Communications in Applied and Industrial Mathematics, ISSN 2038-0909, **vol**, issue, (YYYY) 1–13

DOI: 10.1685/YYYYCAIMXXX

On the G-symplecticity of two-step Runge-Kutta methods

Raffaele D'Ambrosio

Dipartimento di Matematica, Facoltà di Scienze MM.FF.NN.
Università degli Studi di Salerno, Italy
rdambrosio@unisa.it

Communicated by Associated editor

Abstract

This paper investigates the conservative behaviour of two-step Runge-Kutta (TSRK) methods and multistep Runge-Kutta methods (MRK) for the numerical integration of Hamiltonian systems. In particular, the attention is focused on the existence of G-symplectic TSRK and MRK methods, according to the definition provided in Butcher's 2008 monograph.

Keywords: Ordinary differential equations, Hamiltonian problems, two-step Runge-Kutta methods, multistep Runge-Kutta methods, general linear methods, G-symplecticity.

AMS Subject Classification: 65L05

1. Introduction

Let us consider two-step Runge-Kutta (TSRK) methods of the following type:

$$
\left\{
\begin{aligned}
Y_i^{[n]} &= u_i y_{n-1} + (1-u_i) y_n + h \sum_{j=1}^{s} \Big(a_{ij} f(Y_j^{[n]}) + b_{ij} f(Y_j^{[n-1]}) \Big),\\
y_{n+1} &= \vartheta y_{n-1} + (1-\vartheta) y_n + h \sum_{j=1}^{s} \Big(v_j f(Y_j^{[n]}) + w_j f(Y_j^{[n-1]}) \Big),
\end{aligned}
\right.
\tag{1}
$$

$i = 1, 2, \ldots, s$, introduced by Jackiewicz and Tracogna in [1] (compare also [2]), and the family of multistep Runge-Kutta methods (MRK)

$$
\left\{
\begin{aligned}
Y_i^{[n]} &= \sum_{j=1}^{k} u_{ij} y_{n+1-j} + h \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, 2, \ldots, s,\\
y_{n+1} &= \sum_{j=1}^{k} v_j y_{n+1-j} + h \sum_{j=1}^{s} b_j f(Y_j^{[n]}),
\end{aligned}
\right.
\tag{2}
$$

Received YYYY MM DD, in final form YYYY MM DD
Published YYYY MM DD

$i = 1, 2, \ldots, s$, with $k = 2$, introduced by Burrage in [3,4]. It is the purpose of this paper to analyze the conservative behaviour of (1) and (2) when applied to Hamiltonian problems

$$\dot{p}(t) = -\frac{\partial}{\partial q}\mathcal{H}(p(t), q(t), t), \qquad (3)$$
$$\dot{q}(t) = \frac{\partial}{\partial p}\mathcal{H}(p(t), q(t), t),$$

where $\mathcal{H}(p(t), q(t), t)$ is the Hamiltonian of the system. Here, $p(t)$ and $q(t)$ respectively represent generalized momenta and coordinates. The classical numerical approach to Hamiltonian problems mostly consists in using symplectic (or canonical) Runge-Kutta (RK) methods [5–9], i.e. methods numerically preserving some quadratic invariants of the continuous problem. It is known that symplectic RK methods satisfy the following property.

Definition 1.1. (Cooper, 1987; Lasagni, 1988; Sanz-Serna, 1988; Suris, 1988) A RK method (A, b^T, c) is symplectic if the following constrain on the its coefficients holds

$$\text{diag}(b)A + A^T\text{diag}(b) - bb^T = 0, \qquad (4)$$

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

We observe that the matrix $M = diag(b)A + A^T diag(b) - bb^T$ in (4) is also connected to the nonlinear stability properties of a RK method, since it is the matrix to be analyzed to decide whether the corresponding RK method is algebraically stable or not (see [5]).

Symplecticity is mostly a prerogative of one step methods, and therefore of RK methods. In fact, Tang (1993) proved that multistep methods cannot possess a symplectic behaviour. More in general, Butcher and Hewitt [10] proved that multivalue methods cannot be symplectic, unless they actually pass only one single value from the current step to the following one.

