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Energy Conservation in the Numerical Solution of Hamiltonian Boundary Value Problems

Pierluigi Amodio*, Luigi Brugnano† and Felice Iavernaro*

*Dipartimento di Matematica, Università di Bari, Italy
†Dipartimento di Matematica "U. Dini", Università di Firenze, Italy

Abstract. We consider the issue of energy conservation in the numerical solution of Hamiltonian systems coupled with boundary conditions and discuss a few examples arising from astrodynamics.

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INTRODUCTION

In this note we report a few initial results on the implementation of energy conserving Runge-Kutta methods to the solution of Hamiltonian boundary value problems. These methods, named Hamiltonian Boundary Value Methods (HBVMs), have been recently devised for the solution of canonical Hamiltonian systems coupled with initial conditions. They can be interpreted as an extension of the well-known Gauss-Legendre methods with the difference that HBVMs provide a precise energy conservation for polynomial Hamiltonian functions of any high degree and, hence, a practical energy conservation for general Hamiltonian functions.[1] Hereafter, we are interested in applying such methods to the solution of Hamiltonian boundary value problems in the form

$$\dot{y} = J\nabla H(y), \qquad g(y(0), y(T)) = 0, \tag{1}$$

where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ (here I is the identity matrix of dimension m), the scalar function $H : \Omega \subset \mathbb{R}^{2m} \to \mathbb{R}$ is the *Hamiltonian* of the problem and its value is constant along any solution of (1), and $g : \mathbb{R}^{2m} \times \mathbb{R}^{2m} \to \mathbb{R}^{2m}$ defines the boundary conditions.

The state vector y splits in two vectors of length m, $y^T = [q^T, p^T]$ referred to as generalized coordinates and conjugate momenta. Interests in problems such as (1) arise in several research areas and, in the last section, we focus our attention to a couple of applications in astrodynamics. The numerical treatment of Hamiltonian problems is thoroughly discussed in the monographs [6, 9, 11]. In the next section we briefly recall the definition of HBVMs and describe their main feature. For a detailed description of HBVMs and their properties when applied to IVPs, see [2, 3, 4]. The implementation of HBVMs to solve problem (1) will be discussed elsewhere and is not reported here (for an introduction on the solution of boundary value problems by one-step methods see, for example, [1]).

DEFINITION OF HBVMS

We consider the *Legendre* polynomials P_i shifted on the interval $[0,1]$, and scaled in order to be orthonormal:

$$\deg P_i = i, \qquad \int_0^1 P_i(x)P_j(x)\mathrm{d}x = \delta_{ij}, \qquad \forall i, j \geq 0, \tag{2}$$

[1] That is, the error in the Hamiltonian function is within the machine precision.

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where δ_{ij} is the Kronecker symbol. The roots $\{c_1,\dots,c_k\}$ of $P_k(x)$ are all distinct and symmetrically distributed on the interval $(0,1)$. They are referred to as the Gauss-Legendre abscissae on $[0,1]$ and generate the well-known Gauss-Legendre quadrature formulae, whose weights we denote b_i, $i=1,\dots,k$.

Let $s\le k$. We introduce the following matrices, defined by means of the Legendre polynomials evaluated and the k abscissae c_i, $i=1,\dots,k$:

$$\mathscr{P}_s=\begin{pmatrix} P_0(c_1) & \dots & P_{s-1}(c_1)\\ \vdots & & \vdots\\ P_0(c_k) & \dots & P_{s-1}(c_k)\end{pmatrix},\quad \mathscr{I}_s=\begin{pmatrix} \int_0^{c_1}P_0(x)\mathrm{d}x & \dots & \int_0^{c_1}P_{s-1}(x)\mathrm{d}x\\ \vdots & & \vdots\\ \int_0^{c_k}P_0(x)\mathrm{d}x & \dots & \int_0^{c_k}P_{s-1}(x)\mathrm{d}x\end{pmatrix},\quad \Omega=\begin{pmatrix} b_1 & & \\ & \ddots & \\ & & b_k\end{pmatrix}.$$

Notice that $\mathscr{P}_s$ and $\mathscr{I}_s$ are $k\times s$ matrices while $\Omega\in R^{k\times k}$. Finally, let $c=(c_1,\dots,c_k)^T$ and $b=(b_1,\dots,b_k)^T$. The Runge–Kutta formulation of a HBVM is defined by the following Butcher tableau

$$\begin{array}{c|c} c & \mathscr{I}_s\mathscr{P}_s^T\Omega\\ \hline & b^T\end{array} \tag{3}$$

and is denoted by HBVM(k,s) to outline the dependence of the formula on the two integers s (number of Legendre polynomials involved) and k (number of internal abscissae).

