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Numerical integration of Hamiltonian problems by G-symplectic methods

Raffaele D'Ambrosio · Giuseppe De Martino · Beatrice Paternoster

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Abstract It is the purpose of this paper to consider the employ of General Linear Methods (GLMs) as geometric numerical solvers for the treatment of Hamiltonian problems. Indeed, even if the numerical flow generated by a GLM cannot be symplectic, we exploit here a concept of near conservation for such methods which, properly combined with other desirable features (such as symmetry and boundedness of parasitic components), allows to achieve an accurate conservation of the Hamiltonian. In this paper we focus our attention on the connection between order of convergence and Hamiltonian deviation by multivalue methods. Moreover, we derive a semi-implicit GLM which results competitive to symplectic Runge-Kutta methods, which are notoriously implicit.

Keywords Hamiltonian problems · Geometric Numerical Integration · General Linear Methods · B-series methods · Symmetric methods · G-Symplectic methods

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R. D'Ambrosio
Department of Mathematics
University of Salerno
via Giovanni Paolo II, 132 - 84084 Fisciano (Sa), Italy
Tel.: +39089968246
Fax: +39089963303
E-mail: rdambrosio@unisa.it

G. De Martino
Department of Mathematics
University of Salerno
via Giovanni Paolo II, 132 - 84084 Fisciano (Sa), Italy
E-mail: gdemartino@unisa.it

B. Paternoster
Department of Mathematics
University of Salerno
via Giovanni Paolo II, 132 - 84084 Fisciano (Sa), Italy
E-mail: beapat@unisa.it

1 Introduction

The purpose of this paper is the analysis and practical development of multivalue numerical methods exhibiting a nearly conservative behaviour when applied to Hamiltonian problems

$$\begin{aligned} \dot{p}(t) &= -\frac{\partial}{\partial q}\mathcal{H}(p(t),q(t)), \\ \dot{q}(t) &= \frac{\partial}{\partial p}\mathcal{H}(p(t),q(t)), \end{aligned} \tag{1}$$

where $\mathcal{H}:\mathbb{R}^{2d}\to\mathbb{R}$ is the Hamiltonian of the system, $p(t),q(t)\in\mathbb{R}^d$ are generalized momenta and coordinates, respectively. The existing literature regarding the numerical approach to such problems has focused its interest on the employ of symplectic Runge-Kutta (RK) methods [7,28, 32,35], i.e. methods which are meant to numerically maintain quadratic invariants possessed by the continuous problem. However, even though symplectic RK methods accurately preserve such invariants, they have the limit of being implicit, thus they require a remarkable computational effort in the integration process. We overcome this limit by employing, for instance, semi-implicit numerical methods which are able to nearly preserve the invariants of the Hamiltonian problem with a lower computational cost. The spirit of this paper is that of deriving diagonally implicit methods belonging to the family of General Linear Methods (GLMs, compare [6,7,18,30] and references therein)

$$\begin{cases} Y_i^{[n]} = h\sum_{j=1}^{s} a_{ij}F_j^{[n]} + \sum_{j=1}^{r} u_{ij}y_j^{[n]}, \quad i=1,2,\dots,s, \\ y_i^{[n+1]} = h\sum_{j=1}^{s} b_{ij}F_j^{[n]} + \sum_{j=1}^{r} v_{ij}y_j^{[n]}, \; i=1,2,\dots,r, \end{cases} \tag{2}$$

designed for the solution of the first order initial value problems

$$\begin{cases} y'(t) = f(y(t)), \quad t\in[t_0,T], \\ y(t_0) = y_0, \end{cases} \tag{3}$$

where $f:\mathbb{R}^d\to X$, being $(X,<\cdot,\cdot>)$ an inner product space. The formulation (2) is provided in correspondence of the uniform grid $\{t_0+ih, i=0,1,\dots,N\}$, with $h=(T-t_0)/N$. The vector $y^{[n]}=[y_1^{[n]},\dots,y_r^{[n]}]^\intercal$ 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 $t_n+c_ih\in[t_n,t_{n+1}]$, $i=1,2,\dots,s$, 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

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

The paper is organized as follows. Section 2 provides a discussion of the desired properties that a nearly conservative GLM for (1) has to fulfill, such as symmetry, G-symplecticity and boundedness of parasitic components in the numerical solution. Section 3 is devoted to the analysis of the level of accuracy which can be gained by a B-series method; this analysis is then applied to the case of GLMs with bounded parasitic components. Section 4 shows the practical construction of a diagonally implicit and nearly conservative GLM of order 4, by employing the algebraic theory of order reported in [7]. Numerical experiments confirming the effectiveness of this method are presented in Section 5, also in comparison with existing symplectic solvers. Some conclusions of this research are reported in Section 6.

2 G-Symplecticity, Symmetry and parasitism of General Linear Methods

A widely used approach in numerically preserving quadratic invariants of Hamiltonian problems consists in using symplectic (or canonical) RK methods

$$\begin{cases} Y_i = y_n + h \sum_{j=1}^{s} a_{ij} F_j \quad i = 1, 2, \ldots, s, \\ y_{n+1} = y_n + h \sum_{i=1}^{s} b_i F_i, \end{cases}$$

whose coefficients $A = (a_{ij})_{i,j=1}^{s}$, $b = (b_i)_{i=1}^{s}$ satisfy the algebraic constraint [2–4,11,31,35,36]

$$M = \mathrm{diag}(b)A + A^{\intercal}\mathrm{diag}(b) - bb^{\intercal} = 0, \tag{4}$$

where $\mathrm{diag}(x)$ denotes the diagonal matrix having the vector x on the diagonal.

It is worth observing that the matrix M in (4) is directly involved in the nonlinear stability properties of a RK method, as the method is algebraically stable if and only if M is non-negative definite and the weights b_i are all positive. (see, for instance, [7]).

Symplecticity is a prerogative of RK methods: in fact, Tang proved in [37] that linear multistep methods cannot be symplectic, while Butcher and Hewitt [10] proved the following result in the context of GLMs.

Theorem 1 *A zero-stable, irreducible GLM* (2) *with* $r > 1$ *is not symplectic.*

In other words, GLMs cannot be symplectic, unless they reduce to RK methods (for the formal notions of reducibility for GLMs see [5]). However, following the lines drawn for RK methods, i.e. by annihilating the nonlinear stability matrix of a GLM (compare [14,20,30] and references therein, also for collocation-based methods [15,19,21–23])

$$\mathbf{M} = \left[\begin{array}{c|c} DA + A^{\intercal}D - B^{\intercal}GB & DU - B^{\intercal}GV \\ \hline U^{\intercal}D - V^{\intercal}GB & G - V^{\intercal}GV \end{array}\right], \tag{5}$$

a useful property in the context of geometric numerical integration arises, leading to the concept of G-symplecticity. This property, introduced by Butcher in [7] and further investigated in [8, 25], is defined as follows.

