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About the numerical conservation of first integral by a class of symmetric methods

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Summary. We present a class of symmetric methods which are particularly suitable for general conserving systems. Numerical evidence for numerical conservation of first integral within a requested accuracy is provided.

Key words: Conserving dynamical systems, Hamiltonian systems, symmetric methods, conservation of first integral, numerical conservation of energy

1 Introduction

Recently, geometric numerical integration methods have gained an important role in the field of numerical solution of ordinary differential equations. A numerical method is called *geometric* if it preserves exactly (i.e. up to round-off error) one or more physical/geometric properties of the corresponding continuous differential system. Such properties to be preserved are mainly first integrals, symplectic structure, symmetries and reversing symmetries, phase-space volume. Because of their effectiveness, geometric methods are really appreciated in many fields of engineering and physics, including celestial mechanics, molecular dynamics, fluid dynamics, meteorology. Actually, large surveys of geometric methods are provided in [9], [15].

Here we focus on the conservation of first integral. First integrals play an important role in Hamiltonian mechanics, since they lead essentially to a reduction in the number of degrees of freedom. However, conservation of first integral can happen even if the system is non-Hamiltonian . Therefore our focus does not precisely coincide with the study of Hamiltonian systems, but includes them.

We point out that the current most widespread methods for Hamiltonian systems are symplectic methods, but here we neglect them, since it is known [28] that, in general, exact conservation of first integral and symplecticness are conflicting issues, from a numerical point of view. Indeed, there are a number of important exceptions (i.e. splitting methods and implicit midpoint method for quadratic splitted first integrals), but here we want to deal with the most general case of conserving systems. It is worth pointing out that, in the case of Hamiltonian systems, the use of Hamiltonian itself can produce exact conserving numerical methods [24], [14], [12],[13], but here we will use the expression of conserved first integral to check the effectiveness of our computations only.

Actually, we will adopt the traditional approach of numerical analysis which generally assumes that the purpose of simulation is the faithful reproduction of a particular solution or trajectory. Since, for conserving systems, first integral is *necessarily* conserved along numerically correct trajectories, the presence of first integrals (such as energy or other invariant) can provide helpful criteria for assessing the validity of the simulation, particularly in the nonlinear case. However, it should be clear that the numerical conservation alone is not enough of a restriction, since any arbitrary sequence of random data points in the phase space could be projected to the energy surface, but would be not expected to provide a reasonable approximation of a trajectory.

If we restrict to Hamiltonian systems, we observe that there are two extreme ends of possible solutions :i) completely integrable; ii) fully chaotic. For integrable and near-integrable Hamiltonian systems, it is well understood how symplectic methods conserve energy. Indeed, when they are used with a stepsize h much smaller than the inverse of the highest frequency ω (in the linearized system), long -time near conservation of the total energy is obtained up to exponentially small term $O(e^{-c/(h\omega)})$ (e.g. [9], Ch. IX). Unfortunately these results are not useful when large stepsizes can be used, for which the product $h\omega$ is bounded away from 0, and when the considered Hamiltonian system is fully chaotic. In this last case, solutions diverge exponentially everywhere in phase space, even if a large variety of behaviors can be exhibited: slow rates of divergence, fast rates of divergence and islands of periodic orbits also; so areas of weak chaos will alternate to areas of strong chaos and/or ares of stability. In general, the numerical computed trajectory will not stay close to the exact solution over very long time intervals. On the other hand, fully chaotic systems exhibit the so-called *shadowing property* [8], [26]; so, briefly (e.g [15], page 125) numerical trajectories obtained from a symplectic integration method shadow some exact solution of a slightly perturbed fully chaotic Hamiltonian system. Therefore, whenever we want to numerically reproduce a given trajectory as exactly as possible over long time intervals, we clearly use better a non-symplectic method.

Within this frame, here we present a new class of symmetric non-symplectic methods whose properties will be investigated by means of a large number of numerical examples. At the present, the proof of conservation of first integral still lacks, but we think that numerical evidence, provided by reported examples, can be somewhat worthwhile.

These presented methods are improved versions of methods previously introduced in [2] and are called *block-Boundary Value Methods* (block-BVM) [11]. They could also be rewritten [1] in the form of implicit collocation Runge-Kutta methods [4]. So they share all the nice properties of symmetric Runge-Kutta schemes when applied to reversible differential equations ([9], Ch. V). The block-BVM are defined by a set of linear multistep formulas combined in a suitable way. In our implementation, the time integration interval is discretized by using *two different meshes:* an equispaced coarser one and a nonequispaced finer one. The considered linear multistep formulas are then applied on each subinterval defined by the coarser mesh with stepsizes defined by the finer one. First integral is nearly conserved both on the coarse mesh and on the finer mesh.

Finally, there are some other reasons why one might use a symmetric method on a conservative system. First, if the system is Hamiltonian, a symplectic integrator may be prohibitively expensive. This occurs, for example, when the symplectic structured is noncanonical, perhaps as a results of a change of variables. Second, if the system is not Hamiltonian but still has a first integral, then a symmetric integrator is the best choice of geometric method. It is usually much cheaper to preserve symmetry only, which is the dominant property characterizing the dynamics, while energy is merely conserved within a required accuracy.

