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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.

Mathematics subject classification: 65P10, 65L80, 65L06.
Key words: Constrained Hamiltonian systems, Quadratic holonomic constraints, Energy-conserving methods, Line integral methods, Hamiltonian Boundary Value Methods, HBVMs.

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

$$H(q,p) = \frac{1}{2}p^\top M^{-1}p - U(q), \quad q,p \in \mathbb{R}^m, \tag{1.1}$$

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

$$g(q) = 0 \in \mathbb{R}^\nu, \quad \nu \le m, \tag{1.2}$$

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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,

$$\nabla g(q)^\top M^{-1} \nabla g(q) \in \mathbb{R}^{\nu\times\nu} \quad \text{is SPD.} \tag{1.3}$$

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

$$\hat{H}(q,p,\lambda) = H(q,p) + \lambda^\top g(q), \tag{1.4}$$

where λ is the vector of the Lagrange multipliers. The resulting constrained Hamiltonian system reads

$$\dot{q} = M^{-1}p, \quad \dot{p} = \nabla U(q) - \nabla g(q)\lambda, \quad g(q) = 0, \quad t \in [0,T], \tag{1.5}$$

and is subject to consistent initial conditions

$$q(0) = q_0, \quad p(0) = p_0 \tag{1.6}$$

such that

$$g(q_0) = 0, \quad \nabla g(q_0)^\top M^{-1} p_0 = 0. \tag{1.7}$$

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

$$\mathcal{M} = \{q \in \mathbb{R}^m : g(q) = 0\}, \tag{1.8}$$

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:

$$\dot{g}(q) = \nabla g(q)^\top \dot{q} = \nabla g(q)^\top M^{-1} p = 0 \in \mathbb{R}^\nu. \tag{1.9}$$

These latter constraints are usually referred to as hidden constraints, and allow the derivation of the vector of the Lagrange multiplier λ. In fact, from (1.9) and (1.5)-(1.6), one obtains

$$\begin{aligned} 0 &= \nabla g\big(q(t)\big)^\top M^{-1} p(t) \\ &= \nabla g\big(q(t)\big)^\top M^{-1} \left[p_0 + \int_0^t \nabla U\big(q(\zeta)\big)\mathrm{d}\zeta - \int_0^t \nabla g\big(q(\zeta)\big)\lambda(\zeta)\mathrm{d}\zeta \right], \end{aligned} \tag{1.10}$$

from which one derives the integral equation

$$\begin{aligned} &\nabla g\big(q(t)\big)^\top M^{-1} \int_0^t \nabla g\big(q(\zeta)\big)\lambda(\zeta)\mathrm{d}\zeta \\ &= \nabla g\big(q(t)\big)^\top M^{-1} \left[p_0 + \int_0^t \nabla U\big(q(\zeta)\big)\mathrm{d}\zeta \right]. \end{aligned} \tag{1.11}$$