Nearly conservative multivalue methods with extended bounded parasitism

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Abstract

The paper is focused on the analysis of parasitism for multivalue numerical methods intended as geometric numerical integrators for Hamiltonian problems. In particular, the main topic is the design of multivalue numerical methods whose parasitic components remain bounded over certain time intervals, opening the path to the development of nearly conservative multivalue methods able to guarantee a control of parasitism in the long time. The analysis of parasitism as well as the development of the corresponding methods is the core of the treatise. The effectiveness of the approach is also confirmed on selected Hamiltonian problems.

Keywords: Geometric numerical integration, Hamiltonian problems, multivalue methods, symmetry, parasitism.

1. Introduction

Geometric Numerical Integration (GNI; see, for instance, [24, 31] and references therein) is a mature branch of Numerical Analysis that provides a different and more modern perspective on the discretizations to conservative evolutionary operators. Indeed, geometric numerical methods are designed in order to inherit qualitative properties of a conservative differential operator along its discretized solutions, rather than only relying on computing accurate numerical solutions.

A relevant class of conservative differential systems is given by Hamiltonian problems, assuming the form

$$\dot{y}(t) = J^{-1}\nabla\mathcal{H}(y), \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{1.1}$$

where $I \in \mathbb{R}^d$ is the identity matrix and the vector $y(t) \in \mathbb{R}^{2d}$ collects the conjugate momenta and generalized coordinates of a mechanical system with d degrees of freedom. The function $\mathcal{H}$, known as Hamiltonian function of the system, is a first integral of (1.1). The principal task of GNI for Hamiltonian problems is the design of numerical schemes able to perform an excellent long-time conservation of the Hamiltonian function along the corresponding discretized dynamics. A relevant class of geometric methods is given by symplectic (or canonical) Runge-Kutta (RK) methods

[4, 24, 29, 31, 32, 33], which are meant to exactly preserve (clearly, within round-off error) quadratic invariants possessed by (1.1) along the numerical solution. Moreover, a symplectic numerical method is able to preserve Hamiltonian functions over exponentially long times, as proved by Benettin and Giorgilli (see [24], Theorem 8.1, §IX.8), if the solution to (1.1) lies in a compact set.

Symplecticity is a prerogative of certain implicit RK methods, since linear multistep methods and genuine multi-value methods cannot be symplectic [8, 22, 30, 34]. This issue is due to the fact the both multistep and multivalue methods add parasitic components to the numerical solutions growing in time and destroying the accuracy of long-term conservations. However, several contributions in the recent literature have been focused on the design and the analysis of nearly-conservative methods other than RK schemes, as in [4, 5, 6, 7, 1, 13, 14, 15, 18, 19, 23, 24] and references therein, meant to break down the effects of parasitism on long-time intervals and providing a cheaper alternative to symplectic methods.

In this paper we aim to design multivalue numerical methods whose parasitic components remain bounded over certain time intervals, opening the path to the development of nearly conservative multivalue methods able to guarantee a control of parasitism in the long time. The manuscript is organized as follows: Section 2 contains a brief description of multivalue numerical methods and their representation as General Linear Methods (GLMs); Section 3 provides an analysis of the parasitic components and the developments of algebraic constraints on the coefficients of the methods guaranteeing their boundedness; the development of methods is object of Section 4, while their performances are evaluted by the numerical evidence given in Section 5. Some concluding remarks are the topic of Section 6.

2. Methodology: multivalue numerical schemes

Multivalue numerical methods provide a general family of time integrators for the well-posed initial value problem

$$\begin{cases} y'(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \end{cases} \tag{2.2}$$

here supposed to be autonomous, properly including many well-known numerical schemes, e.g., Runge-Kutta and linear multistep methods (compare [4, 17, 28] and references therein). Referring to the step point $t_n \in \mathcal{I}_h$, with

$$\mathcal{I}_h = \left\{ t_n = nh, \quad n = 0, 1, \dots, M, \quad h = \frac{T}{M} \right\},$$

multivalue numerical methods compute a vector of r entries

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \in \mathbb{R}^{rd},$$

assuming that $y^{[n-1]}$ is given. Such a vector does not only (and not necessarily) contain the approximation of the solution in the grid points (as it happens in the case of Runge-Kutta methods, for instance), but also solution related quantities (e.g., linear combination of the derivatives, evaluations of the vector field in off-step points and so on). For instance, a multivalue method discretizing the equation of motion of a system of particles may provide, at each step point, an approximation to the position and the velocity of each particle, i.e., the vector $y^{[n]}$ approximates the solution of the differential equation and its first derivative.

