s-stage trapezoidal methods for the conservation of Hamiltonian functions of polynomial type

Felice Iavernaro and Brigida Pace

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

Abstract. We introduce a class of methods of order two that exactly preserve the Hamiltonian function of separable Hamiltonian systems, in the case where such function is a polynomial. Although each method is a symmetric Runge-Kutta formula involving a number of internal stages, the computational cost is comparable to that of the trapezoidal method. Some numerical results are also presented.

Keywords: Hamiltonian systems, trapezoidal rule, Newton-Cotes formulae.
PACS: 04.20.Ex, 47.10.Df, 45.20.dh.

INTRODUCTION

It is well known that symplectic Runge-Kutta methods conserve the quadratic invariants of a Hamiltonian system. Furthermore, for the class of linear Hamiltonian systems of the form

$$\dot{y} = JCy, \qquad \text{with} \qquad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

where C is a symmetric real matrix, simplecticity of the method is equivalent to symmetry and therefore the quadratic Hamiltonian function $H(y) = \frac{1}{2}y^T Cy$ is exactly conserved by symmetric one step methods like the trapezoidal formula.

For Hamiltonian functions which are polynomial of degree greater than two, such conservation is in general lost both by symmetric and symplectic methods, as shown in Figure 1, where Lobatto IIIA and Gauss methods of order four have been applied to solve the quartic pendulum equation defined by

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4. \tag{1}$$

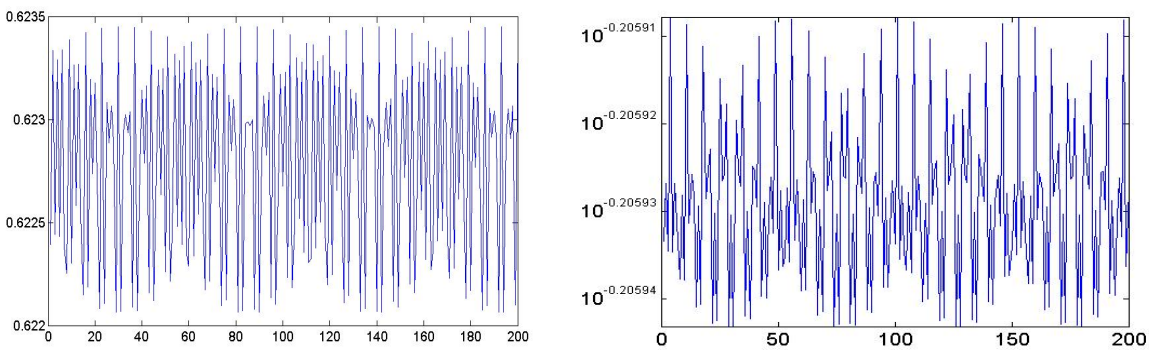

FIGURE 1. Energy function (1) evaluated over the numerical solution obtained by solving the quartic pendulum equation by Lobatto IIIA method of order four (left picture) and Gauss method of order six (right). Stepsize $h = 1$; number of points $n = 200$; initial condition $[p_0, q_0] = [1, 0.5]$.

For the sake of simplicity, in this paper we will confine our study to two-dimensional separable Hamiltonian systems defined by the energy function

$$H(p,q) = \sum_{k=0}^{m_1} \alpha_k p^k + \sum_{k=0}^{m_2} \beta_k q^k. \tag{2}$$

However, the tools exploited for this class of problems are readily extended to (non-separable) problems with more degrees of freedom and so do the theoretical results obtained in this paper: a test problem with six degrees of freedom has been inserted to give a numerical evidence of this.

Our main concern is the introduction of new integration formulae capable to exactly conserve the energy term (2). In the next section we introduce such methods, together with an inspection of their properties. Later we emphasize the reasons why these low-order formulae might be of interest in the integration of Hamiltonian systems defined by (2). Finally we report a few test problems.

s-STAGE TRAPEZOIDAL FORMULAE

As well known, any numerical method for the solution of Ordinary Differential Equations induces a quadrature formula when applied to the problem

$$y' = f(t), \qquad \text{with} \quad t \in [a,b]. \tag{3}$$

To two or more methods for ODEs there may correspond the same quadrature formula: for example the family of Lobatto methods (IIIA IIIB and IIIC) become to Newton-Cotes quadrature formulas when applied to (3).

