Multi-value numerical methods for Hamiltonian systems

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Abstract. We discuss the effectiveness of multi-value numerical methods in the numerical treatment of Hamiltonian problems. Multi-value (or general linear) methods extend the well-known families of Runge-Kutta and linear multistep methods and can be considered as a general framework for the numerical solution of ordinary differential equations. There are some features that needs to be achieved by reliable geometric numerical integrators based on multi-value methods: G-symplecticity, symmetry and boundedness of the parasitic components. In particular, we analyze the effects of the mentioned features for the long term conservation of the energy and provide the numerical evidence confirming the theoretical expectations.

1 Hamiltonian problems

It is the aim of this paper to analyze the effectiveness and the long-term behaviour of multi-value numerical methods for Hamiltonian problems

$$\dot{y}(t) = J^{-1}\nabla H(y), \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{1}$$

where the function H, denoted as Hamiltonian or energy of the system, is exactly preserved along the solution of (1). Geometric numerical integrators for (1) (compare [16] and references therein) are able to perform an excellent long-time conservation of the Hamiltonian along the numerical solution: this is classically the case of symplectic (or canonical) Runge-Kutta (RK) methods [1,16,21,22], which are meant to exactly preserve quadratic invariants possessed by (1) along the numerical solution (within round-off error). Moreover, a symplectic numerical method is able to preserve any Hamiltonian function over exponentially long times with an exponentially decreasing error, as proved by Benettin and Giorgilli (see [16], Theorem 8.1, §IX.8).

Symplecticity is a prerogative of certain RK methods, i.e. those satisfying the algebraic constraint [1,16,19,22,23]

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0. \tag{2}$$

Indeed, linear multistep methods cannot be symplectic [24] as well as genuine multi-value methods cannot be symplectic [14,20,4].

However, many contributions of the recent literature have been devoted to the analysis and the construction of both multistep and multi-value methods

meant to guarantee an excellent near conservation of invariants over long time intervals (compare, for instance, [1–3,7–9,15,16] and references therein). The aim of this paper is that of analyzing the main results achieved so far in the case of multi-value methods and applying them to investigate the long-time behaviour of a method recently developed in [9], both from a theoretical and an experimental point of view.

2 Multi-value methods

Our attention is focused on the family of multi-value methods, which provides a wide range of methods including multistage methods (e.g. Runge-Kutta and multistep Runge-Kutta methods) and multistep methods (compare [1,18] and references therein for a complete analysis of known methods regarded as multi-value methods, extended in [10] to the case of second order ODEs).

The numerical scheme given by a multi-value method for the numerical solution of the initial value problem

$$y' = f(t, y),\ t \geq 0 \qquad y(t_0) = y_0, \tag{3}$$

consists in the following three basic steps:

- a *starting* procedure S_h, $y^{[0]} = S_h(y_0)$,
- a *forward* procedure G_h, $y^{[n+1]} = Vy^{[n]} + h\Phi(h, y^{[n]})$,
- a *finishing* procedure F_h, $y_n = F_h(y^{[n]})$.

Thus, the method transfers along the grid a whole vector $y^{[n]}$ containing the approximations of a set of quantities related to the solution of the problem under investigation. At each step, one can always get the numerical approximation of the solution in the current step point by applying the finishing procedure.

Under some basic hypothesis described in details in [16] (compare Theorem 8.1 in Section XV), one can prove that for any given forward and finishing procedures, there exist a unique starting procedure $S_h^*(y)$ and a unique one-step method $y_{n+1} = \Phi_h^*(y_n)$, such that

$$G_h \circ S_h^* = S_h^* \circ \Phi_h^*, \qquad F_h \circ S_h^* = id.$$

Thus, if the starting vector is computed by $Y^{[0]} = S_h^*(y_0)$, then the numerical solution obtained by the multi-value method is (formally) equal to that of the one-step method Φ_h^*. Hence, Φ_h^* is called *underlying one-step method*.

A widely used representation of multi-value methods is usually given by the family of General Linear Methods (GLMs, compare [1,10,18] and references therein)

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n]}, \quad i = 1, 2, \ldots, s, \\ y_i^{[n+1]} = h \sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n]}, \ i = 1, 2, \ldots, r, \end{cases} \tag{4}$$

The formulation (4) is provided in correspondence of the uniform grid $\{t_0+ih, i=0,1,\ldots,N\}$, with $h=(T-t_0)/N$. The vector $y^{[n]}=[y_1^{[n]},\ldots,y_r^{[n]}]^{\intercal}$ denotes the vector of external approximations containing all the informations we decide to transfer from step n to step $n+1$, $Y_i^{[n]}$ provides an approximation to the solution of (3) in the internal point $t_n+c_ih\in[t_n,t_{n+1}]$, $i=1,2,\ldots,s$, and $F_j=f(Y_j^{[n]})$. A compact representation of GLMs collects their coefficient matrices $A\in\mathbb{R}^{s\times s}$, $U\in\mathbb{R}^{s\times r}$, $B\in\mathbb{R}^{r\times s}$, $V\in\mathbb{R}^{r\times r}$, in the following partitioned $(s+r)\times(s+r)$ matrix