It is also worth observing that the addition of more quantities in the discretized dynamics may allow the introduction of additional degrees of freedom in the method which can be exploited to improve the classical order and stability barriers of multistep and multistage methods [4].

A multivalue numerical method provides a discrete dynamics as described in Figure 1; the corresponding numerical scheme can be formally described through the following maps:

- a *starting* procedure
$$S_h : \mathbb{R}^d \to \mathbb{R}^{rd},$$
providing the starting vector $y^{[0]} = S_h(y_0)$;

- a *forward* map
$$G_h : \mathbb{R}^{rd} \to \mathbb{R}^{rd},$$
updating the vector $y^{[n]}$ in $y^{[n+1]}$. In the remainder, we will usually refer to the notation
$$y^{[n+1]} = Vy^{[n+1]} + h\Phi(h, y^{[n]}), \tag{2.3}$$
where $V \in \mathbb{R}^{rd\times rd}$ and $\Phi(h, y^{[n]}) : [0, +\infty) \times \mathbb{R}^{rd} \to \mathbb{R}^{rd}$ is an increment term. The matrix V has the form
$$V = \widetilde{V} \otimes I_d, \tag{2.4}$$
being $\widetilde{V} \in \mathbb{R}^r$, $I_d \in \mathbb{R}^{d\times d}$ the identity matrix and $\otimes$ the usual Kronecker tensor product. $\widetilde{V}$ has simple eigenvalues, all lying on the unit circle for zero-stability requirements [4, 28];

- a *finishing* procedure
$$F_h : \mathbb{R}^{rd} \to \mathbb{R}^d,$$
projecting the vector $y^{[n]}$ into the numerical solution $y_n \approx y(t_n)$.

It was proved in [24] that, for any given forward and finishing procedures, there exist a unique starting procedure and a unique one-step method

$$y_{n+1} = \varphi_h(y_n),$$

such that

$$G_h \circ S_h = S_h \circ \varphi_h,$$

with $F_h \circ S_h$ equal to the identity map. Such a formal one-step map φ_h is called *underlying one-step method*. In other terms, the numerical solution obtained by the multivalue

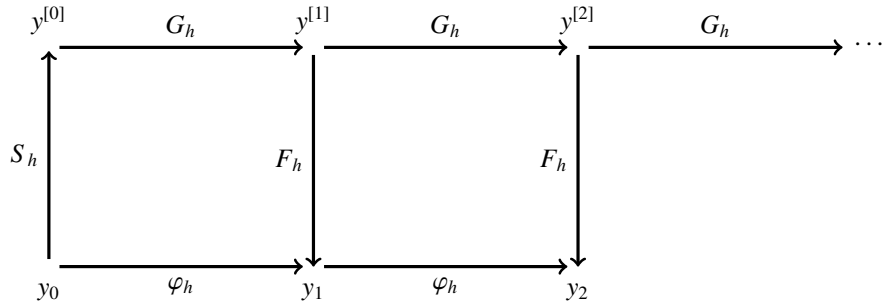

Figure 1: Dynamics of a multivalue numerical method

method is (formally) equal to that of the one-step method φ_h; this issue makes relevant anaylizing the underlying one-step method in order to infer meaningful properties of the forward map.