The class of one-step methods we are interested in are derived from Newton-Cotes formulae as follows. Let us consider, at time t_n, the segment σ_n joining y_n and y_{n+1}: $\sigma_n(c) = (1-c)y_n + cy_{n+1}$, where $c \in [0,1]$ is a parameter. Set $h = t_{n+1} - t_n$; we choose a number, say s, of stages $K_i = \sigma_n(c_i)$, $i = 1,\dots,s$, with $c_i = (i-1)h/(s-1)$.

The abscissae c_i are uniformly distributed in $[0,1]$ and therefore they define the nodes $t_n^{(i)} = (1-c_i)t_n + c_i t_{n+1}$ of Newton-Cotes quadrature formulae over the time interval $[t_n, t_{n+1}]$: let $b_i,\ i = 1,\dots,s$ denote the corresponding weights.

The s-stage trapezoidal method is defined as

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(K_i). \tag{4}$$

When $s = 2$ we obtain the trapezoidal method; for $s = 3$ and $s = 5$ we obtain respectively the methods:

$$y_{n+1} = y_n + \frac{h}{6}\left(f(y_n) + 4f(\frac{y_n + y_{n+1}}{2}) + f(y_{n+1})\right) \tag{5}$$

and

$$y_{n+1} = y_n + \frac{h}{90}\left(7f(y_n) + 32f(\frac{3y_n + y_{n+1}}{4}) + 12f(\frac{y_n + y_{n+1}}{2}) + 32f(\frac{y_n + 3y_{n+1}}{4}) + 7f(y_{n+1})\right) \tag{6}$$

When f is chosen as in (3), (5) and (6) become the Newton-Cotes quadrature formulae of order 4 and 6 respectively. On the other hand, when applied to general ODE problems their order is two. To see this, let us apply (4) to the linear test problem $y' = \lambda y$ and so compute the rational stability function $R(q)$ with $q = h\lambda$. From the definition of the stages K_i we obtain

$$y_{n+1} = R(q)y_n, \qquad \text{with} \quad R(q) = \frac{1 + \sum_{i=1}^{s} b_i(1-c_i)}{1 - \sum_{i=1}^{s} b_i c_i}$$

But $\sum_{i=1}^{s} b_i(1-c_i) = \sum_{i=1}^{s} b_i c_i = \frac{1}{2}$ because these two sums are nothing but the application of the associated Newton-Cotes formulae to the linear functions $g_1(x) = 1-x$ and $g_2(x) = x$ in the interval $[0,1]$. Therefore all methods in the class (4) share the same stability function $R(q) = (1+q/2)/(1-q/2)$ which is the stability function of the trapezoidal method: this justifies the name that we proposed for such methods.

However, when applied to pure quadrature problems (3), method (4) becomes of order s or $s+1$ according to whether s is even or odd.

Written as a Runge-Kutta method, formula (4) is defined by the following Butcher array:

$$
\begin{array}{c|ccccc}
0 & 0 & 0 & \dots & \dots & 0 \\
c_1 & c_1 b_1 & c_1 b_2 & \dots & \dots & c_1 b_s \\
c_2 & c_2 b_1 & c_2 b_2 & \dots & \dots & c_2 b_s \\
\vdots & \vdots & \vdots & & & \vdots \\
c_{s-1} & c_{s-1} b_1 & c_{s-1} b_2 & \dots & \dots & c_{s-1} b_s \\
c_s & b_1 & b_2 & \dots & \dots & b_s \\
\hline
 & b_1 & b_2 & \dots & \dots & b_s
\end{array}
$$

Using either the Butcher array or the formulation (4), it is easily seen that each method under consideration is symmetric.