Definition 1 A GLM (2) is G-symplectic if there exist a positive semi-definite symmetric $r \times r$ matrix G and an $s \times s$ diagonal matrix D such that

$$\begin{aligned} &G = V^{\intercal}GV, \\ &DU = B^{\intercal}GV, \\ &DA + A^{\intercal}D = B^{\intercal}GB. \end{aligned} \tag{6}$$

2.1 What does a G-symplectic methods preserve?

Since a GLM (2) with $r > 1$ cannot be symplectic [10], we now aim to discuss what is the role of G-symplecticity in the numerical conservation of invariants. To this purpose, let us suppose that the quadratic form

$$< y(t), Qy(t) >, \tag{7}$$

with Q symmetric matrix, is invariant along the solution of problem (3). If we approximate the solution by a RK method, for the corresponding numerical counterpart

$$< y_n, Qy_n >$$

the following identity holds (compare [2])

$$< y_n, Qy_n >=< y_{n-1}, Qy_{n-1} > +2h \sum_{i=1}^{s} b_i < f(Y_i), QY_i > -h^2 \sum_{i,j=1}^{s} m_{ij} < f(Y_i), Qf(Y_j) >,$$

with $m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$. If the inner product $< y(t), Qy(t) >$ is preserved along the solution of (3), then $< f(y(t)), Qy(t) >= 0$, and the above identity reduces to

$$< y_n, Qy_n >=< y_{n-1}, Qy_{n-1} > -h^2 \sum_{i,j=1}^{s} m_{ij} < f(Y_i), Qf(Y_j) > .$$

Thus, if the employed RK method is symplectic, the second summand in the right-hand side annihilates and

$$< y_n, Qy_n >=< y_{n-1}, Qy_{n-1} >,$$

i.e. the numerical approximation of the quadratic form (7) by a symplectic RK method is preserved along the numerical solution.

We now turn our attention to GLMs. In correspondence to a symmetric matrix $G \in \mathbb{R}^{r\times r}$, we define the G-inner product

$$< y, z >_G = \sum_{i,j=1}^{r} g_{ij} < y_i, z_j > .$$

Similarly as in the RK case, an analog identity holds for GLMs

$$\begin{aligned} < y^{[n]}, Qy^{[n]} >_G =& < y^{[n-1]}, Qy^{[n-1]} >_G - \sum_{i,j=1}^{r} (G - V^{\intercal} G V)_{ij} < y_i^{[n-1]}, y_j^{[n-1]} > \\ & - 2 \sum_{i=1}^{s} \sum_{j=1}^{r} (DU - B^{\intercal} G V)_{ij} < y_i^{[n-1]}, hF_j^{[n-1]} > \\ & - \sum_{i,j=1}^{s} (DA + A^{\intercal} D - B^{\intercal} G B)_{ij} < hF_i^{[n-1]}, hF_j^{[n-1]} > . \end{aligned}$$

Thus, for a G-symplectic GLM, the above identity reduces to

$$< y^{[n]}, Qy^{[n]} >_G =< y^{[n-1]}, Qy^{[n-1]} >_G .$$

It is evident from the above analysis that a G-symplectic GLM does not provide the conservation of the quadratic form (7) in the same inner product of the space X where the solution of (3) is valued, but the numerical quadratic invariant is given in the sense of the G-inner product. This is strictly connected to the multivalue nature of GLMs (compare [8]). However, even if we have no hope to numerically maintain the form (7) by G-symplectic GLMs, we can still hope to nearly conserve it, as it will be discussed in the remainder of this paper.

2.2 Symmetry

For conservative mechanical systems and, in particular, Hamiltonian systems, a property of time reversibility holds: this means that, by reversing the direction of the flow, the invariants are still preserved. Thus, a desirable property for numerical methods applied to such problems is that of providing a reversible numerical flow. In the context of RK methods, this property is related to that of symmetry, i.e. that of coincidence between the numerical method and its adjoint [28]. A concept of symmetry for GLMs has been defined in [25,28] as follows.

Theorem 2 *Let $L \in \mathbb{R}^{r\times r}$ be an involution matrix and $P \in \mathbb{R}^{s\times s}$ a permutation matrix. If the method* (2) *satisfies*

$$\begin{aligned} &P^{-1}AP = UV^{-1}B - A, && P^{-1}UL = UV^{-1},\\ &L^{-1}BP = B, && L^{-1}VL = V^{-1}, \end{aligned} \tag{8}$$

then it is symmetric.

The importance of symmetry not only lays in its relation with reversibility of the invariants, but also in its strict connection to the order of the method: in fact, a symmetric method has even order (see [28] for RK methods and [25] for GLMs). This provides a remarkable constructive advantage since, for symmetric methods, the only order conditions to be imposed are those related to odd order trees.

2.3 Parasitism

It is known from the literature (compare [8,28]) that the long-term behaviour of multistep and/or multivalue methods is corrupted by parasitic components introduced in the numerical solution. The presence of these components is mainly due to the fact that such methods are notoriously not self-starting, thus they require the employ of starting procedures to recover the missing initial values.

Hairer et al. (compare [28] and references therein) analyzed this phenomenon for multistep methods. This study subsequently led them to retain that the numerical solution of a GLM admits the representation (compare [28], §XV.8.3)

$$y^{[n]} = \tilde{y}(t_n) + \sum_{\ell\in I^*} \zeta_\ell^n z_\ell(t_n),$$

where $\tilde{y}(t)$, $z(t)$ are smooth functions and I^* is an index set (see [27]). In this representation, the numerical solution is expressed as summation of two terms: the first summand is the exact solution of the associated modified equation (compare [26,27]), while the second one is the actual parasitic part of the numerical solution. Such a parasitic part is equal to zero for canonical Runge–Kutta methods, while it does not annihilate for non-symplectic methods and it is responsible of their non-conservative behaviour. Maintaining such parasitic terms bounded is then the first necessary task for the derivation of multistep or multivalue methods with a reliable long-term behaviour (compare [8,17,25,28]).

Butcher (compare [8] and references therein) proposes two different approaches for the control of the parasitic components. The first one, for GLMs with $r = 2$ and $V = \mathrm{diag}(1,-1)$, assures the boundedness of the parasitic components by imposing an algebraic constraint on the coefficients of the method, i.e. $\mu = (BU)_{22} = 0$. In the second approach, a reduction of the effects of parasitism is obtained by composing two G-symplectic methods N and P, both having $\mu \neq 0$:

the numerical scheme computes m steps of the method N and one single step of P, in such a way that, after $m+1$ steps, the sum of the scaled values of μ is exactly cancelled.

We now extend the result reported in [8] (also compare [25]), connected to the first approach by Butcher above discussed, by providing a general algebraic constraint on the coefficients of a GLM in order to make the parasitic components in the numerical approximation bounded. In the following, we will always denote by $\dot{X}$, the matrix obtained by removing the first row and the first column of X.