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right].$$

As mentioned in the previous section, even if GLMs cannot be symplectic (unless they reduce to symplectic one step methods, compare [4,14,20]), the recent literature has emphasized the possibility to effectively employ GLMs for the numerical treatment of Hamiltonian problem (compare, for instance, [1–3,7–9] and references therein). In particular, the state-of-art reveals that some specific properties have to be satisfied by multi-value methods in order to accurately approach Hamiltonian problems:

- G-symplecticity (introduced in the first edition of [16], also see[1–3,5,7–9]), which ensures conjugate-symplecticity of the underlying one-step method associated to the multivalue method (4);
- symmetry of the numerical scheme [16], which is a suitable property providing the discrete counterpart of the reversibility of the exact flow, in case of reversible dynamical systems;
- boundedness of parasitic components over long times [3,11,16], which ensures that the parasitic components generated by the numerical method remain bounded over certain time intervals.

The above mentioned features are considered in the remainder of the treatise.

3 G-symplecticity

As mentioned, the multivalue nature of GLMs does not allow them to be symplectic, unless they reduce to RK methods. However, a near-conservation property achievable by multivalue methods has been provided and analyzed by the recent literature, defined as follows. If $y^{\intercal}Ey$ is a quadratic first integral of the differential problem $y'=f(y)$, where E is a symmetric matrix, G-symplecticity assures that

$$y^{[n+1]^{\intercal}}(G\otimes E)y^{[n+1]}=y^{[n]^{\intercal}}(G\otimes E)y^{[n]}, \tag{5}$$

(compare [12]), being G a symmetric matrix. Taking into account that any GLM (4) satisfies the following identity (compare [9] and references therein)

$$\begin{aligned} y^{[n+1]^\intercal}(G\otimes E)y^{[n+1]} &= y^{[n]^\intercal}(G\otimes E)y^{[n]} + \sum_{i,j=1}^{r}(G - V^\intercal GV)_{ij}y_i^{[n-1]^\intercal}y_j^{[n-1]} \\ &+ 2h\sum_{i=1}^{s}\sum_{j=1}^{r}(DU - B^\intercal GV)_{ij}y_i^{[n-1]^\intercal}F_j^{[n-1]} \\ &+ h^2\sum_{i,j=1}^{s}(DA + A^\intercal D - B^\intercal GB)_{ij}F_i^{[n-1]^\intercal}F_j^{[n-1]}, \end{aligned}$$

the G-symplecticity property (5) is achieved if the algebraic constraints

$$G = V^\intercal GV, \qquad DU = B^\intercal GV, \qquad DA + A^\intercal D = B^\intercal GB \tag{6}$$

are satisfied [1,16].

Condition (5) reveals that G-symplectic multivalue method does not preserve quadratic first integrals, but a related quadratic form $y^{[n]^\intercal}(G\otimes E)y^{[n]}$. It was observed in [12] that the first terms of the expansion in powers of h of the quadratic form $y^{[n]^\intercal}(G\otimes E)y^{[n]}$ is $y^\intercal Ey$ (compare [12]): thus, the more h is small, the more the two forms are close each other. observe that condtions (6) of G-symplecticity are equivalent to annihilating the algebraic stability matrix of a GLM (compare [1,6,13,16]).

There is a strong formal relation between G-symplectic and symplectic maps, which is highlighted in [11]. We report here the main result.

Theorem 1. *Consider a G-symplectic multi-value method* (4) *of order p. Then, for every finishing procedure the underlying one-step method is conjugate-symplectic. More precisely, there exists a change of coordinates* $\chi_h(y) = y + O(h^p)$*, such that* $\chi_h \circ \Phi_h^* \circ \chi_h^{-1}$ *is a symplectic transformation.*

In other words, this results asserts that a G-symplectic method has the same behavior of a symplectic one-step method after a global change of coordinates that is $O(h^p)$ close to the identity [12].

4 Control of parasitism

One-step methods are the only candidates for symplecticity (compare [16,24] for linear multistep methods and [4,15,20] for irreducible multivalue methods). This is due to the fact the multistep and multivalue methods generate parasitic components in the numerical solution which destroy the overall long-time accuracy (see [3,11,16]). Hence, if one aims to derive non-symplectic methods which are capable of nearly preserving invariants over the numerical solution, the parasitic behaviour of such methods has to be taken under control over long time intervals [11].

As announced, due to their multivalue nature, GLMs introduce parasitic components in the numerical solution, which have to be controlled in order to achieve a long-term near conservation of the invariants. Rigorous bounds on parasitic solution components have recently been obtained in [11], where the authors have proved that, for carefully constructed methods, the error in the parasitic components typically grows like $h^{p+4}exp(h^2Lt)$, where p is the order of the method, and L depends on the problem and on the coefficients of the method.