Since the stages $K_i,\ i = 1,\dots,s$ are explicitly determined in terms of y_n and y_{n+1}, implementing the method does not require the solution of a nonlinear system of dimension rs, where r is the dimension of the continuous problem. For example, method (6) requires the computation of one Jacobian matrix per step, if the simplified Newton iteration is considered to solve the associated nonlinear system.

CONSERVATION OF POLYNOMIAL HAMILTONIAN FUNCTIONS

Let us consider a Hamiltonian systems with polynomial Hamiltonian function as specified in (2). It is quite simple to show that method (4) exactly conserve this Hamiltonian function, that is $H(p_{n+1},q_{n+1}) = H(p_n,q_n)$, provided that the degree of $H(p,q)$ does not exceed s (when s is even) or $s+1$ (when s is odd). The gradient $\nabla H(p,q)$ will be of the form $[g_1(p), g_2(q)]^T$ where $g_1(p)$ and $g_2(q)$ are polynomial of degree less than s (when s is even) or $s+1$ (when s is odd).

The key point is the following remark. Substituting $f(y) = J\nabla H(y)$ in (4), and multiplying both members of (4) by $\sum_{i=1}^{s} b_i \nabla H(K_i)^T$ yield

$$
\left(\sum_{i=1}^{s} b_i \nabla H(K_i)^T \right) (y_{n+1} - y_n) = 0. \tag{7}
$$

As we will see in a while, formula (7) is equivalent to $H(p_{n+1},q_{n+1}) = H(p_n,q_n)$. We recall that for a conservative vector field like the one we are considering here, the line integral along any regular line joining the points y_n and y_{n+1} is independent of the particular path considered. We choose the line segment $\sigma_n = (1-c)y_n + cy_{n+1}$, with $c \in [0,1]$. Then we can write:

$$
H(y_{n+1}) - H(y_n) = \int_{y_n \to y_{n+1}} \nabla H(y) dy = \int_0^1 \sigma_n'(c)^T \nabla H(\sigma_n(c))\, dc = (y_{n+1} - y_n)^T \int_0^1 \begin{bmatrix} g_1((1-c)p_n + cp_{n+1}) \\ g_2((1-c)q_n + cq_{n+1}) \end{bmatrix} dc
$$

The last (vectorial) integral involves, as integral functions, polynomials in c for which the corresponding Newton-Cotes formula with s nodes is exact. Therefore

$$
H(y_{n+1}) - H(y_n) = (y_{n+1} - y_n)^T \sum_{i=1}^{s} b_i \begin{bmatrix} g_1((1-c_i)p_n + c_i p_{n+1}) \\ g_2((1-c_i)q_n + c_i q_{n+1}) \end{bmatrix} = (y_{n+1} - y_n)^T \left(\sum_{i=1}^{s} b_i \nabla H(K_i) \right).
$$

From (7) it then follows $H(p_{n+1},q_{n+1}) = H(p_n,q_n)$, as stated above.

NUMERICAL RESULTS

Hereafter we list four problems used for our tests together with a brief description. All of them have separable Hamiltonian function in the form $H(p,q) = 1/2p^T p - U(q)$, with the potential U satisfying the symmetry relation $U(-q) = U(q)$.

TEST 1 (*Pendulum Oscillator*).
We consider the pendulum equation defined by $H(p,q) = 1/2p^2 + 1 - \cos q$ and retain a finite number of terms in the Taylor expansion of the cosine. In particular we consider:
- $H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4$, (quartic pendulum oscillator);