Multivalue methods are usually represented in the form of General Linear Methods (GLMs, compare [4, 17, 28] and references therein)

$$\begin{cases} Y^{[n]} = hAF^{[n]} + Uy^{[n]}, \\ y^{[n+1]} = hBF^{[n]} + Vy^{[n]}, \end{cases} \tag{2.5}$$

that is an extended Runge-Kutta formulation giving a practical scheme to compute the updated vector $y^{[n+1]}$, given $y^{[n]}$ and the vector of internal stages $Y^{[n]} \in \mathbb{R}^{sd}$, where $Y_i^{[n]}$ approximates the solution to (2.2) in the internal point $t_n + c_i h \in [t_n, t_{n+1}]$, $i = 1, 2, \ldots, s$, with c_i usually belonging to the interval $[0, 1]$. $F^{[n]} \in \mathbb{R}^{sd}$ denotes the supervector

$$F^{[n]} = \begin{bmatrix} f(Y_1^{[n]}) \\ f(Y_2^{[n]}) \\ \vdots \\ f(Y_s^{[n]}) \end{bmatrix} \in \mathbb{R}^{sd}.$$

The matrices $A \in \mathbb{R}^{sd\times sd}$, $U \in \mathbb{R}^{sd\times rd}$, $B \in \mathbb{R}^{rd\times sd}$, $V \in \mathbb{R}^{rd\times rd}$ are usually collected in the Butcher tableau

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

When $r = 1$ and the Butcher tableau reduces to

$$\left[\begin{array}{c|c} A & e \otimes I_d \\ \hline b^{\intercal} \otimes I_d & I_d \end{array}\right],$$

being e the unitary vector in $\mathbb{R}^s$, the multivalue method (2.5) is then equivalent to the Runge-Kutta method

$$\begin{cases} Y^{[n]} = hAF^{[n]} + (e \otimes I)y^{[n]}, \\ y^{[n+1]} = h(b^{\intercal} \otimes I)F^{[n]} + y^{[n]}. \end{cases} \tag{2.6}$$

3. Analysis of parasitism

A full backward error analysis for multivalue numerical methods has been given in [18]. It relies on the following ansatz

$$\widehat{y}^{[n]} = Y(t_n) + \sum_{j=2}^{r} \xi_j^n Z_j(t_n), \tag{3.1}$$

where $\widehat{y}^{[n]}$ is an approximation to $y^{[n]}$. In (3.1), a clear separation between the smooth part $Y(t_n)$ and the parasitic ones $Z_j(t_n)$, related to the point t_n, are made visible. The functions $Y(t)$ and $Z_j(t)$ are independent on n, but depend smoothly on the stepsize h. The scalars $\xi_1 = 1, \xi_2, \ldots, \xi_r$ are the eigenvalues of the matrix $\widetilde{V}$ in (2.4), which are supposed to be simple and located on the unit circle for zero-stability requirements [4, 28], as aforementioned. In this representation, we are tacitly assuming that the component $\widehat{y}_1^{[n]}$ approximates the solution to (2.2) in t_n. The ansatz (3.1) is useful in several situations, such as the analysis of the long-term behavior of linear multistep methods [25, 26] and in the study of the long-time behavior of analytic and numerical solutions to highly oscillatory problems by modulated Fourier expansions [27].

In the remainder of the treatise, we will always assume that $r = 2$ and the matrix $\widetilde{V}$ of the form

$$\widetilde{V} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{3.2}$$

Then, the ansatz (3.1) reads

$$\widehat{y}^{[n]} = Y(t_n) + (-1)^n Z(t_n). \tag{3.3}$$

By denoting with v_j and v_j^* the right and left eigenvectors of V (i.e, $Vv_j = \xi_j v_j$ and $v_j^* V = \xi_j v_j^*$) satisfying $v_j^* v_j = 1$, we write $Y(t)$ and $Z(t)$ in terms of the basis of eigenvectors of V, i.e.

$$Y(t) = y_1(t)v_1 + y_2(t)v_2, \qquad Z(t) = z_1(t)v_1 + z_2(t)v_2. \tag{3.4}$$

This representation is useful to get an amenable form of the so-called *modified differential equations*, given by the following theorem [18].

