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Partitioned general linear methods for separable Hamiltonian problems

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Abstract

Partitioned general linear methods possessing the G-symplecticity property are introduced. These are intended for the numerical solution of separable Hamiltonian problems and, as for multivalue methods in general, there is a potential for loss of accuracy because of parasitic solution growth. The solution of mechanical problems over extended time intervals often benefits from interchange symmetry as well as from symplectic behaviour. A special type of symmetry, known as interchange symmetry, is developed from a model Runge–Kutta case to a full multivalue case. Criteria are found for eliminating parasitic behaviour and order conditions are explored.

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1. Introduction

G-symplectic general linear methods [3, 4, 5, 7, 8, 11, 12, 13, 15] are a natural generalization of symplectic Runge–Kutta methods. In this paper we extend these ideas to Runge–Kutta pairs applied to separable problems. We are given a differential equation system, partitioned in the form

$$\widehat{y}'(x) = \widehat{f}(\widetilde{y}(x)), \quad \widetilde{y}'(x) = \widetilde{f}(\widehat{y}(x)), \qquad \widehat{y}(x_0) = \widehat{y}_0 \in \mathbb{R}^N, \quad \widetilde{y}(x_0) = \widetilde{y}_0 \in \mathbb{R}^N. \quad (1.1)$$

The main example is the equations of motion based on a separable Hamiltonian problem

$$p'(t) = -\frac{\partial H}{\partial q}, \qquad q'(t) = \frac{\partial H}{\partial p},$$

where $H(p,q) = T(p) + V(q)$. We could express this in the form (1.1) by writing $\widetilde{y} = p$, $\widehat{y} = q$.

We will consider problems for which there exists a bilinear form $[\widehat{y}, \widetilde{y}]$, which is known to be an invariant, and we will construct methods which attempt to respect this invariant. These methods will be partitioned general linear (that is, multivalue and multistage) and we cannot expect true numerical invariance to be possible. However, we will at least look for invariance in the same sense as for non-partitioned G-symplectic methods.

To achieve theoretical invariance for (1.1) we will assume that for $\widehat{\eta}, \widetilde{\eta} \in \mathbb{R}^N$, it holds that

$$[\widehat{\eta}, \widetilde{f}(\widehat{\eta})] = [\widehat{f}(\widetilde{\eta}), \widetilde{\eta}] = 0, \qquad (1.2)$$

and it follows that

$$\tfrac{d}{dx}[\widehat{y}(x), \widetilde{y}(x)] = [\widehat{f}(\widetilde{y}(x)), \widetilde{y}(x)] + [\widehat{y}(x), \widetilde{f}(\widehat{y}(x))] = 0.$$

In Section 2 we will present a formulation of partitioned general linear methods. This will be followed by Section 3 in which we will state the G-symplectic conditions and show why methods with this property preserve bi-linear invariants. Sections 4 and 5 will analyse the requirement of interchange symmetry and the phenomenon of parasitic behaviour respectively. Order conditions for general linear method pairs are introduced in Section 6. Section 7 is devoted to the construction of general linear method pairs. Some numerical experiments presented in Section 8 will attest to the potential role of these new methods. Some concluding remarks will be given in Section 9.

2. Partitioned general linear methods

A general linear method for the differential equation system

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0 \in \mathbb{R}^M.$$

is characterized by four matrices (A, U, B, V), which indicate the relationship between the vector of r inputs to step number n, denoted by $y^{[n-1]}$, the corresponding outgoing vector $y^{[n]}$ and the vector of s stage values denoted by Y. If the individual stages are Y_1, Y_2, $\ldots$, Y_s, then the vector F of stage derivatives is made up from the subvectors $F_i = f(Y_i)$, $i = 1, 2, \ldots, s$. For simplicity here, and in similar instances throughout the paper, we will write this as $F = F_1 \oplus F_2 \oplus \cdots \oplus F_s$. The equations relating these quantities are

$$Y = h(A \otimes I_M)F + (U \otimes I_M)y^{[0]}, \qquad y^{[1]} = h(B \otimes I_M)F + (V \otimes I_M)y^{[0]}, \qquad (2.3)$$

where we have used $n = 1$ because this is a typical case. Throughout this paper, we will for simplicity omit the Kronecker products and write (2.3) as

$$Y = hAF + Uy^{[0]}, \qquad y^{[1]} = hBF + Vy^{[0]}.$$

To write the partitioned problem in this formulation, let $M = 2N$ and define

$$y = \begin{bmatrix} \widehat{y} \\ \widetilde{y} \end{bmatrix}, \qquad f(y) = \begin{bmatrix} \widehat{f}(\widetilde{y}) \\ \widetilde{f}(\widehat{y}) \end{bmatrix}.$$

Now introduce the tableaux

$$\begin{bmatrix} \widehat{A} & \widehat{U} \\ \widehat{B} & \widehat{V} \end{bmatrix}, \qquad \begin{bmatrix} \widetilde{A} & \widetilde{U} \\ \widetilde{B} & \widetilde{V} \end{bmatrix}.$$

In this partitioned method, $\widehat{y}^{[n]}$ carries information on the variable $\widehat{y}(x)$ and $\widetilde{y}^{[n]}$ carries information on $\widetilde{y}(x)$. Furthermore $\widehat{Y}$ and $\widetilde{Y}$ contain values of the stages and $\widehat{F}_i = \widehat{f}(\widetilde{Y}_i)$ and $\widetilde{F}_i = \widetilde{f}(\widehat{Y}_i)$, the values of the stage derivatives. For the (typical) first step of a computation using this method, the inputs, outputs and stage values are related by

$$\widehat{Y} = h\widehat{A}\widehat{F} + \widehat{U}\widehat{y}^{[0]}, \qquad \widetilde{Y} = h\widetilde{A}\widetilde{F} + \widetilde{U}\widetilde{y}^{[0]}, \tag{2.4}$$

$$\widehat{y}^{[1]} = h\widehat{B}\widehat{F} + \widehat{V}\widehat{y}^{[0]}, \qquad \widetilde{y}^{[1]} = h\widetilde{B}\widetilde{F} + \widetilde{V}\widetilde{y}^{[0]}. \tag{2.5}$$

The fundamental properties of stability, pre-consistency and consistency, can be generalized for partitioned methods and we will only consider method pairs in which these properties hold. The formal meanings are

Definition 2.1. *A partitioned general method pair* $[(\widehat{A},\widehat{U},\widehat{B},\widehat{V})),(\widetilde{A},\widetilde{U},\widetilde{B},\widetilde{V})]$ *is* stable *if* $\widehat{V}$ *and* $\widetilde{V}$ *are each power-bounded.*

Definition 2.2. *A partitioned general method pair* $[(\widehat{A},\widehat{U},\widehat{B},\widehat{V})),(\widetilde{A},\widetilde{U},\widetilde{B},\widetilde{V})]$ *is* pre-consistent *if there exists a pre-consistency vector pair* $[\widehat{q}_0,\widetilde{q}_0]$*, such that*

$$\widehat{V}\widehat{q}_0 = \widehat{q}_0, \qquad \widetilde{V}\widetilde{q}_0 = \widetilde{q}_0,$$
$$\widehat{U}\widehat{q}_0 = \mathbf{1}, \qquad \widetilde{U}\widetilde{q}_0 = \mathbf{1},$$

where $\mathbf{1}$ *is the vector in* $\mathbb{R}^s$ *with each component equal to* 1.

