Conservative block-Boundary Value Methods for the solution of polynomial Hamiltonian systems

Felice Iavernaro and Brigida Pace

Dipartimento di Matematica, Università di Bari, Via Orabona 4, I-70125 Bari, Italy

Abstract. We devise a technique to derive high order one-step methods suitable for the precise conservation of Hamiltonian functions of polynomial type. In many cases of interest Hamiltonian functions are polynomials of the variables $p$ (conjugate momenta) and $q$ (generalized coordinates), or they may be well approximated by polynomials.

In deriving this class of methods, the key idea is to exploit the relation between the method itself and what we called discrete line integral, the discrete counterpart of the the line integral in conservative vector fields. This approach naturally suggests a formulation of such methods in terms of block Boundary Value Methods.

Keywords: Hamiltonian systems, block-Boundary Value Methods, quadrature formulae.

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INTRODUCTION AND MOTIVATIONS

We consider the numerical integration of Hamiltonian systems

\[ \dot{y} = \mathcal{J} \nabla H(y), \quad \mathcal{J} = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \]

where $I$ is the identity matrix of dimension $m$. The vector state $y$ is usually partitioned into two $m$-length vectors $p$ and $q$, the conjugate momenta and the generalized coordinates respectively. Throughout this paper we assume that the Hamiltonian function $H(y) = H(p, q)$ is a polynomial in the variables $p$ and $q$.

Our aim is to find out a general technique to define one-step methods $y_{n+1} = \Phi_h(y_n)$ that conserve the Hamiltonian function:

\[ H(y_{n+1}) = H(y_n), \quad \text{for all } n \text{ and } h > 0, \quad (1) \]

where $y_n$ denotes the numerical solution and $h$ is the stepsize of integration. As far as the authors know, such incoming methods and the problem they solve appear to be new in the literature.

Many interesting Hamiltonian systems arising from different fields of study are defined by polynomial Hamiltonian functions. As an example we consider the Fermi-Pasta-Ulam Problem defined by the Hamiltonian function

\[ H(p, q) = \frac{1}{2} \sum_{i=1}^{m} (p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4} \sum_{i=1}^{m} (q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m} (q_{2i+1} - q_{2i})^4. \quad (2) \]

This problem arises from molecular dynamics and describes the interaction of $2m$ mass points linked with alternating soft nonlinear and stiff linear springs, in a one-dimensional lattice with fixed end points ($q_0 = q_{2m+1} = 0$) [4].

As a further motivation, notice that general Hamiltonian functions may be suitably approximated by polynomials, especially (but not necessarily) when the dynamics takes place in a neighborhood of the equilibrium point. As a simple example we consider the Fermi-Pasta-Ulam Problem defined by the Hamiltonian function

\[ H(p, q) = \frac{1}{2} p^2 + \frac{1}{2} q^2 - \frac{1}{24} q^4 \quad \text{(quartic pendulum oscillator)}, \]

\[ H(p, q) = \frac{1}{2} p^2 + \frac{1}{2} q^2 - \frac{1}{24} q^4 + \frac{1}{720} q^6 \quad \text{(pendulum oscillator of degree 6)}. \quad (3) \]

It is well known that symplectic RK-methods only conserve quadratic Hamiltonian functions: $H(y) = \frac{1}{2} y^T Cy$ but, in general, they fail to yield conservation for higher degree, and so do symmetric methods.
In Figure 1 we report the energy function $H(y_n)$ obtained by applying the LobattoIIIB method of order four to (left picture) the quartic pendulum oscillator (see (3)) and to (right picture) the system defined by the following Hamiltonian function:

$$H(p,q) = \frac{1}{3}p^3 - \frac{1}{2}p + \frac{1}{30}q^6 + \frac{1}{4}q^4 - \frac{1}{3}q^2 + \frac{1}{6}$$ (4)

This problem was introduced in [3] as a counterexample showing how symmetric methods may display the energy drift phenomenon even when the problem is reversible $H(-p,q) = H(p,q)$.

![Figure 1](image)

**Figure 1.** Energy function $H(y_n)$ evaluated over the numerical solution obtained by the Lobatto IIIB method of order four applied to two Hamiltonian systems. Left picture: the quartic pendulum oscillator has been solved with stepsize $h = 1$, number of points $n = 200$ and initial condition $[p_0, q_0] = [1, 0.5]$. Right picture: problem (4) has been solved with stepsize $h = 1$, number of points $n = 1000$ and initial condition $[p_0, q_0] = [1, 0]$. In both plots the horizontal line denotes the theoretical value of the Hamiltonian function.