Theorem 3.1. *For a given multivalue method, represented in the GLM form* (2.5) *with* $r = 2$*, whose matrix* V *assumes the form* (3.2)*, there exist* h*-independent real functions* $f_\ell(y_1)$ *and complex functions* $g_\ell(y_1), a_\ell(y_1)$ *and* $b_\ell(y_1)$*, such that for an arbitrarily chosen truncation index* N *and any solution* $y_k(t), z_k(t)$*,* $k = 1, 2$*, of the system*

$$\begin{aligned} \dot{y}_1 &= f(y_1) + h\, f_1(y_1) + \ldots + h^{N-1} f_{N-1}(y_1), \\ y_2 &= h\, g_1(y_1) + \ldots + h^N g_N(y_1), \\ \dot{z}_1 &= (a_0(y_1) + h\, a_1(y_1) + \ldots + h^{N-1} a_{N-1}(y_1))z_1, \\ z_2 &= (h\, b_1(y_1) + \ldots + h^N b_N(y_1))z_1, \end{aligned} \tag{3.5}$$

the approximation (3.3) satisfy (2.3) *with a small defect, i.e.,*

$$\widehat{y}^{[n+1]} = V\widehat{y}^{[n]} + h\,\Phi(h, \widehat{y}^{[n]}) + O(h^{N+1}) + O(h\|Z\|^2),$$

with $\|Z\| = \max\{|z_1(t_n)|,\ |z_2(t_n)|\}$*, as long as* $y_1(t_n)$ *lies in a compact set.*

A complete proof of this result, for any arbitrary value of r, is given in [18]. We now aim to provide an analysis of the parasitic components in order to translate their boundedness into algebraic conditions on the coefficients of (2.5).

According to Theorem 3.1,

$$\begin{aligned} Y(t_n + h) + (-1)^n Z(t_n + h) = {} & V\,(Y(t_n) + (-1)^n Z(t_n)) \\ & + h\,\Phi\,(h, Y(t_n) + (-1)^n Z(t_n)) + O(h^{N+1}) + O(h\|Z\|^2), \end{aligned}$$

i.e., by Taylor series arguments expansion of Φ around $Y(t)$,

$$\begin{aligned} Y(t_n + h) + (-1)^{n+1} Z(t_n + h) = {} & V\,(Y(t_n) + (-1)^n Z(t_n)) + h\,\Phi\,(h, Y(t_n)) \\ & + (-1)^n h\,\Phi'\,(h, Y(t_n))\,Z(t) + O(h^{N+1}) + O(h\|Z\|^2). \end{aligned}$$

Isolating the parasitic part leads to

$$Z(t_n + h) = -VZ(t_n) - h\,\Phi'\,(h, Y(t_n))\,Z(t) + O(h^{N+1}) + O(h\|Z\|^2).$$

Assuming the form of the increment arising from the GLM formulation (2.5), we have

$$\Phi\,(h, Y(t_n)) = Bf\left(UY(t_n) + hAf(Y^{[n]})\right)$$

and expanding the inner evaluation of f around $UY(t_n)$ leads to

$$\Phi\,(h, Y(t_n)) = Bf\left(UY(t_n) + hAf(UY(t_n)) + h^2 f'(UY(t_n))Af(UY(t_n))\right) + O(h^3)$$

and expanding the outer evaluation of f around $UY(t_n)$ yields

$$\begin{aligned} \Phi\,(h, Y(t_n)) = B\Big(& f\,(UY(t_n)) + hf'\,(UY(t_n))\,Af(UY(t_n)) \\ & + h^2 f'\,(UY(t_n))\,f'(UY(t_n))Af(UY(t_n))\Big) + O(h^3). \end{aligned}$$

As a consequence,

$$\begin{aligned} h\Phi'\,(h, Y(t_n)) = {} & hBf'\,(UY(t_n))\,U + h^2 Bf''\,(UY(t_n))\,(U, Af(UY(t_n))) \\ & + h^2 Bf'\,(UY(t_n))\,Af'\,(UY(t_n))\,U + O(h^3). \end{aligned}$$