When $k=s$ one can show that the method (3) becomes the Gauss collocation method of order $2s$. For any $k\ge s$ the coefficient matrix $A=\mathscr{I}_s\mathscr{P}_s^T\Omega$ has constant rank s and its nonzero eigenvalues coincide with those of the basic s-stage Gauss method [3]. The main property of HBVMs is summarized in the following theorem.

Theorem 1. *HBVM(k,s) is symmetric, of order $2s$ and energy-conserving for all polynomial Hamiltonians of degree $\nu\le\frac{2k}{s}$. In any other case, $H(y_n)-H(y_{n-1})=O(h^{2k+1})$.*

Notice that in the case of non polynomial Hamiltonians, energy conservation can be *practically* obtained by choosing k large enough, provided that the $O(h^{2k+1})$ term in the theorem above, is within roundoff errors.

APPLICATIONS TO ASTRODYNAMICS

We consider the motion of a body with negligible mass (planetoid) in the gravitational field generated by two celestial bodies with finite mass (primaries) rotating around their common center of mass in circular orbits. Such a dynamical system is referred to as the *circular restricted three-body problem* (CRTBP) and its interest goes back to the second quarter of the eighteenth century, in the context of the lunar theory. A renewed interest arose starting from the late 1960s up to present day and is testified by a rich and growing literature on the design and analysis of a variety of orbits connected with the motion of spacecrafts, satellites and asteroids [5, 7, 8, 10, 12].

We consider the case where the two primaries are the Sun and the Earth+Moon whose masses are denoted m_1 and m_2. Usually the units are chosen so that the properties of the resulting dynamical system depend on a single parameter μ, defined as the ratio $\frac{m_2}{m_1+m_2}$. Under this assumption we have $\mu=3.04036\cdot10^{-6}$, the unit of length is the distance between the two primaries $R=1.49589\cdot10^8$km while the unit of time is $1/n$, where $n=1.99099\cdot10^{-7}$rad/s is the constant angular velocity of the Sun and Earth/Moon around their center of mass C_M.

It is also common to write down the equations of motion of the planetoid in a frame where the primaries are stationary. This is accomplished by introducing a rotating (synodic) orthogonal frame centered at C_M, with the $x-y$ axes lying in the plane of the Sun-Earth/Moon orbit, the x axis being oriented from the Sun toward the Earth, and the z axis forming a right-hand frame with the other axes. Thus, the Sun and the Earth are located on the x axis at the abscissae $-\mu$ and $1-\mu$ respectively.

Let $q(t)=[q_1(t),q_2(t),q_3(t)]^T$ be the coordinates of the planetoid at time t and set $p(t)=[p_1(t),p_2(t),p_3(t)]^T\equiv[\dot q_1(t)-q_2(t),\dot q_2(t)+q_1(t),\dot q_3(t)]^T$ the vector of conjugate momenta. The Hamiltonian function in non-dimensional form associated with the dynamical system governing the motion of the planetoid is

$$H(q,p)=p_1q_2-p_2q_1+\frac{1}{2}p^Tp-\frac{1-\mu}{r_1}-\frac{\mu}{r_2}. \tag{4}$$

where $r_1=((q_1+\mu)^2+q_2^2+q_3^2)^{1/2}$ and $r_2=((q_1-(1-\mu))^2+q_2^2+q_3^2)^{1/2}$ are the distances of the planetoid from the Sun and the Earth/Moon respectively.