Theorem 3 *The parasitic components of a GLM* (2) *are bounded if* $\dot{V}$ *is power-bounded and* $\dot{B}\dot{U}$ *is the zero matrix.*

Proof We assume, without loss of generality, that the first component of the vector $y^{[n]}$ is an approximation to $y(t_n)$. Then, we introduce on the external approximation $y_i^{[n]}$, $i=2,\dots,r$, the perturbation $(-1)^n\lambda_i^{[n]}$ and analyze how it propagates along the overall numerical scheme.

We first analyze the influence of the propagations on the internal stages

$$Y_i+\delta Y_i = h\sum_{j=1}^{s} a_{ij}F_j^{[n]} + u_{i1}y_1^{[n]} + \sum_{j=2}^{r} u_{ij}\left(y_j^{[n]}+(-1)^n\lambda_j^{[n]}\right),$$

obtaining

$$\delta Y_i = (-1)^n\sum_{j=2}^{r} u_{ij}\lambda_j^{[n]}.$$

Similarly, for the stage derivatives F_i

$$F_i+\delta F_i = f(Y_i+\delta Y_i) \approx f(Y_i)+\delta Y_i\frac{\partial f}{\partial y},$$

we obtain

$$\delta F_i = \delta Y_i\frac{\partial f}{\partial y} = (-1)^n\sum_{j=2}^{r} u_{ij}\lambda_j^{[n]}\frac{\partial f}{\partial y}.$$

Thus, we get from (2) the difference equation

$$\lambda^{[n+1]} = -\dot{V}\lambda^{[n]} + h\dot{B}\dot{U}\frac{\partial f}{\partial y}\lambda^{[n]}, \tag{9}$$

where $\lambda=[\lambda_2,\dots,\lambda_r]^\intercal$. Due to the hypothesis, the solution of (9) is bounded and the result is given. □

As a consequence, GLMs (2) with $r=2$ produce bounded parasitic components if they satisfy the further constraint

$$\mu = \sum_{i=1}^{2} b_{2i}u_{i2} = 0, \tag{10}$$

that recovers the result obtained in [8,25].

3 Near conservation of invariants by B-series methods

B-series (compare [29] and references therein) are a powerful tool for the theoretical analysis and practical development of numerical methods for ODEs. We employ them to investigate the relation between order of convergence and accuracy of the invariants preservation for B-series methods, with the aim to analyze the behaviour of GLMs with bounded parasitic components.

3.1 B-series methods

A B-series $B(a, y)$ for (3) is a formal series [29]

$$B(a, y(x_1)) = a(\emptyset)y(x_0) + \sum_{\rho(t)\geq 1} \frac{h^{\rho(t)}}{\sigma(t)} a(t)F(t)(y(x_0)), \tag{11}$$

where, in correspondence to the set of rooted trees

$$T = \{\bullet, \quad \begin{smallmatrix}\bullet\\\bullet\end{smallmatrix}, \quad \begin{smallmatrix}&\bullet&\\\bullet&&\bullet\end{smallmatrix}, \quad \begin{smallmatrix}\bullet\\\bullet\\\bullet\end{smallmatrix}, \ldots\},$$

the functions ρ, σ, F and a are defined as follows [29]:

- $\rho(t)$ is the order of $t \in T$, i.e. the number of vertices of t;
- $\sigma(t)$ is the symmetry of $t \in T$, i.e. the cardinality of the symmetry group of t;
- $F(t)$ is the elementary differential of f corresponding to $t \in T$;
- $a(t)$ is the coefficient of the series corresponding to the tree $t \in T$.

It is possible to prove [7,29] that the Taylor series of the exact solution of (3) is the B-series with coefficients

$$a(t) = \frac{1}{\gamma(t)}, \quad t \in T,$$

where $\gamma(t)$ is the density of t (compare [7]). In analogous way, it is possible to show that, in many cases, a numerical approximation $y_1 = \Phi_h(y_0)$ can be written as a B-series: in this case the method is called B-series method. An important example of application of this theory is given by Runge-Kutta methods, for which the coefficients $a(t)$ are called elementary weights and are defined recursively from the coefficients of the method, compare [7,29].

Let us now consider the set of forests (compare [12] and references therein)

$$\mathcal{F} = \{\emptyset, \quad \bullet, \quad \bullet\,\bullet, \quad \begin{smallmatrix}\bullet\\\bullet\end{smallmatrix}, \quad \bullet\,\bullet\,\bullet, \quad \begin{smallmatrix}\bullet\\\bullet\end{smallmatrix}\bullet, \quad \begin{smallmatrix}&\bullet&\\\bullet&&\bullet\end{smallmatrix}, \quad \begin{smallmatrix}\bullet\\\bullet\\\bullet\end{smallmatrix}, \ldots\},$$

where a forest $u = t_1 \cdots t_n \in \mathcal{F}$ is given by the commutative juxtaposition of the rooted trees $t_1, \ldots, t_n$.

Definition 2 Given a forest $u \in \mathcal{F}$ and denoted with $\mathcal{D}$ the set $C^\infty(\mathbb{R}^n, \mathbb{R}^m)$, we define the following differential operator

$$X(u) : \mathcal{D} \to \mathcal{D},$$

$$g \mapsto X(u)[g] = g^{(k)}(F(t_1), \ldots, F(t_k)).$$

The role of the operator X is crucial in the theorem contained in the following section, together with the composition rule (compare [12])

$$g \circ B(a, y) = \sum_{u\in\mathcal{F}} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u)X(u)[g],$$

where $g \in \mathcal{D}$, and

$$\alpha(\emptyset) = 1, \qquad \alpha(t_1 \cdots t_n) = \prod_{i=1}^{n} a(t_i).$$

3.2 Accuracy of invariant conservation by non-parasitic B-series methods

The following theorem clarifies the role of the order of accuracy in the numerical conservation of the Hamiltonian of (1) by a B-series method with annihilated parasitic components, which is the case of Runge-Kutta methods. In the remainder of this section, with a slight abuse of notation, we denote the Hamiltonian of (1) by $\mathcal{H}(y(t))$, where

$$y(t) = \begin{bmatrix} p(t) \\ q(t) \end{bmatrix}.$$

Theorem 4 *Consider an Hamiltonian problem* (1) *whose Hamiltonian function* $\mathcal{H}$ *belongs to* $C^\infty(\mathbb{R}^{2d}, \mathbb{R})$ *and a B-series method* (11) *of order* p*, with coefficients* $b(t)$ *and annihilated parasitic components. Then,*

$$\mathcal{H}(y_1) = \mathcal{H}(y(t_0)) + O(h^{p+1}).$$

Proof We consider the action of the map $\mathcal{H}$ on the B-series of the exact solution $y(t_1)$ and the numerical one y_1, i.e.