A large family of multistep - multivalue numerical methods for the solution of ordinary differential equations is given by General Linear Methods (GLMs)

$$\begin{cases} Y_i^{[n]} = \sum_{j=1}^{s} a_{ij} h F_j^{[n]} + \sum_{j=1}^{r} u_{ij} y_j^{[n]}, \quad i = 1, 2, \ldots, s, \\ y_i^{[n+1]} = \sum_{j=1}^{s} b_{ij} h F_j^{[n]} + \sum_{j=1}^{r} v_{ij} y_j^{[n]}, \; i = 1, 2, \ldots, r, \end{cases} \qquad (5)$$

introduced by Butcher (compare [2,5]), with the aim to create an unifying approach to analyze the properties of a numerical method for ODEs, e.g.

convergence, consistency and stability. Such methods are generally represented by means of their four coefficient matrices $\mathbf{A} \in \mathbb{R}^{s\times s}$, $\mathbf{U} \in \mathbb{R}^{s\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times s}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$, which are put together in the following partitioned $(s+r)\times(s+r)$ matrix

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

We observe that many classical methods can be regarded as GLMs, such as RK methods, TSRK methods (1) and MRK formulae (2) (compare [2]).

According to the results by Tang and Butcher, GLMs cannot be symplectic, unless they reduce to RK methods (the formal notions of equivalence and reducibility for GLMs will be clarified in Definitions 2.1 and 2.2). However, it makes interest to analyze if it is possible to achieve some conservation properties by annihilating the nonlinear stability matrix of a GLM

$$\mathbf{M} = \left[\begin{array}{c|c} D\mathbf{A} + \mathbf{A}^T D - \mathbf{B}^T G\mathbf{B} & D\mathbf{U} - \mathbf{B}^T G\mathbf{V} \\ \hline \mathbf{U}^T D - \mathbf{V}^T G\mathbf{B} & G - \mathbf{V}^T G\mathbf{V} \end{array}\right]. \tag{6}$$

In fact, since the algebraic stability matrix of a symplectic RK method is equal to the zero matrix, it makes interest to investigate the canonical properties of GLMs whose algebraic stability matrix (6) is the zero matrix. This remark gives rise to the notion of *G-symplecticity*, introduced by Butcher in [5].

Definition 1.2. (Butcher, 2008) A GLM $(\mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ 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

$$\begin{aligned} &G = \mathbf{V}^T G\mathbf{V}, \\ &D\mathbf{U} = \mathbf{B}^T G\mathbf{V}, \\ &D\mathbf{A} + \mathbf{A}^T D = \mathbf{B}^T G\mathbf{B}. \end{aligned} \tag{7}$$

It is known that a symplectic method is able to preserve some of the invariants possessed by the continuous problem. Similarly, a G-symplectic method is able to preserve such invariants in a suitable norm, as it has been described in [5] and in particular in [11], where G-symplectic GLMs are introduced, analyzed and tested on several Hamiltonian problems. In [12], partitioned G-symplectic GLMs are introduced for the numerical treatment of separable Hamiltonian problems.

In this paper, we want to investigate the G-symplecticity properties of TSRK methods (1) and MRK methods (2). These formulae, according to the results above provided, cannot be symplectic. However, we aim to analyze theoretically if they can be G-symplectic. This topic is the object of the following sections.

2. Non-existence of irreducible G-symplectic TSRK methods

In this section we analyse the effects of conditions (7) on TSRK methods, in order to understand if irreducible G-symplectic TSRK formulae (1) exist: in fact, if G-symplectic TSRK methods exist, it is our aim to understand whether they are equivalent to canonical RK methods or not. The notions of equivalence and reducibility known in the literature (compare [13]) are formalized as follows.