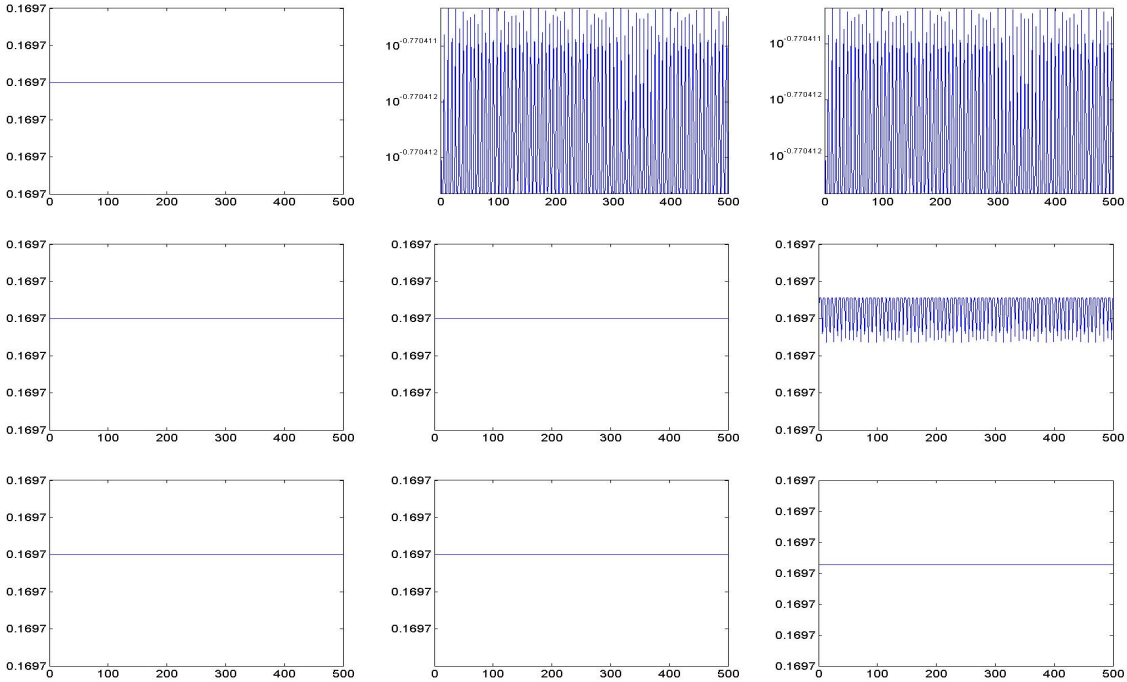

FIGURE 2. 3-stage (first row), 5-stage (second row) and 7-stage (last row) trapezoidal methods for the three equations of Test 1. Stepsizes $h = 0.5$; number of points $n = 500$.

- $H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4 + \frac{1}{720}q^6$, (pendulum oscillator of degree six);
- $H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4 + \frac{1}{720}q^6 - \frac{1}{40320}q^8$, (pendulum oscillator of degree eight).

TEST 2 (*Fermi-Pasta-Ulam Problem*).
This problem 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 ($q_0 = q_{2m+1} = 0$). The Hamiltonian function is

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4. \tag{8}$$

We chose $m = 3$ (6 degrees of freedom) and $\omega = 50$.

As numerical integrators we have used the $3, 5$ and 7-stage trapezoidal methods. In Figure 2 we report the quantity $H(p_n, q_n)$ for the polynomial oscillators described in TEST 1. The three methods have also been successfully applied to the Fermi-Pasta-Ulam problem described in TEST 2: as was to be expected, they all conserved the Hamiltonian function (8) of degree four (we omitted to report the corresponding picture).

REFERENCES

1. E. Faou, E. Hairer, T.-L. Pham, *Energy conservation with non-symplectic methods: examples and counter-examples*, BIT Numerical Mathematics, **44**, pp. 699–709 (2004).
2. E. Hairer, C. Lubich, and G. Wanner, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations.*, Springer Series in Computational Mathematics, **31**, Springer-Verlag, Berlin, 2002.
3. F. Iavernaro and D. Trigiante, *Discrete conservative vector fields induced by the trapezoidal method*, JNAIAM J. Numer. Anal. Ind. Appl. Math. **1**, no. 1, pp. 113–130 (2006).
4. F. Iavernaro and D. Trigiante, *On some conservation properties of the trapezoidal method applied to Hamiltonian systems*, ICNAAM, edited by T. E. Simos, President of ESCMSE, University of Peloponnese, et al., 2005, pp. 254–257.
5. V. Talasila, J. Clemente-Gallardo, A. J. van der Schaft, *Geometry and Hamiltonian mechanics on discrete spaces*, J. Phys. A **37**, no. 41, pp. 9705–9734 (2004).