Definition 2.3. *A partitioned general method pair* $[(\widehat{A},\widehat{U},\widehat{B},\widehat{V})),(\widetilde{A},\widetilde{U},\widetilde{B},\widetilde{V})]$ *is* consistent *if the method is preconsistent with pre-consistency vector pair* $[\widehat{q}_0,\widetilde{q}_0]$*, if there exist consistency vectors* $[\widehat{q}_1,\widetilde{q}_1]$ *such that*

$$\widehat{B}\mathbf{1} + \widehat{V}\widehat{q}_1 = \widehat{q}_1 + \widehat{q}_0, \qquad \widetilde{B}\mathbf{1} + \widetilde{V}\widetilde{q}_1 = \widetilde{q}_1 + \widetilde{q}_0$$

where $\mathbf{1}$ *is the vector in* $\mathbb{R}^s$ *with each component equal to* 1.

The property of convergence for a partitioned general linear method is given by the following definition.

Definition 2.4. *A partitioned general method pair* $[(\widehat{A},\widehat{U},\widehat{B},\widehat{V}),(\widetilde{A},\widetilde{U},\widetilde{B},\widetilde{V})]$ *is* convergent *if for any well-posed initial value problem* (1.1)*, there exist two non-zero vectors* $\widehat{q}_0,\widetilde{q}_0 \in \mathbb{R}^r$ *and two starting procedures* $\widehat{\phi},\widetilde{\phi} : (0,\infty) \to \mathbb{R}^r$*, such that*

$$\lim_{h\to 0} \widehat{\phi}_i(h) = \widehat{q}_{0,i}\widehat{y}(x_0), \qquad \lim_{h\to 0} \widetilde{\phi}_i(h) = \widetilde{q}_{0,i}\widetilde{y}(x_0),$$

for all $i = 1,2,\ldots,r$*, and such that for any* $\bar{x} > x_0$*, the sequences of vectors* $\widehat{y}^{[n]}$*,* $\widetilde{y}^{[n]}$*, computed by using* n *steps with stepsize* $h = (\bar{x}-x_0)/n$*, by employing* $\widehat{y}^{[0]} = \widehat{\phi}(h)$ *and* $\widetilde{y}^{[0]} = \widetilde{\phi}(h)$*, respectively converge to* $\widehat{q}_0\widehat{y}(x)$ *and* $\widetilde{q}_0\widetilde{y}(x)$*.*

It is possible to prove that the classical equivalence between convergence and consistency plus stability also holds true in this case. The proof follows immediately from the lines drawn in the non-partioned case [3].

2.1. Transformations

Let $\widehat{T}$ and $\widetilde{T}$ denote non-singular $r \times r$ matrices which, for full generality, could have complex elements. The information passed from step to step which has been denoted by $\widehat{y}^{[n]}$ and $\widetilde{y}^{[n]}$ at the end of step number n, could be just as well be transformed into the form $\widehat{T}^{-1}\widehat{y}^{[n]}$ and $\widetilde{T}^{-1}\widetilde{y}^{[n]}$. The coefficients of the transformed methods can be seen by rewriting (2.4), (2.5) as follows:

$$\widehat{Y} = h\widehat{A}\widehat{F} + (\widehat{U}\widehat{T})(\widehat{T}^{-1}\widehat{y}^{[0]}), \qquad \widetilde{Y} = h\widetilde{A}\widetilde{F} + (\widetilde{U}\widetilde{T})(\widetilde{T}^{-1}\widetilde{y}^{[0]}),$$
$$(\widehat{T}^{-1}\widehat{y}^{[1]}) = h(\widehat{T}^{-1}\widehat{B})\widehat{F} + (\widehat{T}^{-1}\widehat{V}\widehat{T})(\widehat{T}^{-1}\widehat{y}^{[0]}), \quad (\widetilde{T}^{-1}\widetilde{y}^{[1]}) = h(\widetilde{T}^{-1}\widetilde{B})\widetilde{F} + (\widetilde{T}^{-1}\widetilde{V}\widetilde{T})(\widetilde{T}^{-1}\widetilde{y}^{[0]}).$$

Thus the method $\big((\widehat{A},\widehat{U},\widehat{B},\widehat{V}),(\widetilde{A},\widetilde{U},\widetilde{B},\widetilde{V})\big)$ has been transformed by the matrix pair $(\widehat{T},\widetilde{T})$ as follows

$$\left(\begin{bmatrix} \widehat{A} & \widehat{U} \\ \widehat{B} & \widehat{V} \end{bmatrix}, \begin{bmatrix} \widetilde{A} & \widetilde{U} \\ \widetilde{B} & \widetilde{V} \end{bmatrix}\right) \xrightarrow{(\widehat{T},\widetilde{T})} \left(\begin{bmatrix} \widehat{A} & \widehat{U}\widehat{T} \\ \widehat{T}^{-1}\widehat{B} & \widehat{T}^{-1}\widehat{V}\widehat{T} \end{bmatrix}, \begin{bmatrix} \widetilde{A} & \widetilde{U}\widetilde{T} \\ \widetilde{T}^{-1}\widetilde{B} & \widetilde{T}^{-1}\widetilde{V}\widetilde{T} \end{bmatrix}\right). \tag{2.6}$$

We will regard the original and the transformed methods as equivalent, because the choice of one representation rather than another is only a matter of convenience. This means convenience in derivation and analysis of specific methods, and also in the actual implementation of a method to solve numerical problems.

For the implementation it will never be convenient for the coefficient matrices to have non-real elements; but it will often be convenient for derivation and analysis for $\widehat{V}$ and $\widetilde{V}$ to be diagonal matrices, even if the eigenvalues are not real.

3. Symplectic conditions

Denote by $[\widehat{y},\widetilde{y}]$ a bilinear form which is assumed to be invariant (1.1), that is

$$[\widehat{y},\widetilde{f}(y)] = [\widehat{f}(\widetilde{y}),\widetilde{y}] = 0.$$

Even if we cannot expect from an irreducible GLM with $r > 1$ to preserve this invariant (compare [3, 6]), we aim to find sufficient conditions ensuring that, for the output values provided by the partitioned GLM (2.4)-(2.5), an analogous conservation condition holds. To proceed in this way, we consider a symmetric $r \times r$ matrix G and two diagonal $s \times s$ matrices $\widehat{D} = \operatorname{diag}(\widehat{d})$, $\widetilde{D} = \operatorname{diag}(\widetilde{d})$. Corresponding to these matrices, we introduce the bilinear forms

$$[\eta,\zeta]_G = \sum_{i,j=1}^{r} g_{ij}[\eta_i,\zeta_i], \quad [\widehat{Y},\widetilde{F}]_{\widehat{D}} = \sum_{i=1}^{s} \widehat{d}_i[\widehat{Y}_i,\widetilde{F}_i], \quad [\widehat{F},\widetilde{Y}]_{\widetilde{D}} = \sum_{i=1}^{s} \widetilde{d}_i[\widehat{F}_i,\widetilde{Y}_i].$$

Consider $\widehat{\eta} \in \mathbb{R}^{mN}$, made up from m sub vectors $\widehat{\eta}_1,\widehat{\eta}_2,\ldots,\widehat{\eta}_m \in \mathbb{R}^N$ and similarly for $\widetilde{\eta} \in \mathbb{R}^{nN}$ made up from n sub vectors $\widetilde{\eta}_1,\widetilde{\eta}_2,\ldots,\widetilde{\eta}_n \in \mathbb{R}^N$. If C is an $m \times n$ coefficient matrix, we define an bilinear product on $\mathbb{R}^{mN} \times \mathbb{R}^{nN}$, by

$$[\widehat{\eta},\widetilde{\eta}]_C = \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}[\widehat{\eta}_i,\widetilde{\eta}_j]$$

It will be convenient to make extensive use of the following lemma, which is easy to verify.

Lemma 3.1. *If $\widehat{Q}$ and $\widetilde{Q}$ are $k\times m$ and $l\times n$ matrices respectively, then*

$$[\widehat{Q}\widehat{\eta},\widetilde{Q}\widetilde{\eta}]_C = [\widehat{\eta},\widetilde{\eta}]_{\widehat{Q}^{\top}C\widetilde{Q}}.$$

Recall that the notations $\widehat{Q}\widehat{\eta}$, $\widetilde{Q}\widetilde{\eta}$ denote $(\widehat{Q}\otimes I_M)\widehat{\eta}$, $(\widetilde{Q}\otimes I_M)\widetilde{\eta}$ respectively.