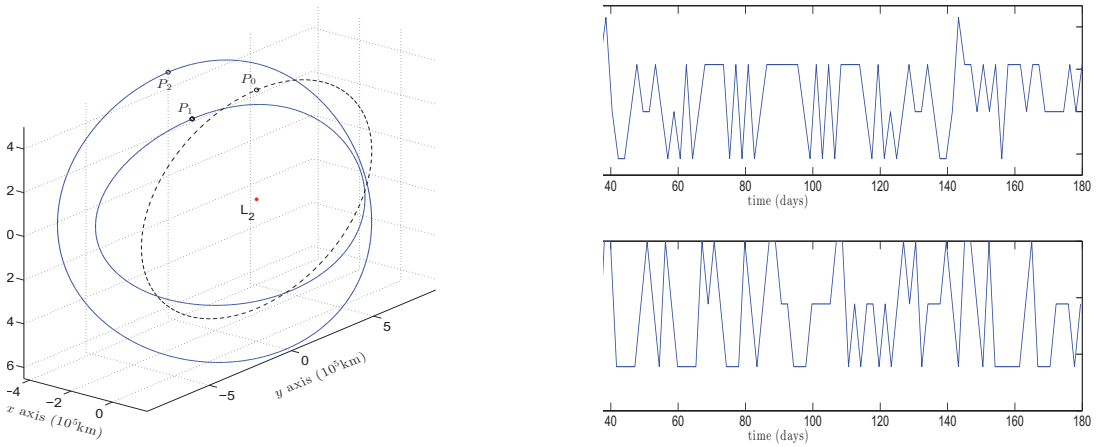

FIGURE 1. Left picture: two halo orbits around the libration point L_2 (solid lines) and the initial guess for the Newton iteration scheme associated to the method (dashed line). Right picture: the Hamiltonian function (4) is precisely conserved along the numerical solutions.

It is well-known that such a dynamical system admits five equilibrium points referred to as *Lagrangian* or *libration* points and denoted L_i, $i = 1,\ldots,5$. Periodic and quasi-periodic orbits around libration points are suited for a number of mission applications. For example, Sun-Earth libration points are commonly used for deep space or Sun activity observations. In the following experiments we consider the dynamics around L_2 which is located beyond the Earth on the x-axis at the abscissa 1.010075. In particular, we are interested in reproducing numerically the so called *halo orbits*. These are out-of-plane periodic orbits which seem to orbit the Earth but are instead quite far from it, tracing a halo around the planet.

We have implemented the $HBVM(6,2)$ formula and adapted the algorithm in order to compute periodic solutions in the two different situations where we are given either the period T of the orbit or its energy level H_0. In the latter case, the step size of integration h is regarded as an extra unknown and the scalar equation $H(q_0,p_0) = H_0$ is added to the set of boundary conditions.

In both cases, an elliptic curve starting (and ending) at P_0 and lying on a plane orthogonal to the x axis and passing through L_2 has been chosen as initial guess in the Newton iteration, while the number of points in the numerical approximation is $n = 100$. The left picture of Figure 1 displays the initial guess (dashed line) together with two halo orbits (solid lines). The inner one is the halo orbit corresponding to a period $T_1 = 180$ days. The energy level of this first numerical approximation is $H_1 \approx -1.500394$. As was discussed above, the outer halo orbit has been computed on the basis of its energy level, which has been set to $H_2 = -1.50036$. Notice that in the non-dimensional system $H_2 \approx H_1(1+2\cdot 10^{-5})$ while the actual distance of the topmost points of the two orbits is $\overline{P_1P_2} = 2\cdot 10^5$km. The period corresponding to the energy level H_2 is $T_2 = 179.19$ days. The right pictures of Figure 1 show that the energy error is close to the machine precision (all experiments have been carried out in Matlab using double precision arithmetic).

An interesting problem in astrodynamics is the *optimal orbit transfer*, which consists in finding the optimal control laws that drives a spacecraft from an initial to a desired final state in a given time T. Here the term *optimal* means that the amount of propellant needed to produce the change in orbital elements is minimized. We are interested in transferring a spacecraft from the inner to the outer halo orbit and, specifically, from the point P_1 to the point P_2.