$$\mathcal{H}(y(t_1)) = \mathcal{H}(y(t_0)) + \sum_{\rho(u)\geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)\,[\mathcal{H}], \tag{12}$$

$$\mathcal{H}(y_1) = \mathcal{H}(y(t_0)) + \sum_{\rho(u)\geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u)\,[\mathcal{H}]. \tag{13}$$

In (12), since the Hamiltonian is constant along the exact solution of (1), we have

$$\sum_{\rho(u)\geq 1} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)\,[\mathcal{H}] = 0.$$

Hence,

$$\sum_{1\leq\rho(u)\leq p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)\,[\mathcal{H}] = -\sum_{\rho(u)>p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)\,[\mathcal{H}]. \tag{14}$$

The method has order p, so $\alpha(u) = \beta(u)$ for all forests u such that $\rho(u) \leq p$. Then, combining (13), (14) and the hypothesis of parasitism absence, we obtain

$$\begin{aligned} \mathcal{H}(y_1) - \mathcal{H}(y(t_0)) &= \sum_{1\leq\rho(u)\leq p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u)\,[\mathcal{H}] + \sum_{\rho(u)>p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u)\,[\mathcal{H}] \\ &= -\sum_{\rho(u)>p} \frac{h^{\rho(u)}}{\sigma(u)} \alpha(u) X(u)\,[\mathcal{H}] + \sum_{\rho(u)>p} \frac{h^{\rho(u)}}{\sigma(u)} \beta(u) X(u)\,[\mathcal{H}] = O(h^{p+1}), \end{aligned} \tag{15}$$

that proves the statement. □

We observe that the hypothesis of being the method non-parasitic is crucial in the proof of Theorem 4, because we notice in (15) the absence of further terms corrupting the accuracy of the Hamiltonian conservation. In other words, if a B-series method has order p and its parasitic components are annihilated, then the Hamiltonian is preserved up to order p.

3.3 The case of GLMs with bounded parasitic components

Section 3.2 deals with the ideal case of B-series methods free from parasitism, which is actually not the case of GLMs with bounded parasitic components. We now aim to check up to which order the Hamiltonian of problem (1) is preserved by a GLM of order p with bounded parasitic components, i.e. we are interested in determining the integer value α such that

$$\|e_n^{\mathcal{H}}\| = O(h^{\alpha}), \tag{16}$$

where

$$e_n^{\mathcal{H}} = \mathcal{H}(p_n, q_n) - \mathcal{H}(p_0, q_0) \tag{17}$$

is the Hamiltonian deviation observed in the n-th step point.

In order to address this issue, we derive the following three-stage symmetric and non G-symplectic GLM (2) of order 4

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} -\frac{41}{150} & \frac{19}{50} & -\frac{11}{25} & 1 & \frac{1}{12} \\ \frac{83}{1100} & \frac{11}{25} & -\frac{17}{1100} & 1 & \frac{1}{12} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 1 & \frac{1}{12} \\ \hline \frac{11}{600} & \frac{289}{300} & \frac{11}{600} & 1 & \frac{1}{6} \\ \frac{1}{2} & -1 & \frac{1}{2} & 0 & -1 \end{array}\right] \tag{18}$$

with abscissa vector $c = \left[-\frac{1}{3}, \quad \frac{1}{2}, \quad \frac{4}{3}\right]^{\intercal}$ and having bounded parasitic components, because it satisfies the hypothesis of Theorem 3. We report in Tables 1 and 2 the numerical evidence obtained by comparing the observed values of α for the two-stage Gauss RK method (which is a symplectic and symmetric method of order 4), the three-stage Lobatto IIIA method (which is a symmetric method of order 4, but non-symplectic) and the GLM (18), when applied to the simple pendulum problem

$$\begin{cases} \dot{p}(t) = -\sin q(t), \quad t \in [0, 50] \\ \dot{q}(t) = p(t), \\ p(0) = 0, \quad q(0) = 2.3, \end{cases} \tag{19}$$

whose Hamiltonian exhibits the form

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

and the Hènon-Heiles Problem [28]

$$\begin{cases} \dot{p_1}(t) = -q_1(t)(1 + 2q_2(t)), \quad t \in [0, 50] \\ \dot{p_2}(t) = -(q_2(t) + q_1^2(t) - q_2^2(t)), \\ \dot{q_i}(t) = p_i(t), \quad i = 1, 2, \\ p_1(0) = \sqrt{0.3185}, \quad p_2(0) = q_1(0) = q_2(0) = 0, \end{cases} \tag{20}$$

with Hamiltonian

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

The result stated in Theorem 4 is confirmed by the numerical evidence in the case of Runge-Kutta methods, that are non-parasitic, i.e. α is equal to the order p of convergence of the

Table 1 Observed values of α in (16) for the simple pendulum problem (19)

	Gauss	Lobatto IIIA	Symmetric GLM
$h = 1/2^3$			
$h = 1/2^4$	4.0016	4.0015	3.2903
$h = 1/2^5$	4.0004	4.0004	3.0328
$h = 1/2^6$	4.0001	4.0001	2.9843
$h = 1/2^7$	4.0025	3.9991	2.9843
$h = 1/2^8$	4.0124	4.0414	2.9905

Table 2 Observed values of α in (16) for the Hènon-Heiles problem (20)

	Gauss	Lobatto IIIA	Symmetric GLM
$h = 1/2^3$			
$h = 1/2^4$	3.9978	3.9978	4.3132
$h = 1/2^5$	3.9995	3.9995	3.8951
$h = 1/2^6$	3.9998	3.9998	3.5158
$h = 1/2^7$	3.9996	4.0008	3.2666
$h = 1/2^8$	4.0033	4.0067	3.1322

methods. In the case of GLM (18), we notice that the observed value of α is no more equal to the order of convergence of the method, but it reduces to $\alpha = p - 1$, due to the fact that the parasitic components in the numerical solution are bounded but not completely removed, as suggested by Theorem 3. This problem is overcome in next section, by deriving a symmetric GLM with bounded parasitic components which is also G-symplectic, providing a cheap alternative to symplectic Runge-Kutta methods, without compromising the accuracy.

4 A nearly conservative GLM method of order 4

We now turn our attention to the construction of an order 4 symmetric and G-symplectic GLM, with bounded parasitic components which provides a valid alternative to symplectic methods in terms of accuracy of invariants preservation, but requiring a lower computational effort. In fact, semi-implicit symplectic RK methods mainly appear in partitioned pairs (compare [28,33] and references therein). It is known that a fourth order partioned method satisfying symmetry and symplecticity properties needs the employ of a pair of 6-stage RK methods, thus globally requiring 12 internal stages (compare [33]). We aim to derive a G-symplectic, symmetric order 4 method (2) which needs a lower number of internal stages, hence requiring a lower computational effort than the mentioned RK pair, but achieving a similar accuracy in the conservation of the Hamiltonian.