Our aim will be to investigate the possible existence of methods such that, for a non-singular $r\times r$ matrix G,

$$[\widehat{y}^{[n]},\widetilde{y}^{[n]}]_G = [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_G \tag{3.7}$$

As a step towards the definition of G-symplectic partitioned methods, and a criterion for (3.7) we introduce:

Lemma 3.2. *Let G denote an $r\times r$ matrix and let $\widehat{D},\widetilde{D}$ denote $s\times s$ diagonal matrices. Also let M be the partitioned $(s+r)\times(s+r)$ matrix*

$$M = \left[\begin{array}{cc} M_{11} & M_{12} \\ M_{21} & M_{22} \end{array}\right] = \left[\begin{array}{cc} \widehat{D}\widetilde{A}+\widehat{A}^{\top}\widetilde{D}-\widehat{B}^{\top}G\widetilde{B} & \widehat{D}\widetilde{U}-\widehat{B}^{\top}G\widetilde{V} \\ \widehat{U}^{\top}\widetilde{D}-\widehat{V}^{\top}G\widetilde{B} & G-\widehat{V}^{\top}G\widetilde{V} \end{array}\right]. \tag{3.8}$$

Then

$$[\widehat{y}^{[n]},\widetilde{y}^{[n]}]_G = [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_G + h[\widehat{Y},\widetilde{F}]_{\widetilde{D}} + h[\widehat{F},\widetilde{Y}]_{\widehat{D}} - [h\widehat{F}\oplus\widehat{Y},h\widetilde{F}\oplus\widetilde{Y}]_M. \tag{3.9}$$

Proof: We will show that

$$[\widehat{y}^{[n]},\widetilde{y}^{[n]}]_G - [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_G - h[\widehat{Y},\widetilde{F}]_{\widetilde{D}} - h[\widehat{F},\widetilde{Y}]_{\widehat{D}} + [h\widehat{F}\oplus\widehat{y}^{[n-1]},h\widetilde{F}\oplus\widetilde{y}^{[n-1]}]_M = 0,$$

or that $C_{11}=0$, $C_{12}=0$, $C_{21}=0$, $C_{22}=0$ where

$$\begin{aligned} h^2[\widehat{F},\widetilde{F}]_{C_{11}} + h[\widehat{F},\widetilde{y}^{[n-1]}]_{C_{12}} + h[\widehat{y}^{[n-1]},\widetilde{F}]_{C_{21}} + [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_{C_{22}} = \\ [h\widehat{B}\widehat{F}+\widehat{V}\widehat{y}^{[n-1]},h\widetilde{B}\widetilde{F}+\widetilde{V}\widetilde{y}^{[n-1]}]_G - [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_G \\ -h[h\widehat{A}\widehat{F}+\widehat{U}\widehat{y}^{[n-1]},\widetilde{F}]_{\widetilde{D}} - h[\widehat{F},h\widetilde{A}\widetilde{F}+\widetilde{U}\widetilde{y}^{[n-1]}]_{\widehat{D}} \\ +h^2[\widehat{F},\widetilde{F}]_{M_{11}} + h[\widehat{F},\widetilde{y}^{[n-1]}]_{M_{12}} + h[\widehat{y}^{[n-1]},\widetilde{F}]_{M_{21}} + [\widehat{y}^{[n-1]},\widetilde{y}^{[n-1]}]_{M_{22}}. \end{aligned}$$

Expand each term making use of Lemma 3.1, and we find

$$C_{11} = \widehat{B}^{\top}G\widetilde{B} - \widehat{A}^{\top}\widetilde{D} - \widehat{D}\widetilde{A} + M_{11} = 0, \tag{3.10}$$

$$C_{12} = \widehat{B}^{\top}G\widetilde{V} - \widehat{D}\widetilde{U} + M_{12} = 0, \tag{3.11}$$

$$C_{21} = \widehat{V}^{\top}G\widetilde{B} - \widehat{U}^{\top}\widetilde{D} + M_{21} = 0, \tag{3.12}$$

$$C_{22} = \widehat{V}^{\top}G\widetilde{V} - G + M_{22} = 0. \tag{3.13}$$

□

Making use of Lemma 3.2, we can now state the central definition and the main theorem:

Definition 3.1. *A partitioned general linear method such that $M = 0$ in* (3.8) *is said to be G-symplectic.*

Theorem 3.1. *Let* $[(\widehat{A}, \widehat{U}, \widehat{B}, \widehat{V}), (\widetilde{A}, \widetilde{U}, \widetilde{B}, \widetilde{V})]$ *be a G-symplectic partitioned general method pair and let* $(\widehat{f}, \widetilde{f})$ *satisfy* (1.2)*, then the solution to* (1.1)*, computed using the method pair, satisfies*

$$[\widehat{y}^{[n]}, \widetilde{y}^{[n]}]_G = [\widehat{y}^{[0]}, \widetilde{y}^{[0]}]_G, \qquad n = 1, 2, 3, \ldots.$$

Proof: From (3.9), we have

$$[\widehat{y}^{[n]}, \widetilde{y}^{[n]}]_G - [\widehat{y}^{[n-1]}, \widetilde{y}^{[n-1]}]_G = h[\widehat{Y}, \widetilde{F}]_{\widetilde{D}} + h[\widehat{F}, \widetilde{Y}]_{\widehat{D}} - [h\widehat{F} \oplus \widehat{Y}, h\widetilde{F} \oplus \widetilde{Y}]_M$$

$$= h\sum_{i=1}^{s} \widetilde{d}_i [\widehat{Y}_i, \widetilde{F}_i] + h\sum_{i=1}^{s} \widehat{d}_i [\widehat{F}_i, \widetilde{Y}_i] = 0.$$

□

4. Interchange symmetry

In addition to G-symplecticity, we also consider symmetry as an important property of Hamiltonian systems which we might wish to preserve in simulations. In this paper, we do not consider pure time-reversal symmetry, but introduce a notion of interchange symmetry motived by the following consideration of classical symplectic Runge-Kutta pairs.

4.1. A model Runge–Kutta method

As a guide to the construction of GLM pairs, Runge-Kutta pairs will be found which automatically satisfy the symplectic condition

$$\operatorname{diag}(\widetilde{b})\widehat{A} + \widetilde{A}^{\mathsf{T}}\operatorname{diag}(\widehat{b}) = \widetilde{b}\widehat{b}^{\mathsf{T}}.$$

Choose arbitrary vectors $\widehat{b}$ and $\widetilde{b}$ and define

$$\widehat{A} = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ \widehat{b}_1 & 0 & \cdots & 0 & 0 \\ \widehat{b}_1 & \widehat{b}_2 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ \widehat{b}_1 & \widehat{b}_2 & \cdots & 0 & 0 \\ \widehat{b}_1 & \widehat{b}_2 & \cdots & \widehat{b}_{s-1} & 0 \end{bmatrix} \qquad \widetilde{A} = \begin{bmatrix} \widetilde{b}_1 & 0 & \cdots & 0 & 0 \\ \widetilde{b}_1 & \widetilde{b}_2 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_{s-1} & 0 \\ \widetilde{b}_1 & \widetilde{b}_2 & \cdots & \widetilde{b}_{s-1} & \widetilde{b}_s \end{bmatrix}$$