Then,

$$Z(t_n) + h\dot{Z}(t_n) + \frac{h^2}{2}\ddot{Z}(t_n) = -VZ(t_n) - h\Lambda Z(t_n) - h^2\Gamma Z(t_n) + O(h^3) + O(h\|Z\|^2). \tag{3.6}$$

with

$$\Lambda = Bf'\,(UY(t_n))\,U \tag{3.7}$$

and

$$\Gamma = Bf''\left(UY(t_n)\right)\left(U, Af(UY(t_n))\right) + Bf'\left(UY(t_n)\right)Af'\left(UY(t_n)\right)U. \tag{3.8}$$

Let us focus on the second component $Z_2(t_n)$, taking into account that $Z_1(t_n) = O(h^2)$. We obtain from (3.6) that

$$h\dot{z}_2(t_n) + \frac{h^2}{2}\ddot{z}_2(t_n) = -h\lambda_{22}z_2(t_n) - h^2\gamma_{22}z_2(t_n) + O(h^3) + O(h\|Z\|^2). \tag{3.9}$$

The coefficient of λ_{22}, appearing in (3.9) as elementary differential associated to the second order rooted tree $[\tau]$, is the so-called *linear growth parameter* (see [7, 15, 18]) and it is responsible of the boundedness of parasitic components as designed so far in the existing literature. Standard computations yields λ_{22} annihilated if

$$v_2^{\intercal}BUv_2 = 0. \tag{3.10}$$

Then, we give the following definition.

Definition 3.1. *A given multivalue method, represented in the GLM form* (2.5) *with* $r = 2$*, whose matrix V assumes the form* (3.2)*, is first order parasitic if* (3.10) *holds true.*

However, as proved in [18], having $\lambda_{22} = 0$ only guarantees to have bounded parasitic components on intervals of length at most $O(h^{-2})$. As observable from [18], if $\lambda_{22} = 0$, then $\ddot{z}_2(t_n) = O(h)$ and (3.9) becomes

$$\dot{z}_2(t_n) = -h\gamma_{22}z_2(t_n) + O(h^2) + O(\|Z\|^2). \tag{3.11}$$

We now aim to annihilate also γ_{22} in order to have a more limited parasitic behaviour over longer time windows than that achievable with first order parasitic methods. Standard computations yields γ_{22} annihilated if the coefficients of the elementary differentials associated to the third order rooted trees $[[\tau]]$ and $[\tau^2]$ are zero, i.e. if the following conditions hold true

$$v_2^{\intercal}BAUv_2 = 0, \qquad v_2^{\intercal}B(Ae \cdot Uv_2) = 0, \tag{3.12}$$

where $\cdot$ denotes componentwise vector multiplication. Then, we give the following definition.

Definition 3.2. *A given multivalue method, represented in the GLM form* (2.5) *with* $r = 2$*, whose matrix V assumes the form* (3.2)*, is second order parasitic if both conditions in* (3.12) *hold true.*

4. Construction of methods

We now focus our attention on the developments of first and second order parasitic methods, represented in the GLM form

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{c|c} \widetilde{A}\otimes I & \widetilde{U}\otimes I \\ \hline \widetilde{B}\otimes I & \widetilde{V}\otimes I \end{array}\right],$$

with $r = 2$, $s = 2$ and

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & 1 & u_{12} \\ a_{21} & a_{22} & 1 & u_{22} \\ \hline b_{11} & b_{12} & 1 & 0 \\ b_{21} & b_{22} & 0 & -1 \end{array}\right].$$

In the remainder of the treatise we assume that the vector of the updates $y^{[n]}$ has the so-called Nordsieck form [28]

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(t_n) \\ hy'(t_n) \end{bmatrix}. \tag{4.1}$$

Due to the form (3.2) of the matrix V, the methods are automatically zero-stable, then they are convergent if they fulfill the preconsistency and consistency requirements [4, 28]

$$U \begin{bmatrix} 1 \\ 0 \end{bmatrix} = e, \quad Be + V \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{4.2}$$