Of course, the right picture depicts a much more dangerous situation with respect to the left one, in that the numerical method alters the marginal stability character of the equilibrium by dissipating energy, thus leading to asymptotic stability. This phenomenon is termed energy drift. Nevertheless, as it is argued, in presence of more equilibrium points, even a small deviation from the level curve may lead to misleading results if the dynamics takes place near the boundary of a stability region of a given equilibrium point.

In this short paper we give an outline about how to approach the problem and, to this aim, we consider a concrete case of a method of order 4 (see the next section). This simple example contains all the essential ingredients to understand how to generalize the approach and devise schemes of any order. A class of methods of order two, called $s$-stage trapezoidal method was already introduced in [5] while a general theory on such methods is in preparation.

**CONSERVATIVE BLOCK-BOUNDARY VALUE METHODS OF ORDER 4**

A key role of the present approach is played by what we called discrete line integral (see [6, 7]). Given a path $\gamma = t \in [0,1] \rightarrow \mathbb{R}^{2n}$ joining the points $y_0$ and $y_1$ in the phase space, we consider the line integral

$$\int_{y_0 \rightarrow y_1} \nabla H(y)dy \equiv \int_0^1 (\dot{\gamma}(t))^T \nabla H(\gamma(t)) dt.$$ (5)

Due to conservativeness of the vector field, such integral is equal to $H(y_1) - H(y_0)$, no matter the choice of $\gamma(t)$. Its discrete counterpart,

$$\sum_{\gamma} f \cdot \Delta y \equiv \sum_{i=0}^{k} A_i(\dot{\gamma}(t_i))^T f(\gamma(t_i)),$$

is obtained by applying to (5) any quadrature formula with weights $A_i$ and abscissae $t_i \in [0,1]$. In general the discrete line integral $\sum_{\gamma} f \cdot \Delta y$ will differ from $H(y_1) - H(y_0)$ but if $\gamma(t)$ is chosen to be a polynomial in $t$, then the integrand $(\dot{\gamma}(t))^T \nabla H(\gamma(t))$ is a polynomial in $t$ of degree

$$k = (\deg(\gamma) - 1) + (\deg(H) - 1) \deg(\gamma).$$ (6)

1 Indeed in [3] the author show that the system deriving from (4) is equivalent to a reversible system. An interesting discussion about the symmetry structure of the problems and its role in the numerical integration can be found in [1].
Hence, if the degree $d$ of the quadrature formula is high enough, that is ($d \geq k$) the quadrature formula is exact and so
\[ \sum_{\gamma} f \cdot \Delta y = H(y_1) - H(y_0). \]

In a sense that will be clear hereafter, we will exploit the fact that a one-step method of given order $p$, if suitably defined, may become a quadrature formula of higher degree if applied to the quadrature problem $\dot{y} = f(t)$.

For the sake of simplicity hereafter we assume that the polynomial $H(p,q)$ has degree 3: generalization to higher degrees is straightforward. Consequently, on the basis of formula (6), we fix $s = 4$ (five stages).

First of all we consider a (quadratic) polynomial path $\gamma(t)$, joining $y_0$ to $y_4 = \Phi_k(y_0)$ and passing through $y_2$. The remaining stages $y_1$ and $y_3$, are to be selected on $\gamma$ in order to improve the degree of the underlying quadrature formula (but not the order). For simplicity we use a uniform distribution of the nodes $t_i = 0, 1/4, 1/2, 3/4, 1$. On the nodes $t_0, t_2$ and $t_4$, the interpolating conditions read
\[ \gamma(0) = y_0, \quad \gamma \left( \frac{1}{2} \right) = y_2, \quad \gamma(1) = y_4. \]

After ordering the nodes as 0, 1 and 1/2, we write $\gamma(t)$ by using divided differences:
\[ \gamma(t) = y_0 + (y_4 - y_0)t + 2(y_4 - 2y_2 + y_0)t(t - 1), \]
and consequently we set
\[ y_1 = \gamma \left( \frac{1}{2} \right) = \frac{3}{8}y_0 + \frac{3}{4}y_2 - \frac{1}{8}y_4, \quad \text{and} \quad y_3 = \gamma \left( \frac{3}{4} \right) = -\frac{1}{8}y_0 + \frac{3}{4}y_2 + \frac{3}{8}y_4. \quad (7) \]

Now we consider the line integral along the curve $\gamma$:
\[ H(y_4) - H(y_0) = \int_{y_0 \to y_4} \nabla H(y) \, dy = \int_0^1 (\gamma(t))^T \nabla H(\gamma(t)) \, dt \]
\[ = (y_4 - y_0)^T \int_0^1 \nabla H(\gamma(t)) \, dt + 2(y_4 - 2y_2 + y_0)^T \int_0^1 (2t - 1) \nabla H(\gamma(t)) \, dt. \]