Definition 2.1. A GLM $(\widehat{\mathbf{A}}, \widehat{\mathbf{U}}, \widehat{\mathbf{B}}, \widehat{\mathbf{V}})$ is equivalent to the GLM $(\mathbf{A}, \mathbf{U}, \mathbf{B}, \mathbf{V})$ if there exist a permutation matrix P and a nonsingular matrix Q such that

$$\left[\begin{array}{c|c} \widehat{\mathbf{A}} & \widehat{\mathbf{U}} \\ \hline \widehat{\mathbf{B}} & \widehat{\mathbf{V}} \end{array}\right] = \left[\begin{array}{c|c} P^T\mathbf{A}P & P^T\mathbf{U}Q \\ \hline Q^{-1}\mathbf{B}P & Q^{-1}\mathbf{V}Q \end{array}\right].$$

Definition 2.2. A GLM is reducible if $s = s_1 + s_2$ and $r = r_1 + r_2 + r_3$ with $s_2 + r_2 + r_3 > 0$, so that an equivalent GLM has sparsity pattern

$$\begin{array}{c} \\ s_1 \\ s_2 \\ r_1 \\ r_2 \\ r_3 \end{array} \begin{array}{c} \begin{array}{ccccc} s_1 & s_2 & r_1 & r_2 & r_3 \end{array} \\ \left[\begin{array}{cc|ccc} A_{11} & 0 & U_{11} & 0 & U_{13} \\ A_{21} & A_{22} & U_{21} & U_{22} & 0 \\ \hline B_{11} & 0 & V_{11} & 0 & V_{13} \\ B_{21} & B_{22} & V_{21} & V_{22} & V_{23} \\ 0 & 0 & 0 & 0 & V_{33} \end{array}\right] \end{array}.$$

In this case the method may be reduced to the GLM $(A_{11}, U_{11}, B_{11}, V_{11})$ with s_1 internal stages and r_1 external ones.

2.1. *TSRK methods with $\vartheta = 0$ and $u = 0$*

We first analyze the G-symplectic behaviour of TSRK methods (1) with $\vartheta = 0$ and $u = 0$

$$\begin{cases} Y_i^{[n]} = y_n + h \sum_{j=1}^{s} \Big(a_{ij} f(Y_j^{[n]}) + b_{ij} f(Y_j^{[n-1]}) \Big), \\ y_{n+1} = y_n + h \sum_{j=1}^{s} \Big(v_j f(Y_j^{[n]}) + w_j f(Y_j^{[n-1]}) \Big), \end{cases}$$

$i = 1, 2, \ldots, s$, which can be represented as GLMs (5) with respect to the Butcher tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & B \\ \hline v^T & 1 & w^T \\ I & 0 & 0 \end{array}\right] \in \mathbb{R}^{(2s+1)\times(2s+1)},$$

where $e = [1, \ldots, 1]^T \in \mathbb{R}^s$. For this family of methods, we prove the following result.

Theorem 2.1. *A TSRK method with $\vartheta = 0$ and $u_i = 0$, $i = 1, 2, \ldots, s$, is G-symplectic if and only if*

$$B = ew^T, \qquad DA + A^T D = \alpha(v + w)(v + w)^T,$$

with

$$D = \alpha \; \mathrm{diag}(v + w), \qquad G = \alpha \begin{bmatrix} 1 & w^T \\ w & ww^T \end{bmatrix}, \qquad \alpha \geq 0. \tag{8}$$

Proof. We assume the following partition for the matrix G

$$G = \begin{bmatrix} g_{11} & G_{12} \\ G_{12}^T & G_{22} \end{bmatrix},$$

with $G_{12} \in \mathbb{R}^s$, $G_{22} \in \mathbb{R}^{s \times s}$ and consider the first condition in (7), whose right hand side assumes the form

$$\mathbf{V}^T G \mathbf{V} = g_{11} \begin{bmatrix} 1 & w^T \\ w & ww^T \end{bmatrix}.$$