We observe that examples of G-symplectic methods (2) of order 2 and bounded parasitic components have already been derived in [17], with different structures of the matrix $\mathbf{A}$: in particular, we report here the following methods taken from [17], characterized by a diagonal matrix $\mathbf{A}$

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{ccc|cc} -\frac{1}{4} & 0 & 0 & 1 & -\frac{1}{4} \\ 0 & \frac{1}{2} & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{4} & 1 & \frac{1}{4} \\ \hline -\frac{1}{3} & \frac{3}{2} & \frac{2}{3} & 1 & -\frac{5}{6} \\ -\frac{2}{3} & 1 & \frac{4}{3} & 0 & -\frac{2}{3} \end{array}\right],$$

and a lower triangular one, with equal diagonal elements

$$\left[\begin{array}{c|c}\mathbf{A}&\mathbf{U}\\\hline\mathbf{B}&\mathbf{V}\end{array}\right]=\left[\begin{array}{ccc|cc}\frac{1}{6}&0&0&1&-\frac{1}{24}\\\frac{1}{3}&\frac{1}{6}&0&1&-\frac{1}{24}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{6}&1&-\frac{1}{24}\\\hline-\frac{1}{4}&\frac{5}{4}&0&1&-\frac{1}{12}\\-14&22&-8&0&-1\end{array}\right].$$

Since GLMs (2) are multivalue methods, they need a starting method to supply the r approximations to the initial values and a finishing method to rebuild the numerical approximation to the solution of the problem from the output vector. Usually (compare [7]) r generalized Runge-Kutta methods of the form

$$\begin{cases}Y_j^{(i)}=y_n^{(i)}+h\sum\limits_{k=1}^{s}a_{jk}^{(i)}f(t_n+c_k^{(i)}h,Y_k^{(i)}),\qquad j=1,2,\ldots,s,\\y_{n+1}^{(i)}=b_0^{(i)}y_n^{(i)}+h\sum\limits_{j=1}^{s}b_j^{(i)}f(t_n+c_j^{(i)}h,Y_j^{(i)}),\end{cases}$$

represented by the Butcher tableau

$$S^{(i)}=\left(\begin{array}{c|c}c^{(i)}&A^{(i)}\\\hline b_0^{(i)}&b^{(i)^{\intercal}},\end{array}\right)\tag{21}$$

are combined in order to provide the missing starting vector. To our purposes, we will always assume that the starting method is *non-degenerate* (compare [7]), i.e. there exists an index i such that $b_0^{(i)}\neq 0$.

The starting method has a remarkable influence on the accuracy of the numerical approximation. Indeed, according to [7], we provide the following definition of order.

Definition 3 A GLM (A,U,B,V) has order p if, and only if, there exists a non-degenerate starting method S such that the numerical approximations obtained via the GLM with starting method S differ from those obtained applying S to the exact solution at the end of the same step by $O(h^{p+1})$.

Following [7], a GLM (2) has order p if

$$\begin{cases}\eta(t)=A\eta D(t)+U\xi(t),\\E\xi(t)=B\eta D(t)+V\xi(t),\end{cases}\tag{22}$$

for any $t\in T$, with $\rho(t)\leq p$. As in [7], η represents the operator associated to the stages, ηD the one associated to the stage-derivatives, ξ is the starting method operator and E the exact solution one. We observe that the product of two operators is defined in [7], §386.

We derive a two-value and three-stage GLM (i.e. $r=2$, $s=3$), assuming that the first component of the numerical solution approximates the exact one, so we do not need any finishing method. The initial value for the second component is computed by means of a generalized 8-stage RK method with elementary weights

$$\{0,\ \theta_1,\ \theta_2,\ \theta_3,\ \theta_4,\ \theta_5,\ \theta_6,\ \theta_7,\ \theta_8\},$$

which are left as free parameters. The values of $\xi_i(t)$ and $E\xi_i(t)$, $i=1,2$, corresponding to trees up to order 4 and depending on such parameters are reported in Table 3.

Table 3 Values of $\xi_i(t)$ and $E\xi_i(t)$, $i = 1, 2$, up to order $p = 4$

	ξ_1	ξ_2	$E\xi_1$	$E\xi_2$
$\emptyset$	1	0	1	0
τ	0	θ_1	1	θ_1
$[\tau]$	0	θ_2	$\frac{1}{2}$	$\theta_1 + \theta_2$
$[\tau^2]$	0	θ_3	$\frac{1}{3}$	$\theta_1 + 2\theta_2 + \theta_3$
$[[\tau]]$	0	θ_4	$\frac{1}{6}$	$\frac{1}{2}\theta_1 + \theta_2 + \theta_4$
$[\tau^3]$	0	θ_5	$\frac{1}{4}$	$\theta_1 + 3\theta_2 + 3\theta_3 + \theta_5$
$[\tau[\tau]]$	0	θ_6	$\frac{1}{8}$	$\frac{1}{2}\theta_1 + \frac{3}{2}\theta_2 + \theta_3 + \theta_4 + \theta_6$
$[\tau[\tau^2]]$	0	θ_7	$\frac{1}{12}$	$\frac{1}{3}\theta_1 + \theta_2 + 2\theta_4 + \theta_7$
$[\tau^4]$	0	θ_8	$\frac{1}{24}$	$\frac{1}{6}\theta_1 + \frac{1}{2}\theta_2 + \theta_4 + \theta_8$

To obtain a basic consistency condition, we solve the second equation in (22) for the empty tree, observing that $\eta D(\emptyset) = 0$ by definition. This leads to

$$\begin{cases} E\xi_1(\emptyset) = v_{11}\xi_1(\emptyset) + v_{12}\xi_2(\emptyset), \\ E\xi_2(\emptyset) = v_{21}\xi_1(\emptyset) + v_{22}\xi_2(\emptyset), \end{cases} \tag{23}$$

and, by taking into account the values in Table 3, we obtain

$$v_{11} = 1, \qquad v_{21} = 0.$$

As a consequence, the matrix V of a preconsistent GLM (2) with $r = 2$ has always the form

$$V = \begin{bmatrix} 1 & v_{12} \\ 0 & v_{22} \end{bmatrix}. \tag{24}$$

At this point, it is worth assuming $v_{22} = -1$. In fact (compare [28], §XV.8.3), in order to limit as much as possible the effects of parasitism, the eigenvalues of the matrix V have to be the r-th roots of unity. Moreover, this choice automatically leads to zero-stable methods (compare [7,30]).