This paper is organized as follows. In Section 2 we introduce our class of symmetric methods. In Section 3 we present several numerical examples relating to different types of conserving systems. In Section 4, we conclude with some final remarks.

2 Numerical methods

Given an ordinary differential system, defined in a space of even dimension, say $2m$,

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t)), \qquad \mathbf{y}(t_0) = \mathbf{y}_0, \tag{1}$$

A block k-step symmetric linear multistep method applied to (1) on the grid $t_0 < t_1 < \cdots < t_{s-1}$ is defined as:

$$\sum_{j=-k_1}^{k_2} \alpha_{j+k_1}^{(i)} \mathbf{y}_{i+j} = h_i \sum_{j=-k_1}^{k_2} \beta_{j+k_1}^{(i)} \mathbf{f}_{i+j}, \quad i = k_1, \ldots, N-k_2, \tag{2}$$

where k is odd, $k_1 = (k+1)/2$ and $k_2 = k-k_1$, $\alpha^{(i)} = (\alpha_0^{(i)}, \ldots, \alpha_k^{(i)})^T$ and $\beta^{(i)} = (\beta_0^{(i)}, \ldots, \beta_k^{(i)})^T$, $i = k_1, \ldots, s-1-k_2$ are the coefficient vectors characterizing the method.
These equations must be associated with the boundary conditions and with $k_1 - 1$ initial and k_2 final equations that are derived using appropriate discretization schemes. Hence we obtain the following one step discretization scheme

$$\begin{cases} y_0 & \textit{given} \\ \sum_{i=0}^{k} \alpha_i^{(n)} y_i = h_n \sum_{i=0}^{k} \beta_i^{(n)} f(t_n) & n = 1, \ldots, k_1 - 1, \\ \sum_{i=0}^{k} \alpha_i^{(n)} y_{n-k_1+i} = h_n \sum_{i=0}^{k} \beta_i^{(n)} f(t_{n-k_1+1}) & n = k_1, \ldots, s-1-k_2, . \\ \sum_{i=0}^{k} \alpha_i^{(n)} y_{s-1-k+i} = h_n \sum_{i=0}^{k} \beta_i^{(n)} f(t_{s-1-k+i}) & n = s-k_2, \ldots, s-1, \end{cases} \tag{3}$$

that could be rewritten in matrix form obtaining

$$(\widetilde{\mathcal{A}} \otimes I_{2m})\mathbf{y} - hD_h(\widetilde{\mathcal{B}} \otimes I_{2m})\mathbf{f} = \mathbf{0} \tag{4}$$

where $\mathbf{y} = (\mathbf{y}_0^T, \mathbf{y}_1^T, \ldots, \mathbf{y}_{s-1}^T)^T$, $\mathbf{f} = (\mathbf{f}_0^T, \mathbf{f}_1^T, \ldots, \mathbf{f}_{s-1}^T)^T$ with $\mathbf{f}_i = \mathbf{f}(t_i, \mathbf{y}_i)$ and $\widetilde{\mathcal{A}}$ and $\widetilde{\mathcal{B}}$ are $s \times (s-1)$ matrices containing the coefficients of the main method plus those of the additional methods, $h = t_{s-1} - t_0$ and $D_h = diag(h_1, \ldots, h_{s-1})/h$. The integer s defines the dimension of the discrete problem. The time interval over which the approximation is computed is $[t_0, t_{s-1}]$. We use the numerical scheme by fixing a priori the value of s. This is a suitable choice for initial values problem. The resulting one step scheme, called block-BVM, can be reformulated as a Runge-Kutta scheme since the matrix $\widetilde{\mathcal{A}} = [a_0,\ \mathcal{A}]$, with $\mathcal{A}$ of size $s-1$, is nonsingular. Moreover the consistency requirement for the main and the additional methods imply that

$$-\mathcal{A}^{-1}a_0 = (1, \ldots, 1)^T = \mathbf{e}$$

and, multiplying by $(\mathcal{A} \otimes I_m)^{-1}$, we have

$$\begin{pmatrix} \mathbf{y}_1 \\ \ldots \\ \mathbf{y}_{s-1} \end{pmatrix} = (\mathbf{e} \otimes I_m)\mathbf{y}_0 + h(\mathcal{A}^{-1}D_h\widetilde{\mathcal{B}} \otimes I_m)\mathbf{f}$$

and

$$\mathbf{y} = (\mathbf{e} \otimes I_{2m})\mathbf{y}_0 + h(A \otimes I_{2m})\mathbf{f}$$

where

$$A = \begin{pmatrix} O_s^T \\ \mathcal{A}^{-1}D_h\widetilde{\mathcal{B}} \end{pmatrix}$$

This corresponds to an implicit Runge-Kutta scheme used with stepsize h. The tableau is ($\mathbf{e}_s = (0, \ldots, 0, 1)^T$):

$$\begin{array}{c|c} c_1 = 0 & \\ c_2 & \\ c_3 & A \\ \vdots & \\ c_s = 1 & \\ \hline & b = \mathbf{e}_s^T A \end{array}$$

with $c_{i+1} = (t_i - t_0)/(t_{s-1} - t_0), i = 0, s-1$

In our code we have implemented three classes of methods called ETR, TOM, BS by always choosing the normalized mesh points c_i satisfying $c_i = 1 - c_{s+1-i}$; with this choice of the mesh, all the methods are symmetric (see Definition 4.1 in [11]) as in the following definition:

DEFINITION 1: Consider the permutation matrix

$$P_s = \begin{pmatrix} 0 & \ldots & 0 & 1 \\ 0 & 0 & \cdot & 0 \\ & & & \\ 0 & 1 & 0 & \vdots \\ 1 & 0 & \ldots & 0 \end{pmatrix}$$

of size $s \times s$, a block-BVM is symmetric if it verifies

$$P_{s-1}\,\widetilde{\mathcal{A}}P_s = -\,\widetilde{\mathcal{A}}$$

$$P_{s-1}\,\widetilde{\mathcal{B}}P_s = \widetilde{\mathcal{B}}$$

$$P_{s-1}D_hP_{s-1} = D_h$$

The following results hold true (see Theorem 4.3 in [11])

THEOREM 2. For a symmetric block-BVM the boundary of the region of A-stability contains the imaginary axis.
Coefficients are computed in the following way:

- ETR: the coefficients $\alpha_i^{(n)}$ are chosen in order to have the matrix $\widetilde{\mathcal{A}}$ with the following structure

$$\widetilde{\mathcal{A}} = \widetilde{\mathcal{A}}_g = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & -1 & 1 \\ & & & & \end{pmatrix}, \tag{5}$$

  order $p = k+1$ and $s_{min} = k+1, s >= s_{min}$ [2].
- TOM: the coefficients of the main method are chosen in order to have the maximum order $p = 2k$, the additional methods are chosen in the ETR class, this implies that $s_{min} = 2k, s >= s_{min}$ [2];
- BS: the coefficients are computed in order to obtain a collocation method using the B spline basis with order $p = k+1$ and $s_{min} = k+1, s >= s_{min}$ ([18], [19]).

An important role assumes the fixed normalized mesh $c_1 < \cdots < c_s$; a suitable choice of it improves the properties of the associated one step scheme. We decided to compute the mesh using the zeros of the orthogonal polynomial $\frac{d^{s-2}}{dx^{s-2}}(x^{s-1}(x-1)^{s-1})$. We note that this way s is in general greater or equal to $k+1$. An important relation beetwen these scheme and classical Runge-Kutta schemes is obtained when the size of the block is $s = s_{min}$ and is described in the following Theorem (see Theorem 1 in [1]) .

THEOREM 3. A block-BVM based on k-step BVM of order p with minimal blosksize and non singular coefficient matrix , is equivalent to a *RK* collocation method.

Moreover, the Runge-Kutta method equivalent to a symmetric block-BVM is symmetric or time reversible.

Using these results, we can state that symmetric block-BVM share all the properties of symmetric Runge-Kutta schemes when applied to reversible differential equations ([9], Ch. V).
If $s = s_{min}$, then all the implemented numerical schemes are equivalent to the Lobatto IIIA scheme. In this case a super-convergence happens; this means that the order in the approximation of the last point t_{s-1} is $2s_{min} - 2$. If $s > s_{min}$, we lose this super-convergence condition. We prefer the block-BVM representation for two main computational reasons. The first one is that we easily compute the coefficients of the methods also when $s > k+1$, the second one is that in this case the matrices $\widetilde{\mathcal{A}}$ and $\widetilde{\mathcal{B}}$ are banded matrices, whereas the corresponding matrix A of the Runge-Kutta tableau is full.

Since all the considered methods are *implicit* and we need to solve non-linear equations, two main problems arise: their efficient numerical solutions and the computation of the starting approximations. For the moment we have considered only a constant stepsize h implementation.

About the solution of the nonlinear equation, we consider both a Newton like iteration and a functional iteration. Even if the latter is usual, because of its cheaper computational cost, our numerical experiments enlightened that, in many cases, a Newton like iteration works better.

The starting approximations are computed using a *BS* Hermite spline quasi-interpolants [21], that compute an approximation of the continuous solution of the same order of the used numerical method and, for the *BS* schemes, collocate the differential equations.

Moreover, since the coefficients of the methods depend on the internal mesh and on the size of the block, an accurate computation of the coefficients is another important issue for high order reliable numerical schemes.

More implementation details will be treated in a further paper where the code will be presented exhaustively; here we focus our attention on the applications of the presented methods.

3 Numerical Experiments

Here we present our results concerning the conservation of first integral of some significant conserving systems, which happen to be Hamiltonian. About the choice of the convenient stepsize, our approach is taken from engineering literature (e.g. [25]) and is based upon the Fourier series representation of periodic, quasi-periodic and nearly quasi-periodic orbits. Once we get an estimation of the (presumed) longest period by an optimization process (over short time intervals), we can use a convenient ratio of that period as stepsize for the numerical integration over long time intervals; this way, we obtained good results, when we used a conveniently stable numerical method of a conveniently high order. Even chaotic orbits can be well simulated by our methods for quite long time intervals, where conservation of first integral is achieved as well, within a required accuracy. Indeed, many general numerical integrators do not preserve at all first integrals of their corresponding continuous differential systems, over long time intervals. Therefore such preservation has been widely used as a tool to measure the accuracy of long-term behavior of these integrators, even though, as stated before, conservation of first integral is just a necessary condition for correctness of orbits (when the degrees of freedom are more than one). The following numerical experiments were carried using an improved version of the code already presented in [17]. All the reported figures are drawn by semilogaritmic scale.