A convenient option is to define $\widetilde{b}_i = \widehat{b}_{s+1-i}$, $i = 1, 2, \ldots, s$ because the two method tableaux become mutually adjoints. Write the elements of $\widehat{b}$ in terms of the abscissae of the second, third, etc stages so that

$$\begin{aligned} \widehat{b}^{\mathsf{T}} &= \begin{bmatrix} c_2 & c_3 - c_2 & \cdots & c_s - c_{s-1} & 1 - c_s \end{bmatrix} \\ \widetilde{b}^{\mathsf{T}} &= \begin{bmatrix} 1 - c_s & c_s - c_{s-1} & \cdots & c_3 - c_2 & c_2 \end{bmatrix} \end{aligned}$$

We will consider the example $s = 4$ so that the tableaux for the method pair become

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ c_2 & c_2 & 0 & 0 & 0 \\ c_3 & c_2 & c_3-c_2 & 0 & 0 \\ c_4 & c_2 & c_3-c_2 & c_4-c_3 & 0 \\ \hline & c_2 & c_3-c_2 & c_4-c_3 & 1-c_4 \end{array} \qquad \begin{array}{c|cccc} 1-c_4 & 1-c_4 & 0 & 0 & 0 \\ 1-c_3 & 1-c_4 & c_4-c_3 & 0 & 0 \\ 1-c_2 & 1-c_4 & c_4-c_3 & c_3-c_2 & 0 \\ 1 & 1-c_4 & c_4-c_3 & c_3-c_2 & c_2 \\ \hline & 1-c_4 & c_4-c_3 & c_3-c_2 & c_2 \end{array}$$

From the method of construction, this design satisfies the symplectic condition for all choices of the parameters and now we consider the order of the pair.

Automatically, the conditions for the tree with one vertex are satisfied. Now try the condition $\widetilde{b}^{\intercal}c = \frac{1}{2}$. This gives

$$2c_2(c_4-c_3) + c_3^2 - \tfrac{1}{2} = 0.$$

The order condition $b^{\intercal}\widetilde{c} = \frac{1}{2}$ gives the same equation and we therefore assume that

$$c_2 = \frac{1-2c_3^2}{4(c_4-c_3)}.$$

Each of the four conditions for order 3 now become the single equation

$$\Big(24c_3^2-12\Big)c_4^2 - \Big(48c_3^2-16\Big)c_4 + \Big(12c_3^4+24c_3^2-16c_3-3\Big).$$

A convenient choice is $c_3 = 1$, leading to

$$c_4 = \tfrac{4}{3} - \tfrac{1}{6}\sqrt{13}.$$

We could also use its conjugate, which is regarded as less suitable because some of the abscissae lie outside the interval $[0,1]$.

The pair now becomes

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{2+\sqrt{13}}{6} & \frac{2+\sqrt{13}}{6} & 0 & 0 & 0 \\ 1 & \frac{2+\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & 0 & 0 \\ \frac{8-\sqrt{13}}{6} & \frac{2+\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & 0 \\ \hline & \frac{2+\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & \frac{-2+\sqrt{13}}{6} \end{array},$$

$$\begin{array}{c|cccc} \frac{-2+\sqrt{13}}{6} & \frac{-2+\sqrt{13}}{6} & 0 & 0 & 0 \\ 0 & \frac{-2+\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & 0 & 0 \\ \frac{4-\sqrt{13}}{6} & \frac{-2+\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & 0 \\ 1 & \frac{-2+\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & \frac{2+\sqrt{13}}{6} \\ \hline & \frac{-2+\sqrt{13}}{6} & \frac{2-\sqrt{13}}{6} & \frac{4-\sqrt{13}}{6} & \frac{2+\sqrt{13}}{6} \end{array}.$$

To test the quality of this method pair, and to set a standard for later tests with G-symplectic GLM pairs, we present a plot of the drift in the value of the Hamiltonian for the Heńon-Heiles problem on the interval $[0,10]$ using a stepsize $h = 10^{-4}$. The results are shown in Figure 1.

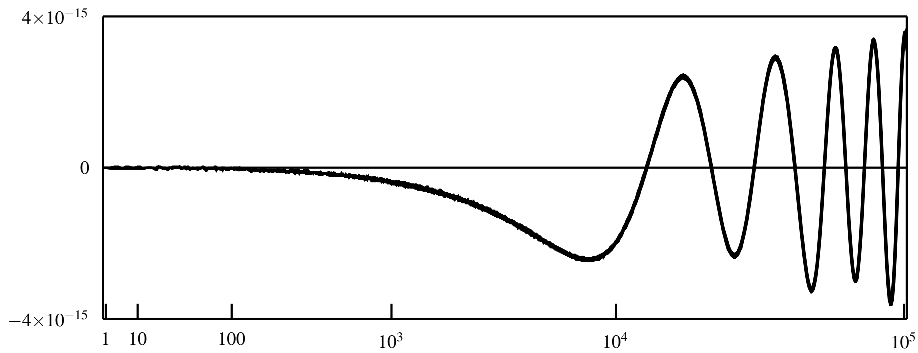


Figure 1: Numerical results for the Heńon-Heiles problem using an RK pair

4.2. Interchange symmetry of partioned GLMs

When we interpret a single step of a method *in the reverse direction*, we cannot expect the stages to exactly correspond to the stages in the forward direction; there might instead be a permutation of the stages involved. Denote P by this permutation and assume that $P^2 = I$, because a double reversal should give the original method. A typical case is where P exactly reverses the order of the stages, i.e. $P_{ij} = \delta_{i,s+1-j}$, $i, j, = 1, 2, \ldots, s$.

In this paper we will consider a limited type of time-reversal symmetry known as "interchange symmetry". This means that when the direction of time is changed, the two methods making up the partitioned are interchanged, but with the stages renumbered according to the permutation matrix P. This gives the equations

$$\widehat{Y} = h\widehat{A}\widehat{F} + \widehat{U}\widehat{y}^{[0]}, \tag{4.14}$$

$$\widehat{y}^{[1]} = h\widehat{B}\widehat{F} + \widehat{V}\widehat{y}^{[0]}, \tag{4.15}$$

$$P\widetilde{Y} = h(P\widetilde{A}P)(P\widetilde{F}) + P\widetilde{U}L\widetilde{y}^{[0]}, \tag{4.16}$$

$$L\widetilde{y}^{[1]} = h(\widetilde{B}P)(P\widetilde{F}) + \widetilde{V}L\widetilde{y}^{[0]},$$

with $L^2 = I$, leading to

$$\widetilde{y}^{[1]} = h(L\widetilde{B}P)(P\widetilde{F}) + (L\widetilde{V}L)\widetilde{y}^{[0]}. \tag{4.17}$$

From (4.14) and (4.15) we find

$$\widehat{Y} = -h\big(\widehat{U}\widehat{V}^{-1}\widehat{B} - \widehat{A}\big)\widehat{F} + \widehat{U}\widehat{V}^{-1}\widehat{y}^{[0]}, \tag{4.18}$$

$$\widehat{y}^{[0]} = -h\widehat{V}^{-1}\widehat{B}\widehat{F} + \widehat{V}^{-1}\widehat{y}^{[1]}, \tag{4.19}$$

By comparing (4.16) and (4.17) with (4.18) and (4.19) with $h \mapsto -h$, we find the symmetry conditions:

$$\widehat{A} + P\widetilde{A}P = \widehat{U}\widehat{V}^{-1}\widehat{B},\ \widehat{U}\widehat{V}^{-1} = P\widetilde{U}L,\ \widehat{V}^{-1}\widehat{B} = L\widetilde{B}P,\ \widehat{V}^{-1} = L\widetilde{V}L.$$

Thus, the following definition holds.

Definition 4.1. *A partitioned GLM* (2.4)-(2.5) *possesses interchange symmetry if*

$$\widehat{A}+P\widetilde{A}P=\widehat{U}\widehat{V}^{-1}\widehat{B}, \tag{4.20}$$

$$\widehat{U}\widehat{V}^{-1}=P\widetilde{U}L, \tag{4.21}$$

$$\widehat{V}^{-1}\widehat{B}=L\widetilde{B}P, \tag{4.22}$$

$$\widehat{V}^{-1}=L\widetilde{V}L. \tag{4.23}$$

It can be verified that these four statements imply the corresponding statements with the two methods interchanged.