This gives the form (8) of the G matrix, with $\alpha = g_{11}$. We next analyze the second condition in (7), which provides that

$$D[e \quad B] = \alpha[v + w \quad (v + w)w^T],$$

or, equivalently, that D assumes the form (8) and $B = ew^T$. Finally, the right hand side of the third condition in (7) assumes the form

$$\mathbf{B}^T G \mathbf{B} = \alpha[v \quad I] \begin{bmatrix} 1 & w^T \\ w & ww^T \end{bmatrix} \begin{bmatrix} v^T \\ I \end{bmatrix} = \alpha(v + w)(v + w)^T,$$

which gives the thesis. □

We remind that a consistent TSRK method satisfies the condition

$$Ae + Be = c,$$

while if it is stage consistent the condition

$$(v + w)^T e = 1$$

holds (compare with [2]). Taking into account these further conditions, the following result is straightforward.

Corollary 2.1. *Consider a stage consistent G-symplectic TSRK method* (1) *with* $\vartheta = 0$ *and* $u_i = 0$, $i = 1, 2, \ldots, s$. *Then,*

$$v^T c + w^T (c - e) = \frac{1}{2}.$$

Another consequence of Theorem 2.1 is that, actually, a G-symplectic TSRK method (1) with $\vartheta = 0$ and $u_i = 0$, $i = 1, 2, \ldots, s$, necessarily reduces to a symplectic RK method, as it is explained in the following result.

Corollary 2.2. *G-symplectic irreducible TSRK method do not exist.*

Proof. In force of Theorem 2.1, the Butcher tableau of a G-symplectic TSRK method (1) with $\vartheta = 0$ and $u_i = 0$, $i = 1, 2, \ldots, s$, regarded as GLM assumes the form

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & ew^T \\ \hline v^T & 1 & w^T \\ I & 0 & 0 \end{array}\right].$$

Such a GLM is equivalent (and, therefore, it reduces to) the GLM

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|c} A & e \\ \hline v^T & 1 \end{array}\right],$$

which is the Butcher tableau of the RK method (c, A, v). □

2.2. *TSRK methods with* $\vartheta \neq 0$ *and* $u \neq 0$

Similar results can be obtained in the more general setting of TSRK methods (1) with $\vartheta \neq 0$ and $u \neq 0$, whose GLM formulation corresponds to the Butcher tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} A & e - u & u & B \\ \hline v^T & 1 - \vartheta & \vartheta & w^T \\ 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{(2s+2)\times(2s+2)}.$$

The following result holds.

Theorem 2.2. *If a TSRK method* (1) *is G-symplectic, then*

$$G = \frac{\alpha}{\vartheta} \begin{bmatrix} 1 & \vartheta & w^T \\ \vartheta & \vartheta^2 & \vartheta w^T \\ w & \vartheta w & w w^T \end{bmatrix}, \qquad \alpha > 0,$$

and

$$D = \frac{\alpha\vartheta}{1+\vartheta}\,\mathrm{diag}(v+w), \qquad u = \frac{\vartheta}{1+\vartheta}\,e, \qquad B = \frac{1}{1+\vartheta}\,ew^T.$$

Proof. The first condition in (7) provides the following representation of the matrix G

$$G = \frac{\alpha}{\vartheta}\begin{bmatrix} 1 & \vartheta & w^T \\ \vartheta & \vartheta^2 & \vartheta w^T \\ w & \vartheta w & ww^T \end{bmatrix}, \qquad \alpha > 0,$$

with $\alpha \in \mathbb{R}$ and $\vartheta \neq 0$. We observe that the spectrum of the matrix G is equal to

$$\sigma(G) = \{\sigma_1, \sigma_2(\vartheta, w)\},$$

where $\sigma_1 = 0$ with multiplicity $r-1$ and

$$\sigma_2(\vartheta, w) = \frac{\alpha}{\vartheta^2}\left(1 + \vartheta^2 + \sum_{i=1}^{s} w_i^2\right).$$

Therefore, the matrix G is positive semi-definite if $\alpha > 0$.