The first vector equation in (22) with $t = \emptyset$, leads to

$$\begin{cases} \eta_1(\emptyset) = u_{11}, \\ \eta_2(\emptyset) = u_{21}, \\ \eta_3(\emptyset) = u_{31}, \end{cases} \tag{25}$$

and, since $\eta_i(\emptyset) = 1$, we get

$$u_{11} = 1, \qquad u_{21} = 1, \qquad u_{31} = 1.$$

Thus, by imposing preconsistency, G-symplecticity, symmetry and condition (10) to bound the parasitic components, we obtain the GLM

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} \frac{1}{2}\alpha & 0 & 0 & 1 & u_{32} \\ \alpha & \frac{1}{2}\beta & 0 & 1 & u_{32} \\ \alpha & \beta & \frac{1}{2}\alpha & 1 & u_{32} \\ \hline b_{13} & b_{12} & b_{13} & 1 & 2u_{32} \\ b_{23} & -2b_{23} & b_{23} & 0 & -1 \end{array}\right] \tag{26}$$

Table 4 Elementary weights of the starting procedure for the computation of $y_2^{[0]}$

θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8
0	0	$\frac{1}{24}\left(2-\sqrt[3]{2}\right)$	$-\frac{1}{24}\left(\sqrt[3]{2}+\sqrt[3]{4}\right)$	0	0	0	0

where $\alpha = b_{13} + b_{23}u_{32}$ and $\beta = b_{12} - 2b_{23}u_{32}$, and the system (22) assumes the form

$$\begin{cases} \eta_1(t) = \frac{1}{2}\alpha\eta_1 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ \eta_2(t) = \alpha\eta_1 D(t) + \frac{1}{2}\beta\eta_2 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ \eta_3(t) = \alpha\eta_1 D(t) + \beta\eta_2 D(t) + \frac{1}{2}\eta_3 D(t) + \xi_1(t) + u_{32}\xi_2(t), \\ E\xi_1(t) = b_{13}\eta_1 D(t) + b_{12}\eta_2 D(t) + b_{13}\eta_3 D(t) + \xi_1(t) + 2u_{32}\xi_2(t), \\ E\xi_2(t) = b_{23}\eta_1 D(t) - 2b_{23}\eta_2 D(t) + b_{23}\eta_3 D(t) - \xi_2(t). \end{cases} \tag{27}$$

Due to symmetry, we imposed order conditions associated to odd order trees only. This led to

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} \frac{1}{6}\gamma & 0 & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & -\frac{1}{6}\delta & 0 & 1 & \frac{1}{24} \\ \frac{1}{3}\gamma & \frac{1}{6}\delta & \frac{1}{6}\gamma & 1 & \frac{1}{24} \\ \hline \frac{1}{6}\varphi & -\frac{1}{4} - \frac{2\sqrt[3]{2}}{3} - \frac{\sqrt[3]{4}}{3} & \frac{1}{6}\varphi & 1 & \frac{1}{12} \\ 1 & -2 & 1 & 0 & -1 \end{array}\right], \tag{28}$$

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

$$c = \left[\, \tfrac{1}{6}\gamma, \quad \tfrac{1}{2}, \quad -\tfrac{1}{12}\left(\sqrt[3]{2}-2\right)\left(4+\sqrt[3]{2}\right) \,\right]^{\intercal}.$$

This method is G-symplectic with respect to the matrices

$$G = \begin{bmatrix} 1 & \frac{1}{24} \\ \frac{1}{24} & \frac{1}{576} \end{bmatrix}, \qquad D = \begin{bmatrix} \frac{1}{3}\gamma & 0 & 0 \\ 0 & -\frac{1}{3}\delta & 0 \\ 0 & 0 & \frac{1}{3}\gamma \end{bmatrix},$$

and symmetric with $L = I$ and

$$P = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

4.1 Starting procedure

As announced, we derive as starting method for the initial value of the second external approximation $y_2^{[0]}$ the generalized Runge-Kutta method with elementary weights $0, \theta_1, \ldots, \theta_8$ given in Table 4.

We introduce the following eight-stage generalized RK method with

$$A=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ \frac{1}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ \frac{1}{4} & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0\\ \frac{5}{6} & -\frac{8}{3} & \frac{5}{2} & 0 & 0 & 0 & 0 & 0\\ -\frac{8}{5} & \frac{3}{5} & 1 & \frac{1}{5} & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{1}{4} & \frac{1}{2} & -\frac{1}{4} & 0 & 0 & 0\\ -1 & 0 & 1 & -\frac{1}{6} & \frac{1}{2} & 0 & 0 & 0\\ 0 & -\frac{1}{5} & \frac{3}{5} & 0 & 0 & 0 & \frac{2}{5} & 0 \end{bmatrix}, \qquad c=\begin{bmatrix} 0\\ \frac{1}{6}\\ -\frac{1}{4}\\ \frac{2}{3}\\ \frac{1}{5}\\ \frac{1}{2}\\ \frac{1}{3}\\ \frac{4}{5} \end{bmatrix},$$

and weights obtained by solving the linear system

$$\begin{cases} b_1+b_2+b_3+b_4+b_5+b_6+b_7+b_8=0\\ 10b_2-15b_3+40b_4+12b_5+30b_6+20b_7+48b_8=0\\ \frac{b_2}{36}+\frac{b_3}{16}+\frac{4b_4}{9}+\frac{b_5}{25}+\frac{b_6}{4}+\frac{b_7}{9}+\frac{16b_8}{25}+\frac{1}{24}\left(-2+\sqrt[3]{2}\right)=0\\ -60b_3-770b_4-12b_5+159b_6-188b_7-36b_8+30\left(\sqrt[3]{2}+\sqrt[3]{4}\right)=0\\ \frac{b_2}{216}-\frac{b_3}{64}+\frac{8b_4}{27}+\frac{b_5}{125}+\frac{b_6}{8}+\frac{b_7}{27}+\frac{64b_8}{125}=0\\ 450b_3-15400b_4-72b_5+2385b_6-1880b_7-864b_8=0\\ -600b_3+3550b_4+7260b_5+9843b_6+364b_7+3300b_8=0\\ -2250b_4-3210b_5-5955b_6+935b_7-1668b_8=0 \end{cases}$$

The linearity of this system is due to the fact that the number of employed internal stages in the starting procedure (eight) equals the number of order conditions to impose to gain order 4 in the approximation of the starting value $y_2^{[0]}$.

5 Numerical experiments

We now provide some numerical experiments comparing the GLM (28) derived in Section 4 with the partitioned RK method [33,34]

$$\frac{\left|A\right|}{\left|b\right|}=\left|\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0\\ \frac{1}{3} & 0 & 0 & 0 & 0 & 0\\ \frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 & 0\\ \frac{1}{3} & -\frac{1}{3} & 1 & 0 & 0 & 0\\ \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & 0 & 0\\ \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0\\ \hline \frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} & \frac{1}{3} & 0 \end{array}\right| \qquad \frac{\left|A\right|}{\left|b\right|}=\left|\begin{array}{cccccc} \frac{7}{48} & 0 & 0 & 0 & 0 & 0\\ \frac{7}{48} & \frac{3}{8} & 0 & 0 & 0 & 0\\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & 0 & 0 & 0\\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & 0 & 0\\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & 0\\ \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & \frac{7}{48}\\ \hline \frac{7}{48} & \frac{3}{8} & -\frac{1}{48} & -\frac{1}{48} & \frac{3}{8} & \frac{7}{48} \end{array}\right| \tag{29}$$

which originates by coupling a diagonally implicit method with an explicit one, thus leading to an overall explicit scheme in case of separable Hamiltonians. Such partitioned pairs are indeed

of practical interest only for separable Hamiltonian problems (compare, for instance, [28] and references therein). Both methods, i.e. our GLM (28) and the partioned RK (29) are symmetric and of order 4. Moreover, the GLM is G-symplectic with zero growth parameter for the parasitic components, while the RK method is symplectic.