4.3. Transformations of methods with interchange symmetry

In the transformation provided by (2.6) there is, in general, not reason to restrict the values of the non-singular matrices $\widehat{T}$ and $\widetilde{T}$. However, if the untransformed method-pair possesses interchange symmetry, and they are to be transformed into a pair which retains this property, we can always assume that $\widetilde{T}=\widehat{T}$. To verify this fact, apply the $\widehat{T}$ transformation to $\widehat{U}$, $\widehat{B}$, $\widehat{V}$ in (4.21)–(4.23). It is found that $\widetilde{U}$, $\widetilde{B}$, $\widetilde{V}$ transform according to $\widetilde{U}\to\widetilde{U}T$, $\widetilde{B}\to T^{-1}\widetilde{B}$, $\widetilde{V}\to T^{-1}\widetilde{V}T$.

4.4. Symmetric and G-symplectic methods depending on two input values

We now aim to determine the coefficient matrices of a G-symplectic partioned GLM (2.4)-(2.5) satisfying time-reversal symmetry and depending on two input values. We first observe that, for these methods, we can always assume without loss of generality that

$$\widehat{V}=\widetilde{V}=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},$$

since, from (4.23), both $\widehat{V}$ and $\widetilde{V}$ have to be power bounded. As a consequence, (3.13) leads to

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

Then, by using the notation $\mathbf{d}$ =diag, the following result holds.

Proposition 4.1. *A G-symplectic partitioned GLM* (2.4)-(2.5) *with* $r=2$ *possesses interchange symmetry if its coefficient matrices have the following form*

$$\left[\begin{array}{c|c}\widehat{A} & \widehat{U}\\ \hline \widehat{B} & \widehat{V}\end{array}\right]=\left[\begin{array}{c|cc}\widehat{A} & \mathbf{1} & -g\widetilde{x}\\ \hline \widehat{b}^{\top}\widehat{x} & 1 & 0\\ \widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x}) & 0 & -1\end{array}\right],\qquad \left[\begin{array}{c|c}\widetilde{A} & \widetilde{U}\\ \hline \widetilde{B} & \widetilde{V}\end{array}\right]=\left[\begin{array}{c|cc}\widetilde{A} & \mathbf{1} & -g\widehat{x}\\ \hline \widetilde{b} & 1 & 0\\ \widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x}) & 0 & -1\end{array}\right] \tag{4.24}$$

and satisfy

$$\widehat{A}=\widehat{U}\widehat{V}\widehat{B}-P\widetilde{A}P, \tag{4.25}$$

$$\widetilde{D}P\widetilde{A}P=\widetilde{A}^{\mathsf{T}}\widehat{D}, \tag{4.26}$$

with

$$G = \begin{bmatrix} 1 & 0 \\ 0 & g \end{bmatrix}, \qquad \widehat{D} = \mathbf{d}(\widehat{b}), \qquad \widetilde{D} = \mathbf{d}(\widetilde{b}),$$

and $\widehat{b} = P\widetilde{b}$, $\widehat{x} = -P\widetilde{x}$.

Proof: Once it is assumed that $\widehat{B} = \begin{bmatrix} \widehat{b}^{\mathsf{T}} \\ \widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x}) \end{bmatrix}$, we obtain

$$\widehat{D} = \widehat{B}^{\mathsf{T}} G \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \mathbf{d}(\widehat{b}),$$

and $\widehat{B} = \widehat{X}\widehat{D}$, where

$$\widehat{X} = \begin{bmatrix} \mathbf{1}^{\mathsf{T}} \\ \widehat{x}^{\mathsf{T}} \end{bmatrix}.$$

Under the previous assumptions, equation (3.13) is trivial, while (3.12) takes the form $\widehat{D}\widetilde{U} = \widehat{D}\widehat{X}^{\mathsf{T}}G\widehat{V}$, and implies that

$$\widetilde{U} = \widehat{X}^{\mathsf{T}}G\widehat{V} = \begin{bmatrix} \mathbf{1} \\ -g\widehat{x} \end{bmatrix}.$$

Moreover, by exploiting the hypothesis of time-reversal symmetry (4.22), equation (3.11) can be regarded as $\widetilde{D}\widehat{U} = P\widehat{B}^{\mathsf{T}}G$, and implies that $\widetilde{D} = P\widehat{D}P = \mathbf{d}(\widetilde{b})$, and

$$\widehat{U} = \begin{bmatrix} \mathbf{1} \\ g\widetilde{x} \end{bmatrix}.$$

Finally, equations (4.20) and (3.10) leads to (4.25) and (4.26).

□

5. Parasitic behaviour of partitioned general linear methods

Multivalue methods for which V has multiple eigenvalues on the unit circle suffer from parasitic behaviour, which destroys overall accuracy. Our approach will be to study the growth of perturbations in the output values. Consider the partitioned method in (2.4)-(2.5) and add a perturbation $(-1)^{n-1}\widehat{\lambda}_j^{[n-1]}$ to the external approximations $\widehat{y}_j^{[n-1]}$, $j = 2, \ldots, r$, and a perturbation $(-1)^{n-1}\widetilde{\lambda}_j^{[n-1]}$ to the external approximation $\widetilde{y}_j^{[n-1]}$, $j = 2, \ldots, r$. This means that the inputs of these components in step number $n-1$ then become

$$\widehat{y}_j^{[n-1]} + (-1)^{n-1}\widehat{\lambda}_j^{[n-1]}, \qquad \widetilde{y}_j^{[n-1]} + (-1)^{n-1}\widetilde{\lambda}_j^{[n-1]}, \quad j = 2, \ldots, r.$$

Denote the effects of these perturbations on internal stage number i by $\widehat{\delta Y}_i$ and $\delta\widetilde{Y}_i$, respectively. These are equal to

$$\widehat{\delta Y}_i = (-1)^{n-1}\sum_{j=2}^{r}\widehat{u}_{ij}\widehat{\lambda}_j^{[n-1]} + O(h) \qquad \delta\widetilde{Y}_i = (-1)^{n-1}\sum_{j=2}^{r}\widetilde{u}_{ij}\widetilde{\lambda}_j^{[n-1]} + O(h).$$

As a consequence of the perturbation of the internal stages, the stage derivatives will also be perturbed. Denote the deviations to $\widehat{f}(\widetilde{Y}_i)$ and $\widetilde{f}(\widehat{Y}_i)$ by $\delta\widehat{f}_i$ and $\delta\widetilde{f}_i$ respectively. Thus, we have

$$\delta\widehat{f}_i = (-1)^{n-1}\frac{\partial\widehat{f}}{\partial\widetilde{y}}\sum_{j=2}^{r}\widehat{u}_{ij}\widehat{\lambda}_j^{[n-1]}, \qquad \delta\widetilde{f}_i = (-1)^{n-1}\frac{\partial\widetilde{f}}{\partial\widehat{y}}\sum_{j=2}^{r}\widetilde{u}_{ij}\widetilde{\lambda}_j^{[n-1]}$$