Then, the first column of U is the unit vector in $\mathbb{R}^s$, while the condition on B leads to

$$b_{11} + b_{12} = 1, \quad b_{21} + b_{22} = 2.$$

Correspondingly, the family of two-stage and two-value methods in the GLM form (2.5), is first order parasitic if their Butcher tableau assumes the form

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & 1 & u_{12} \\ a_{21} & a_{22} & 1 & u_{22} \\ \hline 1 - b_{12} & b_{12} & 1 & 0 \\ -\dfrac{2u_{22}}{u_{12} - u_{22}} & \dfrac{2u_{12}}{u_{12} - u_{22}} & 0 & -1 \end{array}\right]$$

while it is second order parasitic if

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & -\dfrac{u_{12}(a_{11} - a_{22})}{u_{12} + u_{22}} & 1 & u_{12} \\ \dfrac{u_{22}(a_{11} - a_{22})}{u_{12} + u_{22}} & a_{22} & 1 & u_{22} \\ \hline 1 - b_{12} & b_{12} & 1 & 0 \\ -\dfrac{2u_{22}}{u_{12} - u_{22}} & \dfrac{2u_{12}}{u_{12} - u_{22}} & 0 & -1 \end{array}\right].$$

According to [4, 28], together with the above discussed minimal requirements of accuracy and stability, we enforce our methods to attain order 2 of convergence, by imposing the condition

$$\begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix} - B(A + I)e = 0,$$

where I is the identity matrix of dimension s. Then, the family of two-stage and two-value second order methods (2.5), is a class of first order parasitic formulae if their Butcher tableau depends on

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} \dfrac{u_{22}-u_{12}+2a_{21}u_{12}-2a_{12}u_{22}+2a_{22}u_{12}}{2u_{22}} & a_{12} & 1 & u_{12} \\ a_{21} & a_{22} & 1 & u_{22} \\ \hline -\dfrac{u_{22}}{u_{12}-u_{22}} & \dfrac{u_{12}}{u_{12}-u_{22}} & 1 & 0 \\ -\dfrac{2u_{22}}{u_{12}-u_{22}} & \dfrac{2u_{12}}{u_{12}-u_{22}} & 0 & -1 \end{array}\right],$$

while it is second order parasitic if

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} \dfrac{u_{12}+u_{22}-2a_{22}u_{12}}{2u_{22}} & \dfrac{u_{12}(2a_{22}-1)}{2u_{22}} & 1 & u_{12} \\ 1/2-a_{22} & a_{22} & 1 & u_{22} \\ \hline -\dfrac{u_{22}}{u_{12}-u_{22}} & \dfrac{u_{12}}{u_{12}-u_{22}} & 1 & 0 \\ -\dfrac{2u_{22}}{u_{12}-u_{22}} & \dfrac{2u_{12}}{u_{12}-u_{22}} & 0 & -1 \end{array}\right].$$

Two examples of methods falling in the aforementioned classes are given by

- `GLM1`

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} 19/30 & -1/3 & 1 & 1/2 \\ 1/5 & 1/2 & 1 & -1/2 \\ \hline 1/2 & 1/2 & 1 & 0 \\ 1 & 1 & 0 & -1 \end{array}\right].$$

  that is first order parasitic and of order 2;

- `GLM2`

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} 19/50 & 3/25 & 1 & 1/5 \\ 3/10 & 1/5 & 1 & -1/2 \\ \hline 5/7 & 2/7 & 1 & 0 \\ 10/7 & 4/7 & 0 & -1 \end{array}\right].$$

  that is second order parasitic and of order 2.