Example 1. We consider the one-degree-of-freedom Hamiltonian system with the given Hamiltonian $H(p,q) = T(p) + U(q)$, where $T(p) = \frac{p^3}{3} - \frac{p}{2}$ and $U(q) = \frac{q^6}{30} + \frac{q^4}{4} - \frac{q^3}{3} + \frac{1}{6}$. Since the Hamiltonian H is not an even function in p, the system is not reversible. We applied our symmetric methods with initial conditions $p(0) = 1$ and $q(0) = 0$. We notice that in this case $H(0) = 0$, so we can compute absolute Hamiltonian error only. The periodic orbit has a period whose first five correct digits were estimated 8.8808. This integrable Hamiltonian system was firstly studied in [7] , where they investigated examples when symmetric methods produce an energy drift, and then in [3]. In Fig. 1 we report our results relating to method *BS* with stepsize $h = 8.8808/24$. The important point to note here is the expression of h, which is

taken as a convenient integer submultiple of the estimated period. At first we used a method of order 4 with $s = 10$ and then a method of order 10 with $s = 14$. It is clear that in the first case an energy drift appears (the increasing straight line interpolating the maxima is also drawn), whereas in the second case no drift is present, because of the higher order of the method. In [7] authors report that LOBATTO IIIA method of order 4 exhibits an evident energy drift. In Fig. 2 we report our results relating to ETR method of order 8 with $s = 8$, which means a minimum blocksize; the chosen stepsize was $h = 8.8808/20$, i.e. a little larger stepsize, but still an integer submultiple of the estimated period. This method corresponds to a Lobatto IIIA method of an order higher than the presently available ones. By the way, we notice that ETR method of order 4 with $s = 4$ corresponds to a Lobatto IIIA method of order 6. It is clear that no drift appears over more than 10^5 periods.

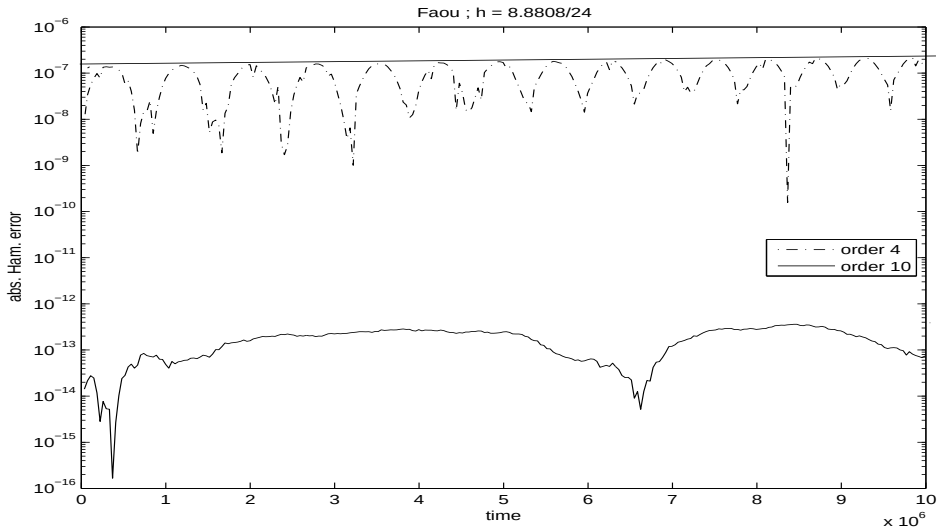

Fig. 1 Example 1- Method BS

Example 2. The second example is an Hamiltonian system, which was firstly presented in [27] , where it was deeply investigated from a theoretical point of view. The considered system is the following:

$$\ddot{q_1} + 4q_1 = q_2^2$$
$$\ddot{q_2} + q_2 = 2q_1q_2$$

The Hamiltonian is $H = \frac{1}{2}(p_1^2 + 4q_1^2) + \frac{1}{2}(p_2^2 + q_2^2) - q_1q_2^2$, .
The Hamiltonian H is an even function in p, so the system is reversible.
Moreover this system is nonintegrable, but it can be considered nearly-integrable in the neighborhood of the origin, since the origin is a stable equilibrium point.
Here we take under consideration three sets of initial conditions, corresponding to increasing values of initial Hamiltonian, which means that we are moving from nearly periodicity towards chaotic behavior:

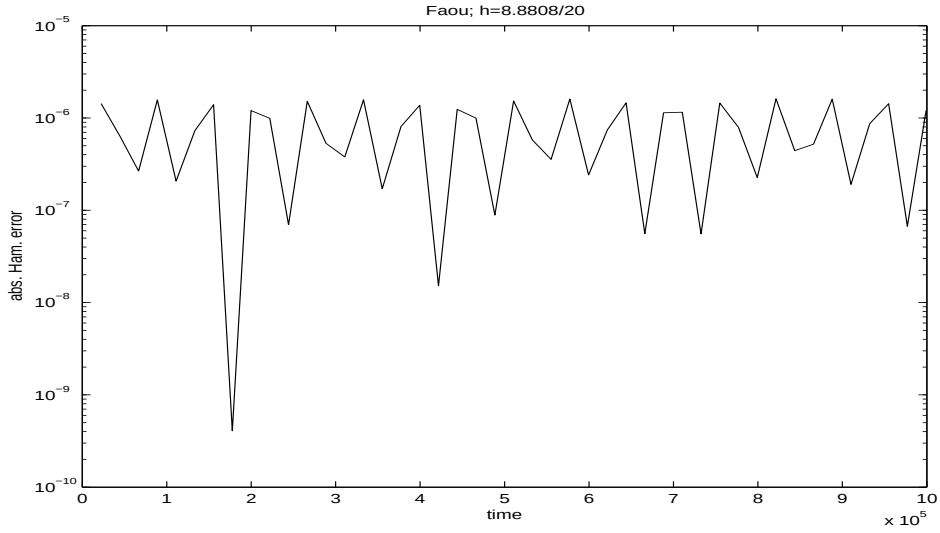

Fig. 2 Example 1- Method ETR, order 8, minimum blocksize

a) $q_1(0) = 0; q_2(0) = 0; p_1(0) = 1.5e-4; p_2(0) = 1.5e-4$, with initial Hamiltonian $H_0 = 2.25e-8$. We used *BS* method of order 10 and $s = 14$ with stepsize $h = \pi/12$. This example was already treated in [22], where it was shown that the longest period is $T = 2\pi$ (plus neglegible perturbations). Therefore the choice of $\pi/12$ is chosen analogously to the previous example. In Fig. 3 we report the behavior of relative Hamiltonian error over more than 10^6 cycles and we show that no drift appears, since the error remains permanently bounded (within the considered interval).

b) $q_1(0) = 0; q_2(0) = 0; p_1(0) = 0.08; p_2(0) = 0.08$, with initial Hamiltonian $H_0 = 6.4e-3$. We used ETR method of order 8 with $s = 8$, which means a minimum blocksize. For this example, the longest period was estimated $T = 6.3263$. Therefore the stepsize was chosen $h = T/8$. From Fig. 4 it is clear that even in this case we have no energy drift, over more than 10^6 cycles.

c) $q_1(0) = 0; q_2(0) = 0; p_1(0) = 0.5; p_2(0) = 0.5$, with initial Hamiltonian $H_0 = 0.25$. We used TOM method of order 6 with $s = 10$. Here the orbit exhibits a behavior which suggests transition to chaos and the presumed longest period is about $T = 60$. Therefore the stepsize was chosen $h = 2$. Since the order of the method is quite low, we expect that the relative Hamiltonian error is quite high. Indeed, from Fig. 5 it is clear that again no energy drift appears, even for high values of relative errors, over more than 10^4 cycles .

Example 3. The third example is an Hamiltonian system taken from the field of structural engineering. This highly nonlinear system was deeply studied in [5] and can be rewritten in the following form:

$$\begin{aligned} 4\ddot{q_1} + \ddot{q_2} &= -\beta[4q_1^3 - 6q_1^2 q_2 + 4q_1 q_2^2 - q_2^3] - 5k\, q_1 + 3k\, q_2 \\ \ddot{q_1} + 2\ddot{q_2} &= -\beta[q_2^3 - 3q_2^2 q_1 + 4q_2 q_1^2 - 2q_1^3] + 3k\, q_1 - 2k\, q_2 \end{aligned}$$