We next analyze the second condition in (7), which assumes the following compact form

$$D[e-u \quad u \quad B] = \left[\frac{\alpha}{\vartheta}(v+w) \quad \alpha(v+w) \quad \frac{\alpha}{\vartheta}(v+w)w^T\right],$$

and provides the last part of the thesis. □

Theorem 2.2 provides some necessary conditions of G-symplecticity for TSRK methods, according to which the tableau of a G-symplectic TSRK method must exhibit the form

(9) $$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} A & \frac{1}{1+\vartheta}e & \frac{\vartheta}{1+\vartheta}e & \frac{1}{\vartheta}ew^T \\ \hline v^T & 1-\vartheta & \vartheta & w^T \\ 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 \end{array}\right],$$

with the additional constraint given by the third equality in (7). Once the input value

$$z_n = \vartheta y_{n-1} + y_n + h\sum_{j=1}^{s} w_j f(Y_j^{n-1}), \quad n > 1,$$

is provided at each time step, then method (9) is equivalent to apply the following method

$$
\begin{aligned}
(1+\vartheta)Y_i^{[n]} &= z_n + h\sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i=1,2,\dots,s,\\
y_{n+1} &= z_n - \vartheta y_n + h\sum_{i=1}^{s} v_i f(Y_i^{[n]}),
\end{aligned} \tag{10}
$$

which can be represented as the GLM corresponding to the tableau

$$
\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & 1 & 0 \\ \hline v^T & 1 & -\vartheta \\ 0 & 1 & 0 \end{array}\right],
$$

with input vector $[z_n \quad y_n]^T$. This tableau is representative of the GLM formulation of MRK methods (2) with $k=2$, thus G-symplectic TSRK methods reduce to (and, therefore, are equivalent to) MRK methods of the form (10).

3. G-symplectic multistep Runge-Kutta methods

The results contained in the previous section essentially assert that TSRK methods cannot be G-symplectic, unless they reduce to canonical RK methods or MRK methods corresponding to the GLM (10). MRK methods (2) with $k=2$ depend on the approximations to the solution in two consecutive step points but, unlike TSRK methods (1), they do not contain any dependency on past stage derivatives.

We focus our attention of MRK methods (2) with $k=s=2$, whose GLM representation is given by the tableau

$$
\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & u_{11} & u_{12} \\ a_{21} & a_{22} & u_{21} & u_{22} \\ \hline b_1 & b_2 & v_1 & v_2 \\ 0 & 0 & 1 & 0 \end{array}\right], \tag{11}
$$

in correspondence of the input vector $y^{[n-1]} = [y_n \quad y_{n-1}]^T$.

We aim to investigate if MRK methods (2) can be genuine G-symplectic methods or if they reduce to known canonical formulae. We prove in the remainder of this paper the existence of such methods in a constructive way, i.e. by exhibiting an example of G-symplectic method falling in the class (11). It is worth remarking that Burrage in [3] was able to find many algebraically stable methods belonging to the family (2): for this reason, the investigation of the G-symplecticity properties of such methods seems particularly reasonable, since G-symplecticity and algebraic stability are strongly connected each other, as we have seen.

We first ensure the convergence of (11), by applying the GLM convergence analysis described in [2,5], i.e. by assuming the following preconsistency, consistency and stage consistency conditions

$$\begin{aligned} u_{11} + u_{12} &= 1, \\ u_{21} + u_{22} &= 1, \\ v_1 + v_2 &= 1, \\ b_1 + b_2 + v_1 &= 2, \\ a_{11} + a_{12} - u_{12} &= c_1, \\ a_{21} + a_{22} - u_{22} &= c_2, \end{aligned}$$

with $-1 < v_2 \leq 1$ for zero-stability requirements. In order to avoid reduction to GLMs with $r = 1$, we assume in advance two values for v_1 and v_2, e.g. $v_1 = 1/3$ and $v_2 = 2/3$; we remark that such assumptions are in accordance with zero-stability and preconsisistency requirements, thus they do not affect the convergence of the scheme. We solve the above equalities with respect to u_{11}, u_{21}, b_1, a_{11}, a_{21} and, under these assumptions, the resulting methods are consistent and zero-stable and, therefore, convergent (see Theorem 2.3.4 in [2]). We use the remaining parameters to achieve G-symplecticity via conditions (7), order 2 and stage order 2 by assuming

