, in the same domain the potential \( U \) will be assumed to be analytic.

It is well-known that the problem defined by (1.1)-(1.2) can be cast in Hamiltonian form by defining the augmented Hamiltonian  
\[
\hat{H}(q,p,\lambda) = H(q,p) + \lambda^\top g(q),
\]  
(1.4)
where \( \lambda \) is the vector of the Lagrange multipliers. The resulting constrained Hamiltonian system reads  
\[
\dot{q} = M^{-1}p, \quad \dot{p} = \nabla U(q) - \nabla g(q)\lambda, \quad g(q) = 0, \quad t \in [0, T],
\]  
(1.5)
and is subject to consistent initial conditions  
\[
q(0) = q_0, \quad p(0) = p_0
\]  
(1.6)
such that  
\[
g(q_0) = 0, \quad \nabla g(q_0)^\top M^{-1}p_0 = 0.
\]  
(1.7)
Clearly, \( H(q,p) \equiv \hat{H}(q,p,\lambda) \), provided that the constraints (1.2) are satisfied, and a straightforward calculation proves that both are conserved along the solution trajectory.

We notice that the condition \( g(q_0) = 0 \) ensures that \( q_0 \) belongs to the manifold  
\[
\mathcal{M} = \{ q \in \mathbb{R}^m : g(q) = 0 \},
\]  
(1.8)
as required by the constraints, whereas the condition \( \nabla g(q_0)^\top M^{-1}p_0 = 0 \) means that the motion initially stays on the tangent space to \( \mathcal{M} \) at \( q_0 \). This condition is satisfied by all points on the solution trajectory, since, in order for the constraints to be conserved, the following condition needs to be satisfied as well:  
\[
\dot{g}(q) = \nabla g(q)^\top \dot{q} = \nabla g(q)^\top M^{-1}p = 0 \in \mathbb{R}^\nu.
\]  
(1.9)
These latter constraints are usually referred to as hidden constraints, and allow the derivation of the vector of the Lagrange multiplier \( \lambda \). In fact, from (1.9) and (1.5)-(1.6), one obtains  
\[
0 = \nabla g(q(t))^\top M^{-1}p(t)
= \nabla g(q(t))^\top M^{-1} \left[ p_0 + \int_0^t \nabla U(q(\zeta))d\zeta - \int_0^t \nabla g(q(\zeta))\lambda(\zeta)d\zeta \right],
\]  
(1.10)
from which one derives the integral equation  
\[
\nabla g(q(t))^\top M^{-1} \int_0^t \nabla g(q(\zeta))\lambda(\zeta)d\zeta
= \nabla g(q(t))^\top M^{-1} \left[ p_0 + \int_0^t \nabla U(q(\zeta))d\zeta \right].
\]  
(1.11)