We are now in a position to calculate the perturbations $\widehat{\lambda}_i^{[n]}$ and $\widetilde{\lambda}_i^{[n]}$ to $\widehat{y}_i^{[n]}$ and $\widetilde{y}_i^{[n]}$, respectively. These are

$$\begin{aligned}
\widehat{\lambda}^{[n]} &= -\dot{\widehat{V}}\widehat{\lambda}^{[n-1]} + h\dot{\widehat{B}}\dot{\widetilde{U}}\frac{\partial\widehat{f}}{\partial\widetilde{y}}\widetilde{\lambda}^{[n-1]},\\
\widetilde{\lambda}^{[n]} &= h\dot{\widetilde{B}}\dot{\widehat{U}}\frac{\partial\widetilde{f}}{\partial\widehat{y}}\lambda^{[n-1]} - \dot{\widetilde{V}}\widetilde{\lambda}^{[n-1]},
\end{aligned}$$

or, equivalently, in matrix notation,

$$\begin{bmatrix} \widehat{\lambda}^{[n]} \\ \widetilde{\lambda}^{[n]} \end{bmatrix} = \begin{bmatrix} -\dot{\widehat{V}} & h\widehat{\Gamma}\frac{\partial\widehat{f}}{\partial\widetilde{y}} \\ h\widetilde{\Gamma}\frac{\partial\widetilde{f}}{\partial\widehat{y}} & -\dot{\widetilde{V}} \end{bmatrix}\begin{bmatrix} \widehat{\lambda}^{[n-1]} \\ \widetilde{\lambda}^{[n-1]} \end{bmatrix},$$

where $\widehat{\Gamma} = \dot{\widehat{B}}\dot{\widetilde{U}}$ and $\widetilde{\Gamma} = \dot{\widetilde{B}}\dot{\widehat{U}}$. The dotted matrix is obtained by removing the first column and the first row. Thus, the growth of parasitism is removed if $\dot{\widehat{V}}$ and $\dot{\widetilde{V}}$ are power bounded and $\widehat{\Gamma} = 0$ or $\widetilde{\Gamma} = 0$. We observe that in the special case of G-symplectic methods with interchange symmetry depending on two input values, which are described in Proposition 4.1, we obtain

$$\widehat{\Gamma} = \widetilde{\Gamma} = -\big(\widehat{b}_1\widehat{x}_1^2 + \widehat{b}_2\widehat{x}_2^2 + \ldots + \widehat{b}_s\widehat{x}_s^2\big).$$

Thus, the following result holds.

Theorem 5.1. *A G-symplectic partitioned GLM* (2.4)-(2.5) *with $r = 2$ and possessing interchange symmetry is free from parasitism if*

$$\sum_{i=1}^{s}\widehat{b}_i\widehat{x}_i^2 = 0. \tag{5.27}$$

6. Order conditions

6.1. Trees, elementary differentials and B-series

At the heart of the theory involving orders of Runge–Kutta and related methods is the formula

$$y(x_0+h) = y_0 + \sum_{t\in T}\frac{h^{|t|}}{\sigma(t)t!}\mathsf{F}(t)(y_0) \tag{6.28}$$

Although (6.28) is relevant to solutions of the initial value problem

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0,$$

it applies equally to the system

$$\begin{aligned}
\widehat{y}'(x) &= \widehat{f}(\widetilde{y}), \qquad \widehat{y}(x_0) = \widehat{y}_0,\\
\widetilde{y}'(x) &= \widetilde{f}(\widehat{y}), \qquad \widetilde{y}(x_0) = \widetilde{y}_0,
\end{aligned}$$

and can be used alongside the expansions for $\widehat{y}(x_0+h)$ and $\widetilde{y}(x_0+h)$ given by

$$\begin{aligned}
\widehat{y}(x_0+h) &= \widehat{y}_0 + \sum_{t\in T} \frac{h^{|t|}}{\sigma(t)t!}\widehat{\mathbf{F}}(t)(\widehat{y}_0),\\
\widetilde{y}(x_0+h) &= \widetilde{y}_0 + \sum_{t\in T} \frac{h^{|t|}}{\sigma(t)t!}\widetilde{\mathbf{F}}(t)(\widetilde{y}_0),
\end{aligned} \tag{6.29}$$

assuming that the elementary differentials are defined using the following recursions

$$\begin{aligned}
\widehat{\mathbf{F}}(\tau) &= \widehat{\mathbf{f}},\\
\widetilde{\mathbf{F}}(\tau) &= \widetilde{\mathbf{f}},\\
\widehat{\mathbf{F}}([t_1,t_2,\dots,t_m]) &= \widehat{\mathbf{f}}^{(m)}(\widetilde{F}(t_1),\widetilde{F}(t_2),\dots,\widetilde{F}(t_m)),\\
\widetilde{\mathbf{F}}([t_1,t_2,\dots,t_m]) &= \widetilde{\mathbf{f}}^{(m)}(\widehat{F}(t_1),\widehat{F}(t_2),\dots,\widehat{F}(t_m)).
\end{aligned}$$

The Taylor expansions (6.28) and (6.29) can be generalized to give

$$\begin{aligned}
\frac{h^{|u|}}{\sigma(u)}\widehat{\mathbf{F}}(u)\widehat{y}(x_0+h) &= \sum_{t\in T} C(u,t)\frac{h^{|t|}}{\sigma(t)}\widehat{\mathbf{F}}(t)(\widehat{y}_0),\\
\frac{h^{|u|}}{\sigma(u)}\widetilde{\mathbf{F}}(u)\widetilde{y}(x_0+h) &= \sum_{t\in T} C(u,t)\frac{h^{|t|}}{\sigma(t)}\widetilde{\mathbf{F}}(t)(\widetilde{y}_0).
\end{aligned}$$

The values of $C(u,t)$ up to $|u|,|t| \le 4$ are shown in Table 1. The special case in which $y(x_0+h)$ is written in accordance with (6.28) is included using the well-known convention that $\mathbf{F}(\emptyset)(y_0) = y_0$. Given a mapping $\alpha : \{\emptyset\}\cup T \to \mathbb{R}$, a B-series $\mathbf{B}(\alpha, y_0)$ is defined by

$$\mathbf{B}(\alpha, y_0) = \alpha(\emptyset)y_0 + \sum_{t\in T} \frac{\alpha(t)h^{|t|}}{\sigma(t)}\mathbf{F}(t)(y_0).$$

The particular choice of α corresponding to (6.28) will be denoted by $\mathbf{E}$, so that

$$\begin{aligned}
\mathbf{E}(\emptyset) &= 1,\\
\mathbf{E}(t) &= \frac{1}{t!}.
\end{aligned}$$

In dealing with classical (first order) differential equation systems, the B-series defined by $\emptyset \mapsto 0$, $\tau \mapsto 1$, $t \mapsto 0$ for all other trees, plays a central role; but this cannot be

$u \backslash t$	$\emptyset$	$\bullet$							
$\emptyset$	1	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{12}$	$\frac{1}{24}$
$\bullet$		1	1	1	$\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$
			1	2	1	3	$\frac{3}{2}$	1	$\frac{1}{2}$
				1	0	3	1	0	0
					1	0	1	2	1
						1	0	0	0
							1	0	0
								1	0
									1

Table 1: Values of $C(u,t)$ for $|u|,|t| \le 4$

extended in a simple way to partitioned systems because the two series, for expansions based on functions of $\widehat{y}_0$ and on $\widetilde{y}_0$, are interrelated. The composition of a B-series $\mathbf{B}(\alpha, y_0) = y_0 + \cdots$ with $\mathbf{D}$, in the classical case, is equal to $\mathbf{B}(\alpha\mathbf{D}, y_0)$, where $\alpha\mathbf{D}$ is given according to the formula

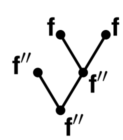
$$(\alpha D)(\emptyset) = 0,$$
$$(\alpha D)(\tau) = 1,$$
$$(\alpha D)([t_1, t_2, \ldots, t_m]) = \prod_{i=1}^{m} \alpha(t_i).$$

However, in applications to partitioned methods we will need to involve a pair of B-series, $\mathbf{B}(\widehat{\alpha}, \widehat{y}_0) = \widehat{\alpha}(\emptyset)\widehat{y}_0 + \cdots$ and $\mathbf{B}(\widetilde{\alpha}, \widetilde{y}_0) = \widetilde{\alpha}(\emptyset)\widetilde{y}_0 + \cdots$. In this case

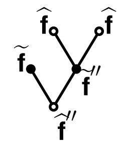
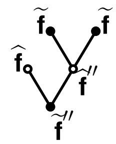
$$\left(\begin{bmatrix} \widehat{\alpha} \\ \widetilde{\alpha} \end{bmatrix} \mathbf{D} \right)([t_1, t_2, \ldots, t_m]) = \begin{bmatrix} \prod_{i=1}^{m} \widetilde{\alpha}(t_i) \\ \prod_{i=1}^{m} \widehat{\alpha}(t_i). \end{bmatrix}. \tag{6.30}$$

To avoid clumsiness, we will, throughout this section observe the convention that $\widehat{\alpha}$ and $\widetilde{\alpha}$ always come in pairs and that $\widehat{\alpha}\mathbf{D}$ and $\widetilde{\alpha}\mathbf{D}$ are the two components on the right of (6.30).