$$\begin{aligned} Ac - Uq_2 &= \frac{c^2}{2}, \\ Bc + Vq_2 &= q_2 + q_1 + \frac{q_0}{2}, \end{aligned}$$

with $q_0 = [1 \quad 1]^T$, $q_1 = [0 \quad -1]^T$, $q_2 = [0 \quad \frac{1}{2}]^T$. Then, we finally obtain the G-symplectic MRK method corresponding to the following GLM representation

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|cc} \frac{1}{4} & \frac{15-14\sqrt{30}}{60} & \frac{3}{5} & \frac{2}{5} \\ \frac{15+14\sqrt{30}}{60} & \frac{1}{4} & \frac{3}{5} & \frac{2}{5} \\ \hline \frac{5}{6} & \frac{5}{6} & \frac{1}{3} & \frac{2}{3} \\ 0 & 0 & 1 & 0 \end{array}\right], \tag{12}$$

with abscissa vector

$$c = \begin{bmatrix} \frac{3-\sqrt{7}}{30} & \frac{3+\sqrt{7}}{30} \end{bmatrix}^T,$$

and

$$G = \begin{bmatrix} \frac{3}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{4}{15} \end{bmatrix}, \qquad D = \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{27}{8} \end{bmatrix}.$$

We now show the numerical evidence originated from the application of the derived MRK method to the simple pendulum problem

$$\begin{cases} \dot{p}(t) = -\sin(q(t)), \\ \dot{q}(t) = p(t), \\ p(0) = 0, \\ q(0) = 2.3, \end{cases} \tag{13}$$

with $t \in [0, 1000]$. It is known that the Hamiltonian of this dynamical system, i.e.

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

which provides the total energy of the system, is preserved along the time. Table 1 reports the infinity norm of the vector $e^{\mathcal{H}}$ of the Hamiltonian deviations

$$e_n^{\mathcal{H}} = \frac{\mathcal{H}_n - \mathcal{H}(p(0), q(0))}{\mathcal{H}(p(0), q(0))}, \quad n = 1, \ldots, N,$$

where $\mathcal{H}_n$ is approximated value of the Hamiltonian computed in the point t_n of the discretization and $N = 1000/h$, being $h = 1/2^k$ the (fixed) value of the stepsize and k an integer value. The results confirm the ability of method (12) to preserve for long time the total energy of the dynamical system described by (13).

We also notice that the total energy is accurately preserved for long time since the method (12) does not exhibit any parasitic behaviour, as it happens for the G-symplectic GLM

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & -\frac{3+2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right], \tag{14}$$

described in [5]. Figures 1 and 2 show the Hamiltonian deviation associated to methods (12) and (14) respectively, when applied to problem (13) with

DOI: 10.1685/YYYYCAIMXXX

Table 1. Numerical results for the G-symplectic MRK method (12) on problem (13)

k	$\|e^{\mathcal{H}}\|_\infty$
5	$2.66 \cdot 10^{-3}$
6	$6.66 \cdot 10^{-4}$
7	$1.66 \cdot 10^{-4}$
8	$4.16 \cdot 10^{-5}$
9	$1.04 \cdot 10^{-5}$
10	$2.60 \cdot 10^{-6}$

stepsize $h = 10^{-2}$. It can be advised that method (14) exhibits a parasitic behaviour which destroys the overall accuracy of the conservation, since $\|e^{\mathcal{H}}\|_\infty = 2.99$. Such a behaviour is not advisable on our method (12) and the infinity norm of the achieved Hamiltonian error is $\|e^{\mathcal{H}}\|_\infty = 2.73 \cdot 10^{-4}$.