Since the fuel consumption is proportional to changes in the velocity, an input vector $u(t) = [u_1(t),u_2(t),u_3(t)]^T$ enters the dynamical system to control the acceleration of the vehicle along the three axes. This is accomplished by considering a new non-autonomous Hamiltonian function $\bar{H}(q,p) = H(q,p) + q^T u$, where $H(q,p)$ is as in (4). Our optimal control problem is formulated as:

> *Minimize the quadratic cost* $J = \frac{1}{2}\int_0^T ||u(t)||_2^2 \mathrm{d}t$, *subject to the dynamics induced by* $\bar{H}(q,p)$ *and the boundary conditions corresponding to the states at* P_1 *and* P_2.

We assume that the control input is unconstrained and regular. The Pontryagin maximum principle is often used to

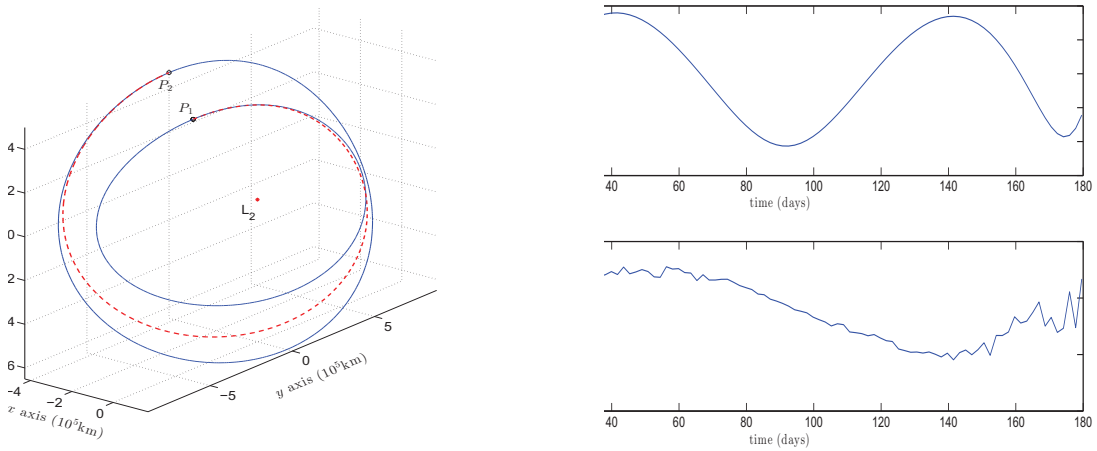

FIGURE 2. Left picture: optimal orbit transfer between two halo orbits (dashed line). Right picture: norm of the optimal control variable $u(t)$ and error in the Hamiltonian function (5).

attack this problem. Setting $y^T = [q^T, p^T]$ (state variables) and $\lambda = [\lambda_1, \ldots, \lambda_6]^T$ (costate variables), one considers the augmented Hamiltonian function $\widetilde{H}(y, \lambda, u) = \frac{1}{2}u^T u + \lambda^T J \nabla \bar{H}(q, p)$. Then, the necessary conditions for optimality are

$$\dot{y} = \frac{\partial \widetilde{H}}{\partial \lambda}, \quad \dot{\lambda} = -\frac{\partial \widetilde{H}}{\partial Y}, \quad \frac{\partial \widetilde{H}}{\partial u} = 0.$$

The third equation gives $u_i = -\lambda_{(3+i)}$, $i = 1, 2, 3$, so that the resulting system is autonomous and only depends on the state and costate variables. It is defined by the Hamiltonian

$$\widehat{H}(y, \lambda) = \frac{1}{2}(\lambda_4^2 + \lambda_5^2 + \lambda_6^2) + \lambda^T (J \nabla H(q, p) - [0, 0, 0, \lambda_4, \lambda_5, \lambda_6]^T) = \lambda^T J \nabla H(q, p) - \frac{1}{2}(\lambda_4^2 + \lambda_5^2 + \lambda_6^2). \quad (5)$$

In Figure 2 we show the optimal control trajectory joining the points P_1 and P_2 in a time $T = (T_1 + T_2)/2$ (left picture, dashed line) together with the norm of the optimal control variable $u(t)$ and the error $\widehat{H}(y_n) - \widehat{H}(y_0)$ (right picture).

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