The reported tests have been carried out on a node with CPU Intel Xeon 6 core X5690 3,46GHz, belonging to the E4 multi-GPU cluster of Mathematics Department of Salerno University. In particular, it is our aim to show the accuracy gained in the numerical conservation of the Hamiltonian of the following dynamical systems:

- the simple pendulum problem (19);
- the Kepler problem [28]

$$\begin{cases} \dot{p_1}(t) = -\dfrac{q_1(t)}{(q_1^2(t)+q_2^2(t))^{\frac{3}{2}}}, \\ \dot{p_2}(t) = -\dfrac{q_2(t)}{(q_1^2(t)+q_2^2(t))^{\frac{3}{2}}}, \\ \dot{q_i}(t) = p_i(t), \quad i = 1,2, \\ p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \quad q_1(0) = 1-e, \quad q_2(0) = 0, \end{cases} \tag{30}$$

  where the value of the eccentricity $e \in [0,1[$ is fixed to $\frac{1}{2}$. The Hamiltonian of this problem is

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

- the Hènon-Heiles Problem (20);
- the planar three-body problem

$$\begin{cases} \dot{p_i}(t) = \displaystyle\sum_{j\neq i} \frac{q_i - q_j}{r_{ij}^3}, \quad i = 1,2,3, \\ \dot{q_i}(t) = p_i(t), \quad i = 1,2,3, \end{cases} \tag{31}$$

  with $r_{ij} = \|q_i - q_j\|_2$, describing the motion of three coplanar bodies having unitary mass under a Newtonian gravitational force field. The Hamiltonian of this problem assumes the form

$$\mathcal{H}(p(t),q(t)) = \sum_{i=1}^{3} \frac{1}{2} p_i^\intercal p_i - \sum_{i<j} \frac{1}{r_{ij}}.$$

  We consider the initial conditions computed by Carles Simó (compare [13])

$$\begin{aligned} p_1(0) &= [\ 0.46620368,\ 0.43236573\ ]^\intercal, & q_1(0) &= [\ 0.97000436,\ -0.24308753\ ]^\intercal, \\ p_2(0) &= [\ 0.46620368,\ 0.43236573\ ]^\intercal, & q_2(0) &= [\ -0.97000436,\ 0.24308753\ ]^\intercal, \\ p_3(0) &= [-0.93240737,\ -0.86473146\ ]^\intercal, & q_3(0) &= [\ 0,\ 0\ ]^\intercal, \end{aligned}$$

  which provides a figure-of-eight orbit;

Table 5 Numerical comparison of the partitioned RK method (29) with respect to the G-symplectic GLM (28)

	PRK	GLM
Simple pendulum	$\|e^{\mathcal{H}}\|_\infty = 9.51e-14$ $fe = 12000000$	$\|e^{\mathcal{H}}\|_\infty = 1.28e-13$ $fe = 10697133$
Kepler problem	$\|e^{\mathcal{H}}\|_\infty = 5.73e-14$ $fe = 12000000$	$\|e^{\mathcal{H}}\|_\infty = 1.88e-13$ $fe = 11017887$
Hènon-Heiles problem	$\|e^{\mathcal{H}}\|_\infty = 1.48e-14$ $fe = 12000000$	$\|e^{\mathcal{H}}\|_\infty = 5.02e-14$ $fe = 9088029$
3-body problem	$\|e^{\mathcal{H}}\|_\infty = 2.43e-13$ $fe = 12000000$	$\|e^{\mathcal{H}}\|_\infty = 7.48e-13$ $fe = 11988456$
Bead on wire	non-separable	$\|e^{\mathcal{H}}\|_\infty = 1.11e-14$ $fe = 8999952$
Non-reversible problem	$\|e^{\mathcal{H}}\|_\infty = 3.64e-14$ $fe = 12000000$	$\|e^{\mathcal{H}}\|_\infty = 4.59e-013$ $fe = 8999871$

– the non-separable problem whose Hamiltonian is given by

$$\mathcal{H}(p(t),q(t)) = \frac{p^2}{2(1+U'(q)^2)} + U(q), \quad U(q) = 0.1(q(q-2))^2 + 0.008q^3, \tag{32}$$

with initial values

$$p(0) = 0.49, \quad q(0) = 0,$$

describing the path of a particle of unit mass moving on a wire of shape $U(q)$ [1];

– the non-reversible problem [24]

$$\begin{cases} \dot{p}(t) = -\dfrac{q(t)^5}{5} - q(t)^3 + q(t)^2, \\ \dot{q}(t) = p(t)^2 - \dfrac{1}{2}, \\ p(0) = 1, \quad q(0) = 0, \end{cases} \tag{33}$$

whose Hamiltonian function is

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

We perform one million steps of the mentioned numerical methods and compute the Hamiltonian deviation (17). The values of the observed Hamiltonian deviations and the number of function evaluations (fe in Table 5) required by the overall integration schemes are reported in Table 5. We observe that the accuracy gained in preserving the Hamiltonian of the above dynamical systems is essentially the same for both the RK method and the GLM. However the main novelty here is that the derived GLM requires a lower computational effort, due to the lower number of stages: each step of the GLM requires 3 internal stages, while the RK method involves 12 stages.

It is also worth observing that the hypothesis of bounded parasitic components is absolutely crucial: parasitic methods, such as the G-symplectic GLM presented in [7], fail in preserving the Hamiltonian over suitably long time intervals and, moreover, completely destroy the symplecticity of the phase space. This is also visible from the orbit patterns, reported in Figures 1, 2 and 3.