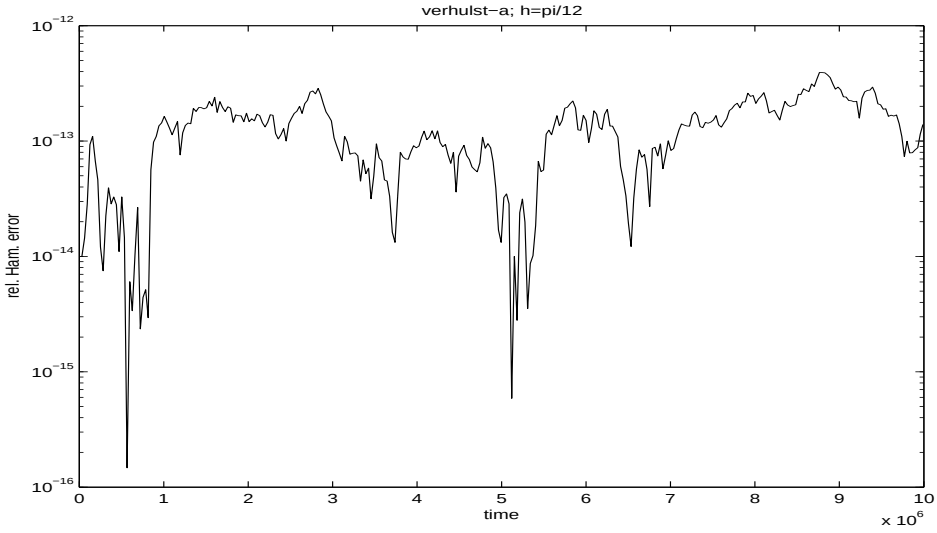

Fig. 3 Example 2- Method BS, order 10

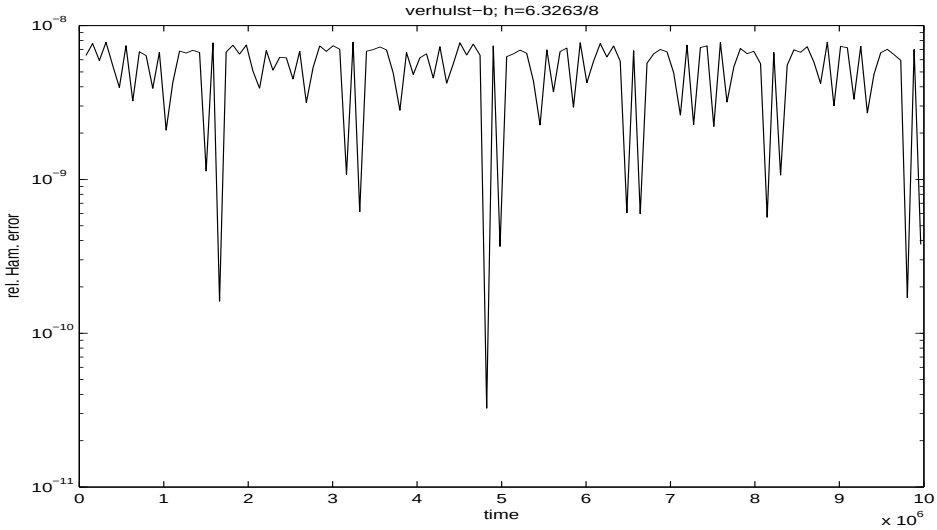

Fig. 4 Example 2- Method ETR, order 8, minimum blocksize

where $\beta = 3.5555556 \times 10^{12}$, $k = 2.611235\,56 \times 10^{7}$.

The initial conditions are $q_1(0) = 0; q_2(0) = 0; p_1(0) = 3.576526614260458; p_2(0) = 1.733$, corresponding to a total energy $H = 1000$. Analogously to the previous example, this system is nonintegrable, but it can be considered nearly-integrable in the neighborhood of the origin, since the origin is a stable equilibrium point. However in this case the initial conditions are chosen quite far from the origin, so that the Hamiltonian exhibits a high value. In this case the presumed longest period was estimated of the order of 10^{-4} [23]. Given that, we chose

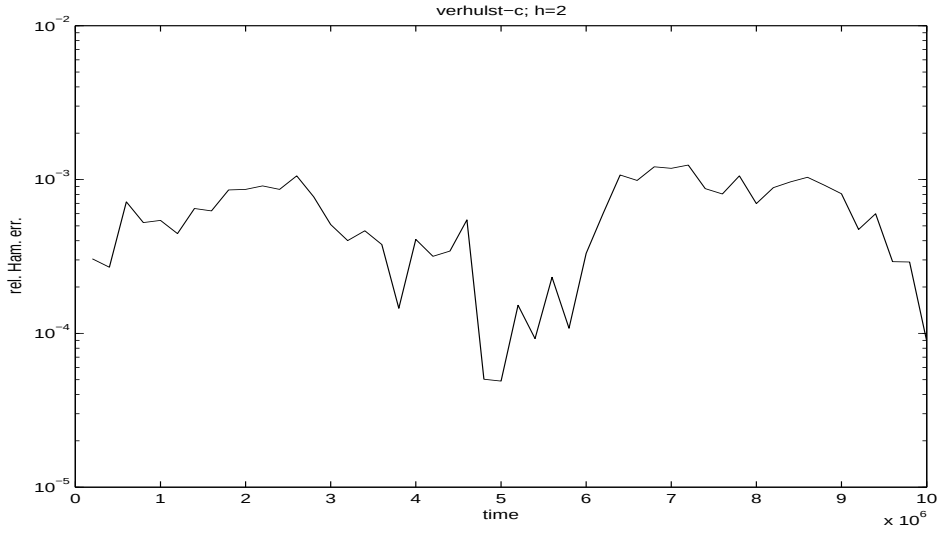

Fig. 5 Example 2- Method TOM, order 6

a *BS* method of order 10 and $s = 14$ with stepsize $h = 9e-6$, that is a quite high order with a quite small stepsize. In Fig. 6 the relative Hamiltonian error is reported until $t = 1$ sec, which means about 10^4 cycles, but it is worth noticing that the physical problem suggests that solutions are interesting until 0.1 sec only.
It is clear that , even though a clear transition to chaos happens, no drift in numerical computation of Hamiltonian appears.

Moreover, in Fig. 7 we report the Poincarè map of the same flow obatined by a special options of our code, which allows the *BS* method to get a Poincarè map in continuous sense (i.e. of continuous orbits), without interpolation and approximation. It is clear that, even though a hyperbolic point is present, the provided Poincarè map turns out satisfactorily clean and significant.

Example 4. We consider the Hénon-Heiles model whose Hamiltonian is

$$H(p,q) = \frac{1}{2}\,(p_1^2+p_2^2) + \frac{1}{2}\,(q_1^2+q_2^2) + q_1^2 q_2 - \frac{1}{3}\,q_2^3$$

and we chose initial values $q_1(0) = 0$, $q_2(0) = 0.3$, $p_2(0) = 0.2$ and the positive value $p_1(0)$ such that the Hamiltonian takes the value $H_0 = 1/8$: the solution is chaotic ([9], Section I.3). In [10] for this same problem, they present some simulations carried out by the Gauss-Runge-Kutta method of order 8 and by an explicit composition method (based on Störmer-Verlet approach) of order 8. Stepsize is taken $h = 2\pi/240$ for both methods and integration is carried out on an interval of length $2\pi e + 6$. In [10] they aim at showing the influence of round-off error on the conservation of first integrals for long time integrations. They find that for the explicit composition method the round-off contribution increases, as expected for random walk, like the square root of time, whereas for the implicit Runge-Kutta method the round-off contribution is a superposition of a statistical error, which grows like a square root of time, and of a deterministic error which grows linearly with time. We found different