The latter integrand has degree 5 and is exactly computed by the Newton-Cotes formula with 5 nodes:\[ y_4 = y_0 + h \sum_{i=0}^4 \beta_i f(t_i), \quad h = \frac{b - a}{4}, \quad [\beta_0, \beta_1, \beta_2, \beta_3, \beta_4] = \frac{1}{90}[7, 32, 12, 32, 7]. \]

Therefore we get
\[ H(y_4) - H(y_0) = h(y_4 - y_0)^T \sum_{i=0}^4 \beta_i \nabla H(\gamma(t_i)) + 2h(y_4 - 2y_2 + y_0)^T \sum_{i=0}^4 \beta_i (2t_i - 1) \nabla H(\gamma(t_i)). \]

Requiring that $H(y_4) = H(y_0)$ results in the following two conditions:
\[ (y_4 - y_0)^T \sum_{i=0}^4 \beta_i \nabla H(\gamma(t_i)) = 0, \quad \text{and} \quad (y_4 - 2y_2 + y_0)^T \sum_{i=0}^4 \beta_i (2t_i - 1) \nabla H(\gamma(t_i)) = 0. \quad (8) \]

The first condition is satisfied if we assume that the state vector $y_4$ is computed by the formula
\[ y_4 - y_0 = h \sum_{i=0}^4 \beta_i J \nabla H(y_i). \]
To see why, multiply both terms on the left by $(y_4 - y_0)^T J^T$ and observe that $y_i = \gamma(t_i), i = 0, \ldots, 4$. This is an implicit linear multistep method in the unknowns $y_1, y_2, y_3, y_4$, therefore, referring to the theory on block-BVMs (see [2]),

2 The scaling factor $h$ will coincide with the (internal) stepsize of integration of the associated block-BVM [2].
we need three additional methods to determine these unknowns. One additional method is suggested by the second condition

\[ y_4 - 2y_2 + y_0 = h \sum_{i=0}^{4} \beta_i' J \nabla H(y_i), \quad \text{with} \quad \beta_i' = \eta \delta_i (2i - 1), \]

where \( \eta \) is a suitable constant which will be chosen in order to maximize the order. Again, one easily verifies that this equation implies the second condition in (8). The remaining additional methods were already been set up in (7). The coefficient \( \eta \) is selected by maximizing the order of the corresponding formula, which yields \( \eta = 3/2 \).

Our block-BVM is the collection of the multistep formulae derived above:

\[
[a_0][A] \otimes \begin{pmatrix} y_0 \\ Y \end{pmatrix} - h([b_0][B] \otimes J) \begin{pmatrix} \nabla H(y_0) \\ \nabla H(Y) \end{pmatrix} = 0, \tag{9}
\]

where

\[
[a_0][A] = \begin{pmatrix} -3/2 & 1 & -1/2 & 0 & 1/2 \\ -1 & 0 & -1/2 & 1 & -1/2 \end{pmatrix}, \quad [b_0][B] = \begin{pmatrix} -7/6 & 0 & 0 & 0 & 0 \\ -7/6 & -4/3 & 4/3 & 7/6 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}, \quad \nabla H(Y) = \begin{pmatrix} \nabla H(y_1) \\ \nabla H(y_2) \\ \nabla H(y_3) \\ \nabla H(y_4) \end{pmatrix}.
\]

To optimize the implementation notice that, by exploiting (7), the stages \( y_1 \) and \( y_3 \) may be canceled out, therefore the cost is comparable to a standard Runge-Kutta method of order 4 with 3 stages. By construction, method (9) conserve polynomial Hamiltonian functions up to the degree 3. As a test problem we choose a simplified version of problem (4), in order to handle with a cubic Hamiltonian function:

\[
H(p,q) = \frac{1}{3} p^3 - \frac{1}{2} p - \frac{1}{3} q^3 + \frac{1}{2} q^2 + \frac{1}{6}.
\]

The left picture in Figure 2 shows that, once again, the Lobatto IIIB method of order 4 produces a drift in the energy function, while the right picture confirms the exact conservation of the energy by method (9). By adding a sufficient number of stages on the quadratic curve \( y(t) \), one easily obtains block-BVMs of order 4 that conserve polynomial Hamiltonian functions of higher degree, like those presented in the previous section.

Figure 2. Energy function \( H(y_n) \) evaluated over the numerical solution obtained by the Lobatto IIIB method and the block-BVM (9) of order four applied to problem (10). Stepsize \( h = 1 \), number of points \( n = 5000 \); initial condition \( [p_0, q_0] = [1, 0] \).

REFERENCES