It is customary to represent elementary differentials for separable problems using bi-coloured trees. For example, consider the tree $t = [\tau[\tau^2]]$, for which, for the classical (non-separable) problem, $F(t)$ is represented by the tree, with operators attached to the vertices,



In the case of separable methods, the two elementary differentials $\widehat{\mathbf{F}}(t)$ and $\widetilde{\mathbf{F}}(t)$ are represented by bi-coloured trees as follows:

$\widehat{\mathbf{F}}(t) =$  $\qquad \widetilde{\mathbf{F}}(t) =$ 

6.2. Order of partitioned general linear methods

Given a pair of starting methods, represented by vectors of B-series coefficients $\widehat{\psi}$ and $\widetilde{\psi}$, we write the stage values, represented by $\widehat{\eta}, \widetilde{\eta}$, and the output value order p conditions as follows:

$$\widehat{\eta} = \widehat{A}\widehat{\eta}\mathbf{D} + \widehat{U}\widehat{\psi}, \tag{6.31}$$

$$\widetilde{\eta} = \widetilde{A}\widetilde{\eta}\mathbf{D} + \widetilde{U}\widetilde{\psi}, \tag{6.32}$$

$$\widehat{B}\widehat{\eta}\mathbf{D} + \widehat{V}\widehat{\psi} = E\widehat{\psi}, \tag{6.33}$$

$$\widetilde{B}\widetilde{\eta}\mathbf{D} + \widetilde{V}\widetilde{\psi} = E\widetilde{\psi} \tag{6.34}$$

where (6.33) and (6.34) each hold up to trees of order p. This extends the standard definition of order to the partitioned case. For Runge–Kutta methods, classical oder requires $\widehat{\psi} = \widetilde{\psi} = 1$, the identity B-series and the definition which allows more general $\widehat{\psi}, \widetilde{\psi}$ is known as “effective order”.

In this paper we will aim only to make a slight extension to what is standard for Runge–Kutta methods. We will make several assumptions to achieve this aim; these are

1. $r = 2$,
2. $\widehat{V} = \widetilde{V} = \operatorname{diag}(1, -1)$,
3. $\widehat{\psi}e_1 = \widetilde{\psi}e_1 = 1$,
4. $\widehat{U}e_1 = \widetilde{U}e_1 = \mathbf{1}$,
5. $(\widehat{B}\widehat{\psi}\mathbf{D} + \widehat{V}\widehat{\psi} - \mathbf{E}\widehat{\psi})e_2 = (\widetilde{B}\widetilde{\psi}\mathbf{D} + \widetilde{V}\widetilde{\psi} - \mathbf{E}\widetilde{\psi})e_2 = 0$.

We will also assume that the method-pair is G-symplectic with $G = \operatorname{diag}(1, g)$, $D = \operatorname{diag}(b)$, $\widetilde{D} = \operatorname{diag}(\widetilde{b})$. According to Proposition 4.1, write the method pair in the form

$$\left(\left[\begin{array}{c|cc} \widehat{A} & \mathbf{1} & -g\widetilde{x} \\ \hline \widehat{b}^{\mathsf{T}} & 1 & 0 \\ \widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x}) & 0 & -1 \end{array} \right], \left[\begin{array}{c|cc} \widetilde{A} & \mathbf{1} & -g\widehat{x} \\ \hline \widetilde{b}^{\mathsf{T}} & 1 & 0 \\ \widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x}) & 0 & -1 \end{array} \right] \right),$$

so that all the G-symplectic conditions are satisfied as long as

$$\widehat{D}\widetilde{A} + \widehat{A}^{\mathsf{T}}\widetilde{D} = \widehat{B}^{\mathsf{T}}G\widetilde{B}.$$

Write the second components of the starting methods as

$$\widehat{\psi}e_2 = \widehat{\xi}, \qquad \widetilde{\psi}e_2 = \widetilde{\xi}.$$

With these choices, rewrite (6.31) – (6.34), where each of the components of (6.33) and (6.34) are written out separately. It will always be required, that $\widehat{\eta}(\emptyset)=\widetilde{\eta}(\emptyset)=1$ and that $\widehat{\xi}(\emptyset)=\widetilde{\xi}(\emptyset)=0$:

$$\widehat{\eta}(t)=\widehat{A}(\widehat{\eta}\mathsf{D})(t)-g\widetilde{x}\widehat{\xi}(t), \tag{6.35}$$

$$\widetilde{\eta}(t)=\widetilde{A}(\widetilde{\eta}\mathsf{D})(t)-g\widehat{x}\widetilde{\xi}(t), \tag{6.36}$$

$$(\widehat{b}^{\intercal}\widehat{\eta}\mathsf{D})(t)=\frac{1}{t!}, \tag{6.37}$$

$$(\widetilde{b}^{\intercal}\widetilde{\eta}\mathsf{D})(t)=\frac{1}{t!}, \tag{6.38}$$

$$\widehat{\xi}(t)+(\mathsf{E}\widehat{\xi})(t)=\widehat{b}^{\intercal}\mathbf{d}(\widehat{x})(\widehat{\eta}\mathsf{D})(t), \tag{6.39}$$

$$\widetilde{\xi}(t)+(\mathsf{E}\widetilde{\xi})(t)=\widetilde{b}^{\intercal}\mathbf{d}(\widetilde{x})(\widetilde{\eta}\mathsf{D})(t) \tag{6.40}$$

6.3. Conditions up to order 4

Now apply equations (6.35) – (6.40) to find the various B-series coefficients for $\widehat{\xi}$, $\widetilde{\xi}$, $\widehat{\eta}$, $\widetilde{\eta}$ in the case of $t=\tau,[\tau],[\tau^2],[[\tau]]$. Later we will use the results for $\widehat{\eta}(t),\widetilde{\eta}(t)$ to write down the remaining conditions required for order 4. Throughout the calculations, we will write

$$\widehat{c}=\widehat{A}\mathbf{1}-\tfrac{1}{2}g(b^{\intercal}\widehat{x})\widetilde{x},$$
$$\widetilde{c}=\widetilde{A}\mathbf{1}-\tfrac{1}{2}g(\widetilde{b}^{\intercal}\widetilde{x})\widehat{x}.$$

We are presenting only the formulae for $\widehat{\xi}(t)$ etc because the corresponding results for $\widetilde{\xi}(t)$ etc are identical subject to interchanging $\widehat{c}$ with $\widetilde{c}$ etc. From (6.39), we find, making use of Table 1,

$$2\widehat{\xi}(\tau)=\widehat{b}^{\intercal}\mathbf{d}(\widehat{x})(\widehat{\eta}\mathsf{D})(\tau), \tag{6.41}$$

$$2\widehat{\xi}([\tau])+\widehat{\xi}(\tau)=\widehat{b}^{\intercal}\mathbf{d}(\widehat{x})(\widehat{\eta}\mathsf{D})([\tau]), \tag{6.42}$$

$$2\widehat{\xi}([\tau^2])+2\widehat{\xi}([\tau])+\widehat{\xi}(\tau)=\widehat{b}^{\intercal}\mathbf{d}(\widehat{x})(\widehat{\eta}\mathsf{D})([\tau^2]), \tag{6.43}$$

$$2\widehat{\xi}([[\tau]])+\widehat{\xi}([\tau])+\tfrac{1}{2}\widehat{\xi}(\tau)=\widehat{b}^{\intercal}\mathbf{d}(\widehat{x})(\widehat{\eta}\mathsf{D})([[\tau]]). \tag{6.44}$$