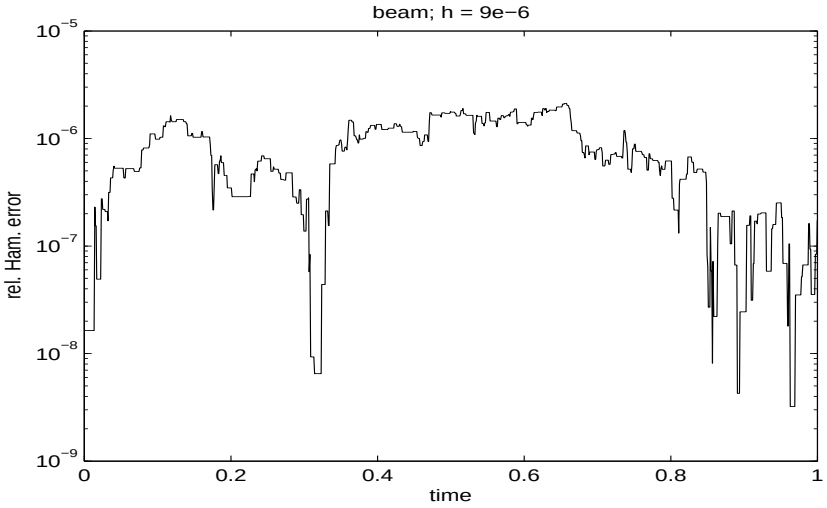

Fig. 6 Example 3- Method BS, order 10

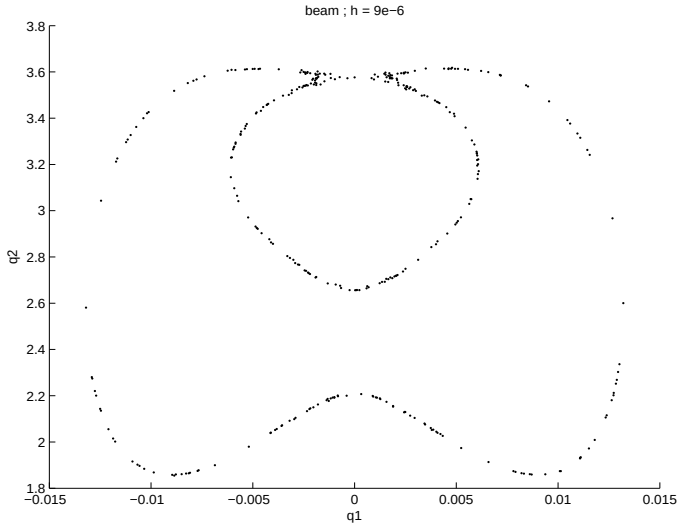

Fig. 7 Example 3- Method BS, order 10

results. Here in Fig. 8 we report the relative Hamiltonian error, referring to our simulation carried out by method *BS* of order 4 with $s = 10$ and stepsize $h = 0.05$ up to $t = 7e+6$ sec. It is clear that no drift in Hamiltonian error appears , which means that our method, equipped with a suitable stepsize, is able to provide good numerical approximations, even though solution is chaotic.

We notice that the Hénon-Heiles system has a critical energy value $H_c = 1/6$, at which the qualitative nature of solutions changes, from bounded to unbounded orbits. In [24] they