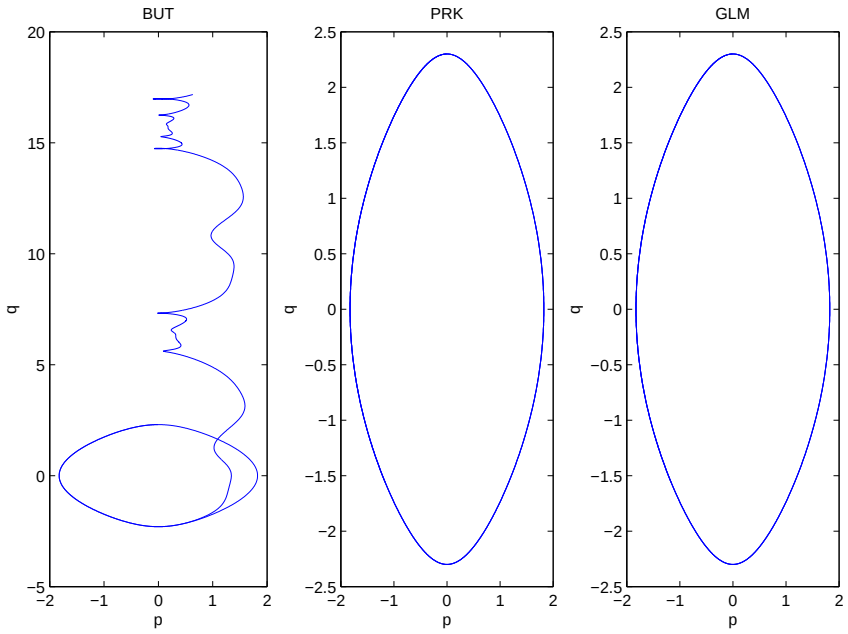

Fig. 1 Orbit patterns for problem (19), gained by the G-symplectic method presented in [7] (BUT), the symplectic PRK method (29) and the GLM (28)

6 Conclusions

This paper is concerned with the actual possibility to employ GLMs for the numerical treatment of Hamiltonian problems. The ingredients we have used in order to derive a GLM competitive with canonical RK methods are G-symplecticity, symmetry, boundedness of parasitic components and a semi-implicit structure. A theoretical investigation of these aspects, benefiting from the B-series theory, has been carried out and a GLM possessing such requirements has been derived. The effectiveness of our approach has been confirmed by the numerical evidence.

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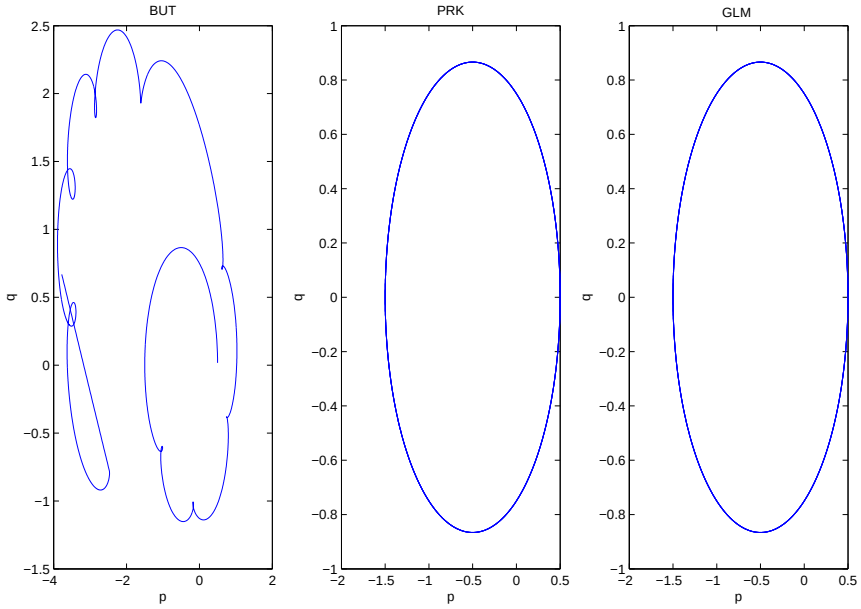

Fig. 2 Orbit patterns for problem (30), gained by the G-symplectic method presented in [7] (BUT), the symplectic PRK method (29) and the GLM (28)

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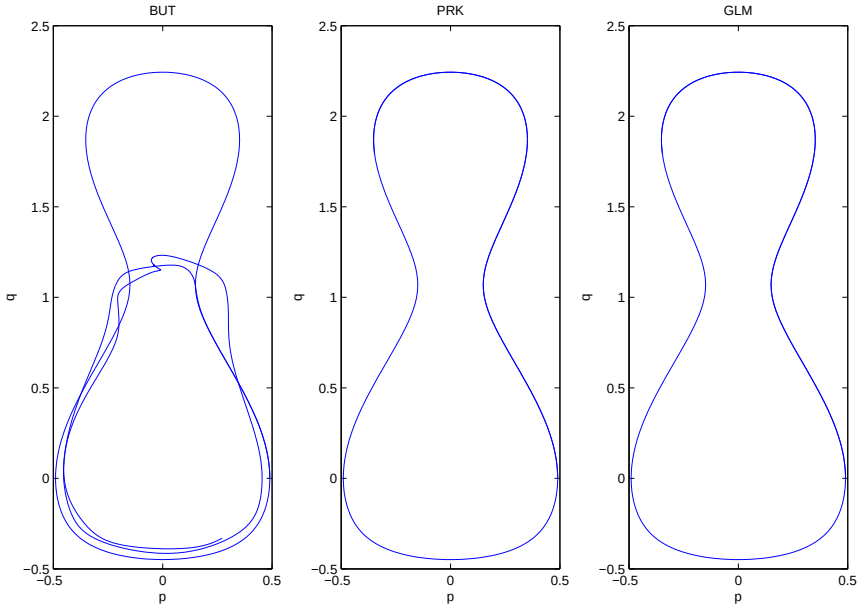

Fig. 3 Orbit patterns for problem (32), gained by the G-symplectic method presented in [7] (BUT), the symplectic PRK method (29) and the GLM (28)

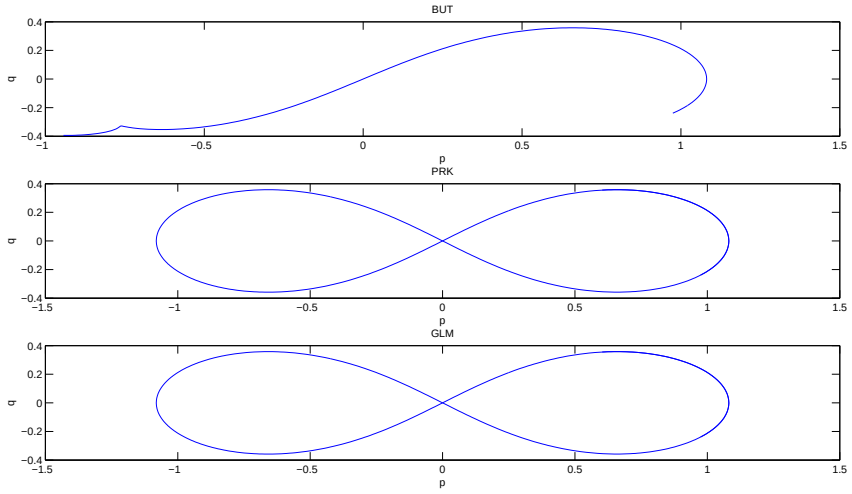

Fig. 4 Orbit patterns for problem (31), gained by the G-symplectic method presented in [7] (BUT), the symplectic PRK method (29) and the GLM (28)

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