5. Numerical evidence

We now aim to show the results of selected numerical experiments, in order to highlight the features of `GLM1` and `GLM2` methods provided in the previous section,

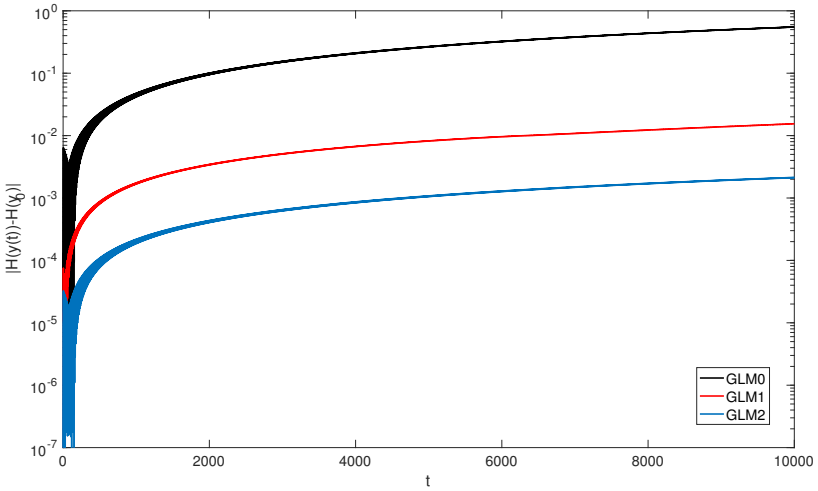

Figure 2: Pattern of the Hamiltonian deviation for the multivalue methods `GLM0` (top), `GLM1` (middle) and `GLM2` (bottom) applied to the simple pendulum, with Hamiltonian function (5.1), in a fixed stepsize environment of steplength $h = 0.05$.

when applied to given Hamiltonian problems. Both methods are also compared with the following multivalue method (see [28])

$$\left[\begin{array}{c|c} \widetilde{A} & \widetilde{U} \\ \hline \widetilde{B} & \widetilde{V} \end{array}\right] = \left[\begin{array}{cc|cc} 19/50 & 3/25 & 1 & 1/5 \\ 3/10 & 1/5 & 1 & -1/2 \\ \hline 5/7 & 2/7 & 1 & 0 \\ 10/7 & 4/7 & 0 & -1 \end{array}\right],$$

denoted in the remainder as `GLM0`, whose parasitism has not been bounded in any way. All the experiments are carried out in a fixed stepsize environment in the time interval [0,10000], with stepsize specified on the case by case basis.

We first consider the standard mathematical pendulum [24], depending on the Hamiltonian function

$$\mathcal{H}(y) = \frac{y_1^2}{2} - \cos(y_2), \tag{5.1}$$

with initial value $y(0) = [0 \;\; 3]^{\intercal}$. Figure 2 shows the pattern of the Hamiltonian deviation in time, computed by the multivalue methods `GLM0`, `GLM1` and `GLM2` with stepsize $h = 0.05$. It is visible that the parasitic components, though growing in each case, are more bounded the more the parasitic order is higher. Without any parasitic order, as in the case of `GLM0`, the corresponding method does not guarantee any long-term conservation.

We next consider the following modified pendulum [24], depending on the Hamiltonian function

$$\mathcal{H}(y) = \frac{y_1^2}{2} - \cos(y_2) + \frac{1}{5}\sin(2y_2), \tag{5.2}$$