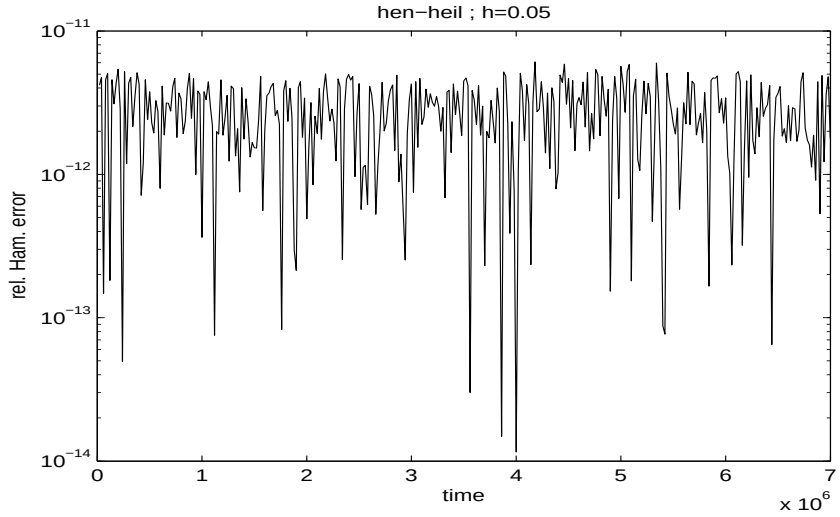

Fig. 8 Example 4- Method BS, order 4

choose initial values $q_1(0) = 0.1$, $q_2(0) = -0.5$, $p_1(0) = p_2(0) = 0$, corresponding exactly to the critical energy $H_c = 1/6$. In particular initial spatial coordinates (q_1, q_2) are taken at a point on the boundary of the critical triangular region (see [16], Section 1.4*a*). In [24] they solve this system by a new class of energy-preserving $B-$series numerical method and compare their features with those of an analogous second order sympletic method, the leapfrog method (e.g [9]) up to $t = 71$ sec and with stepsize $h = 0.16$. Finally they show that their B-series solution not only preserves energy, but also stays within the stable zone, whilst leapfrog solution stays outside and soon becomes completely unstable. We repeated the same simulations by our *BS* method of order 4 and $s = 10$ with stepsize $h = 0.16$, and our results are reported in Fig. 9 and Fig.10. It is clear that by our method, not only energy is preserved, but also the stable zone superbly embraces the solution for a much longer time, i.e. up to $t = 71e+6$ sec (for convenience, the border of triangular stable zone is also drawn [16]).

4 Conclusion and remarks

When simulations are carried out for reversible integrable systems, almost all methods work properly, but when systems are nonintegrable or nearly integrable and non reversible and even chaotic, then numerical troubles become dominant. This is the reason why we presented previous examples. Actually, we carried out a large amount of numerical tests where the crucial choices were always two: the stepsize and the order of the method. We tried to find out efficient solutions time by time, but no general rules appeared, except that stepsize has to be conveniently chosen, according to the (presumed) longest period. For our block-BVM, both the the order p and the parameter s are input data, so a very large number of possible combinations are available. Even though conservative systems are very sensitive to non-conservative perturbations, such those introduced by some numerical integrators, our numerical evidence

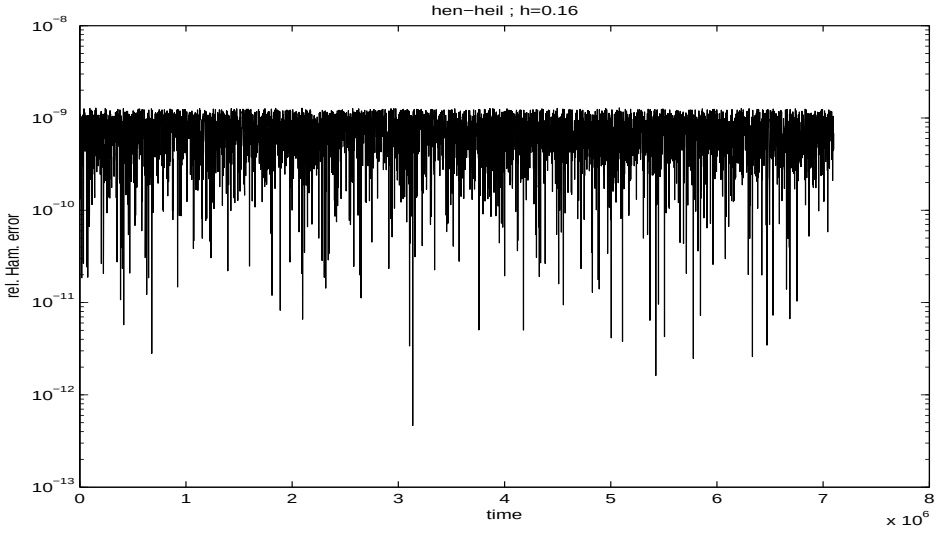

Fig. 9 Example 4- Method BS, order 4

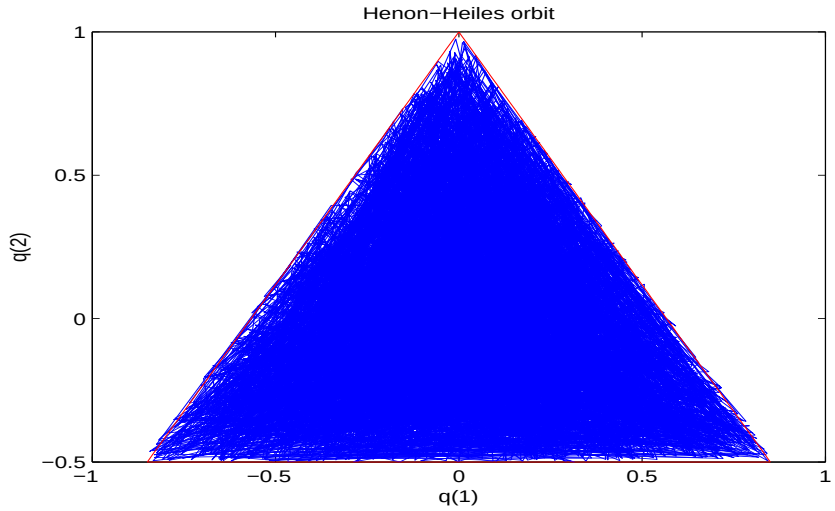

Fig. 10 Example 4- Method BS, order 4 : configuration space orbit

suggests that we are always able to find a convenient combination of order p, parameter s and stepsize h such that the first integral is preserved within a required accuracy, over long-time intervals. One of the main advantages of our methods is given by their numerical stability, as was shown in Example 4. Another significant advantage is that our class of methods provides reliable methods of higher orders than the usual ones. We did not present any explicit comparisons with other methods, because here we restrict to the presentation of the features of our class of symmetric methods only.

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