A basic property of boundedness for the parasitic components of multivalue methods is achieved by annihilating the so-called growth parameters [11,16]

$$\mu_j = \xi_j^{-1} v_j^* BU v_j, \tag{7}$$

where ξ_j are the eigenvalues of the matrix V such that $\xi_j \neq 1$, v_j and v_j^* are the right and left eigenvectors, respectively ($Vv_j = \xi_j v_j$ and $v_j^* V = \xi_j v_j^*$) satisfying $v_j^* v_j = 1$. Examples of methods with zero-growth parameters, in the context of multivalue methods, have been provided in [2,3,8,9]. In particular, a G-symplectic, symmetric (i.e. the underlying one-step method is symmetric, compare [16]), order 4 method (4) with zero growth parameter has been introduced in [9]. Denoted by

$$\gamma = 2 + \frac{\sqrt[3]{4}}{2} + \sqrt[3]{2}, \qquad \delta = \left(1 + \sqrt[3]{2}\right)^2, \qquad \varphi = \frac{15}{4} + 2\sqrt[3]{2} + \sqrt[3]{4},$$

such a method depends on the following coefficient matrices

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} \frac{1}{6}\gamma & 0 & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & -\frac{1}{6}\delta & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & \frac{1}{6}\delta & \frac{1}{6}\gamma & 1 & \frac{1}{24} \\ \hline \frac{1}{6}\varphi & -\frac{1}{4} - \frac{2\sqrt[3]{2}}{3} - \frac{\sqrt[3]{4}}{3} & \frac{1}{6}\varphi & 1 & \frac{1}{12} \\ 1 & -2 & 1 & 0 & -1 \end{array}\right]. \tag{8}$$

A starting procedure is given in details in [9].

5 Long-term behaviour

As explained in the previous section, ideal multi-value methods generate small and bounded parasitic components over long time intervals. In order to derive sharp long-term error estimates for multi-value methods, we have suitably applied in [11] backward error analysis, a powerful tool successfully applied to one-step and linear multistep methods (compare [16,15] and references therein) which provides a crucial ingredient for the study of the long-time behavior of numerical integrators. In [11], we have derived sharp estimates for the parasitic components and the error in the Hamiltonian numerically

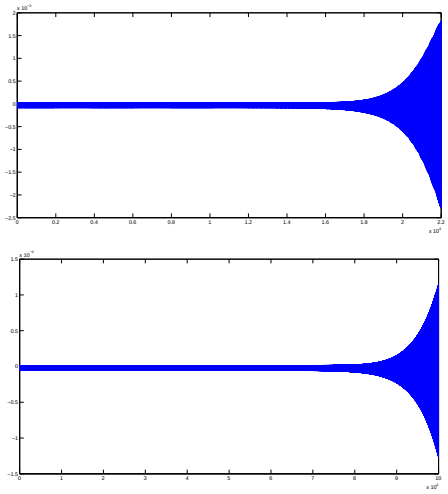

Fig. 1. Error in the Hamiltonian (9) for the method (8) with stepsizes $h = 0.25$ (top) and $h = 0.125$ (bottom)

computed by a multi-value method: we realized that, for carefully constructed methods (i.e. symmetric and with zero growth parameters) the error in the parasitic components typically grows like $h^{p+4}\exp(h^2Lt)$.

In particular, for the multi-value method (8), the following result holds (compare [11]).

Theorem 2. *If* (8) *is applied to a Hamiltonian system* (1)*, then the energy is nearly preserved according to*

$$H(y_n) - H(y_0) = O(h^4) + O(th^8) + O\big(h^8\exp(h^2Lt)\big)$$

as long as $t = nh = O(h^{-2})$.

Thus, for method (8), parasitic components remain bounded on intervals of steplength $O(h^{-2})$, which is also confirmed by the numerical evidence. We apply method (8) to the simple pendulum problem, depending on the Hamiltonian function

$$H(p,q) = \frac{1}{2}\,p^2 - \cos q, \tag{9}$$

and initial values $q(0) = 3$, $p(0) = 0$.

Figure 1 shows the Hamiltonian error obtained by using the step sizes $h = 0.25$ and $h = 0.125$: confirming the predicted estimate of Theorem 2, the error behaves like $O(h^4)$ on intervals of length $O(h^{-2})$, and then follows an exponential growth. We observe that method (8) is also able to preserve the symplecticity of the phase space, as visible from the orbit pattern in Figure 2.

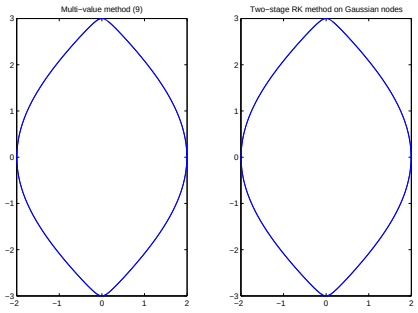

Fig. 2. Orbit patterns of the mathematical pendulum (1) obtained by the multi-value method (8) (left) and the symplectic Runge-Kutta method on two Gaussian points (right)

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