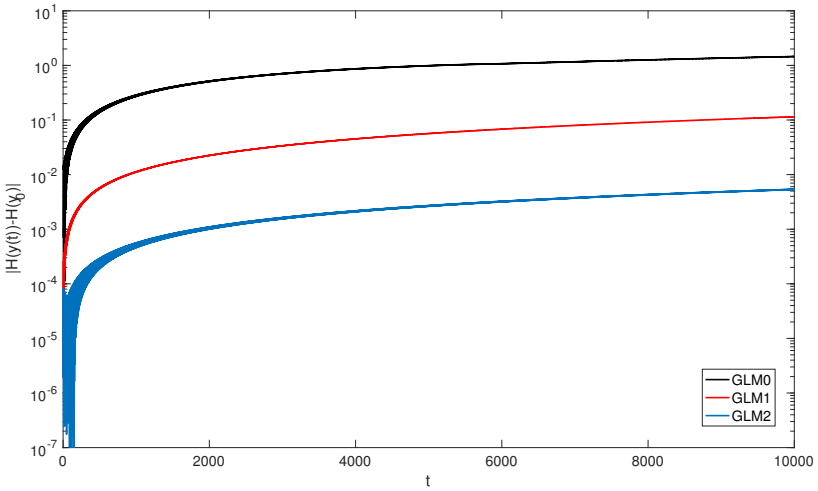

Figure 3: Pattern of the Hamiltonian deviation for the multivalue methods `GLM0` (top), `GLM1` (middle) and `GLM2` (bottom) applied to the modified pendulum, with Hamiltonian function (5.2), in a fixed stepsize environment of steplength $h = 0.05$.

with initial value $y(0) = [2.5 \;\; 0]^{\intercal}$. The pattern of the Hamiltonian deviation, displayed in Figure 3, has essentially the same behaviour as in the previous case, confirming a better performance for the higher parasitic order method. Also in this case, the employed stepsize is $h = 0.05$.

We finally aim to provide a comparison between `GLM1` and `GLM2`, in order to check if the second parasitic order method maintains the parasitic components bounded over longer time intervals than `GLM1`. To this purpose, we consider a non-reversible problem [21], depending on the following Hamiltonian function

$$\mathcal{H}(y) = \frac{y_1^3}{3} - \frac{y_1}{2} + \frac{y_2^6}{30} + \frac{y_2^4}{4} - \frac{y_2^3}{3} + \frac{1}{6}, \tag{5.3}$$

with initial value $y(0) = [1 \;\; 0]^{\intercal}$. From the numerical evidence, depicted in Figure 4, it is visible that the parasitic components generated by `GLM1` blow up more rapidly than those associated to `GLM2`.

6. Concluding remarks

We have focused our attention on the ability of multivalue numerical methods to act as geometric numerical integrators for Hamiltonian problems. In particular, we have provided conditions on the coefficients of the method in such a way that the corresponding methods have more bounded parasitic components, with respect to other cases known in the literature. The analysis of parasitism as well as the development of the corresponding methods have been given and their effectiveness confirmed on

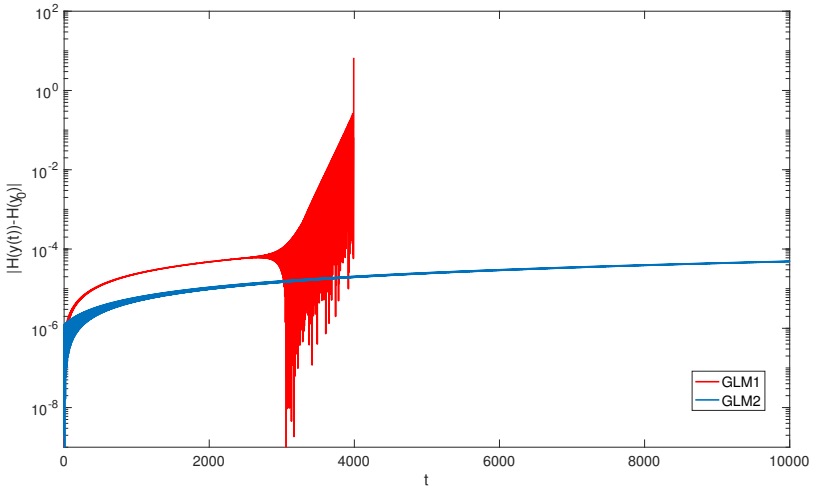

Figure 4: Pattern of the Hamiltonian deviation for the multivalue methods `GLM1` (top) and `GLM2` (bottom) applied to the non-reversible problem with Hamiltonian function (5.3), in a fixed stepsize environment of steplength $h = 0.01$.

selected Hamiltonian problems. Future developments of this research will be oriented to merging higher order parasitism and symmetry, in order to have large intervals in which parasitic components remain properly bounded, as well as to applying these ideas to discrezation of other deterministic and stochastic evolutionary operators [2, 3, 9, 10, 11, 12, 16, 20].

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