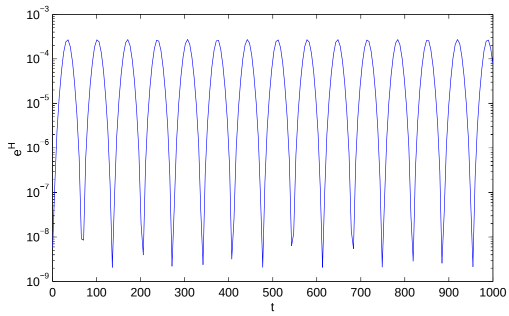

Figure 1. Hamiltonian error of the method (12) applied to (13) with stepsize $h = 10^{-2}$.

4. Conclusions

We have focused our attention on the conservative properties of TSRK methods, proving that irreducible G-symplectic TSRK methods do not exist, since such methods are equivalent to (and, therefore, they reduce to) symplectic RK methods or G-symplectic two-step MRK methods. The existence of genuine G-symplectic MRK methods (2) is discussed in Section 3 by means of constructive arguments: in particular, an example of G-symplectic MRK method has been provided, tested and compared with a known G-symplectic method due to Butcher [5]. Future investigations will concern the extensive analysis of the conservative properties of MRK methods, also

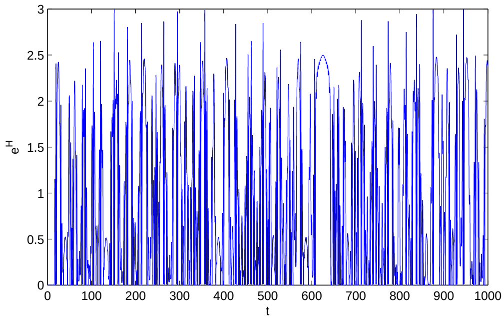

Figure 2. Hamiltonian error of the method (14) applied to (13) with stepsize $h = 10^{-2}$.

in comparison to known canonical formulae. Our purpose will also be the investigation of G-simplecticity of other classes of non-symplectic methods already known in the literature (such as DIMSIMs, peer methods, almost RK methods, and so on [2,5]).

Acknowledgements

The author expresses his warmest gratitude to John C. Butcher, who deeply introduced him into the topic of G-symplecticity.

REFERENCES

1. Z. Jackiewicz and S. Tracogna, A general class of two-step Runge-Kutta methods for ordinary differential equations, *SIAM J. Numer. Anal.*, vol. 32, pp. 1390–1427, 1995.
2. Z. Jackiewicz, *General Linear Methods for Ordinary Differential Equations*. John Wiley & Sons, 2009.
3. K. Burrage, High order algebraically stable multistep Runge-Kutta methods, *SIAM J. Numer. Anal.*, vol. 24, pp. 106–115, 1987.
4. K. Burrage, Order properties of implicit multivalue methods for ordinary differential equations, *IMA J. Numer. Anal.*, vol. 8, pp. 43–69, 1988.
5. J. C. Butcher, *Numerical methods for Ordinary Differential Equations, Second Edition*. Wiley, 2008.
6. C. L. E. Hairer and G. Wanner, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations, Second Edition*. Springer Series in Computational Mathematics 31, Springer-Verlag, 2006.

7. F. M. Lasagni, Canonical Runge-Kutta methods, *Z. Angew. Math. Phys.*, vol. 39, pp. 952–953, 1988.
8. R. I. McLachlan and G. R. W. Quispel, Geometric integrators for ODEs, *J. Phys. A: Math. Gen.*, vol. 39, no. 19, pp. 5251–5285, 2006.
9. J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems.* Chapman & Hall, 1994.
10. J. C. Butcher and L. L. Hewitt, The existence of symplectic general linear methods, *Numer. Algor.*, vol. 51, pp. 77–84, 2009.
11. Y. Habib, *Long-term behaviour of G-symplectic methods.* PhD thesis, The University of Auckland, 2010.
12. J. C. Butcher and R. D'Ambrosio, Partitioned general linear methods for separable Hamiltonian problems, *submitted.*
13. J. C. Butcher, The equivalence of algebraic stability and AN-stability, *BIT*, vol. 27, pp. 510–533, 1987.