From (6.41)–(6.44) and (6.37) we find in turn

$$\widehat{\xi}(\tau) = \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\widehat{x}, \tag{6.45}$$

$$\widehat{\eta}(\tau) = \widehat{A}\mathbf{1} - \tfrac{1}{2}g(\widehat{b}^{\mathsf{T}}\widehat{x})\widetilde{x} = \widehat{c}, \tag{6.46}$$

$$(\widehat{\eta}\mathsf{D})([\tau]) = \widetilde{c}, \tag{6.47}$$

$$(\widehat{\eta}\mathsf{D})([\tau^2]) = \widetilde{c}^2, \tag{6.48}$$

$$(\widehat{\eta}\mathsf{D})([\tau^3]) = \widetilde{c}^3, \tag{6.49}$$

$$\widehat{\xi}([\tau]) = \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\widehat{x}, \tag{6.50}$$

$$\widehat{\xi}([\tau^2]) = \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^2 - \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}, \tag{6.51}$$

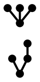
$$\widehat{\eta}([\tau]) = \widehat{A}\widetilde{c} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\widehat{x}\big)\widetilde{x}, \tag{6.52}$$

$$\widehat{\eta}([\tau^2]) = \widehat{A}\widetilde{c}^2 - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^2 - \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}\big)\widetilde{x}, \tag{6.53}$$

$$\widehat{\xi}([[\tau]]) = \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^2 - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}, \tag{6.54}$$

$$\widehat{\eta}([[\tau]]) = \widehat{A}\big(\widetilde{A}\widehat{c} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)\widehat{x}\big) - g\big(\tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^2 - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}\big)\widetilde{x}. \tag{6.55}$$

We are now in a position to evaluate $(\widehat{\eta}\mathsf{D})(t)$ for the trees of order up to 4. Trees will be written in both algebraic form and pictorial form.

Tree	t	$(\widehat{\eta}\mathsf{D})(t)$
	τ	$\mathbf{1}$
	$[\tau]$	$\widetilde{c}$
	$[\tau^2]$	$\widetilde{c}^2$
	$[[\tau]]$	$\widetilde{A}\widehat{c} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)\widehat{x}$
	$[\tau^3]$	$\widetilde{c}^3$
	$[\tau[\tau]]$	$\mathbf{d}(\widetilde{c})\widetilde{A}c - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)\mathbf{d}(\widetilde{c})\widehat{x}$
	$[[\tau^2]]$	$\widetilde{A}\widehat{c}^2 - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}^2 - \tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}\big)\widehat{x}$
	$[[[\tau]]]$	$\widetilde{A}\big(\widehat{A}\widetilde{c} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\widehat{x}\big)\widetilde{x}\big) - g\big(\tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}^2 - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}\big)\widehat{x}$

Now write down the 16 order conditions, corresponding to the bi-coloured trees of orders 1 to 4.

$$\widehat{b}^{\mathsf{T}}\mathbf{1} = 1 \tag{6.56}$$

$$\widetilde{b}^{\mathsf{T}}\mathbf{1} = 1 \tag{6.57}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{c} = \frac{1}{2} \tag{6.58}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{c} = \frac{1}{2} \tag{6.59}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{c}^{2} = \frac{1}{3} \tag{6.60}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{c}^{2} = \frac{1}{3} \tag{6.61}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{A}\widehat{c} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)b^{\mathsf{T}}x = \frac{1}{6} \tag{6.62}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{A}\widetilde{c} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\widehat{x}\big)\widetilde{b}^{\mathsf{T}}\widetilde{x} = \frac{1}{6} \tag{6.63}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{c}^{3} = \frac{1}{4} \tag{6.64}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{c}^{3} = \frac{1}{4} \tag{6.65}$$

$$\widehat{b}^{\mathsf{T}}\mathbf{d}(\widetilde{c})\widetilde{A}\widehat{c} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)b^{\mathsf{T}}\mathbf{d}(\widetilde{c})\widehat{x} = \frac{1}{8} \tag{6.66}$$

$$\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widehat{c})\widehat{A}\widetilde{c} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\widehat{x}\big)\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widehat{c})\widetilde{x} = \frac{1}{8} \tag{6.67}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{A}\widehat{c}^{2} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}^{2} - \tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}\big)\widehat{b}^{\mathsf{T}}\widehat{x} = \frac{1}{12} \tag{6.68}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{A}\widetilde{c}^{2} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^{2} - \tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}\big)\widetilde{b}^{\mathsf{T}}\widetilde{x} = \frac{1}{12} \tag{6.69}$$

$$\widehat{b}^{\mathsf{T}}\widetilde{A}\big(\widehat{A}\widetilde{c} - g\big(\tfrac{1}{2}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}x\big)\widetilde{x}\big) - g\big(\tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}^{2} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c}\big)\widehat{b}^{\mathsf{T}}\widehat{x} = \frac{1}{24} \tag{6.70}$$

$$\widetilde{b}^{\mathsf{T}}\widehat{A}\big(\widetilde{A}\widehat{c} - g\big(\tfrac{1}{2}\widetilde{b}^{\mathsf{T}}\mathbf{d}(\widetilde{x})\widehat{c} - \tfrac{1}{4}\widetilde{b}^{\mathsf{T}}\widetilde{x}\big)\widehat{x}\big) - g\big(\tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}^{2} - \tfrac{1}{4}\widehat{b}^{\mathsf{T}}\mathbf{d}(\widehat{x})\widetilde{c}\big)\widetilde{b}^{\mathsf{T}}\widehat{x} = \frac{1}{24} \tag{6.71}$$

7. Construction of methods

We apply the results developed in the previous sections in order to derive G-symplectic partitioned GLMs (2.4)-(2.5) with $r = 2$, satisfying interchange symmetry and free of parasitism. We also require that the matrix A is strictly lower triangular and the matrix $\widetilde{A}$ is lower triangular: in this way, the whole numerical scheme results to be fully explicit. In our construction, following the lines drawn for the RK model in the previous section, we always assume that $\widetilde{c} = \mathbf{1} - c$.

We first focus our attention on the family of two-stage G-symplectic methods (2.4)-(2.5) satisfying interchange symmetry. According to Proposition 4.1, such methods satisfy (4.24) with

$$A = \begin{bmatrix} 0 & 0 \\ b_1(1 - gx_1^2) & 0 \end{bmatrix}, \qquad \widetilde{A} = \begin{bmatrix} b_2(1 - gx_1x_2) & 0 \\ b_2(1 - gx_2^2) & b_1(1 - gx_1x_2) \end{bmatrix}.$$

In order to eliminate the parasitic behaviour of the methods, we next solve Equation (5.27) and finally impose as many order conditions as possible from the set of equations

(6.56)-(6.71). Due to the number of degrees of freedom, we are able to derive a family of methods of order 2. A member of this family is the partitioned GLM

$$M = \left[\begin{array}{cc|cc} 0 & 0 & 1 & \frac{463}{2232} \\ \frac{33}{217} & 0 & 1 & \frac{463}{2976} \\ \hline \frac{16}{7} & -\frac{9}{7} & 1 & 0 \\ \frac{96}{7} & -\frac{72}{7} & 0 & -1 \end{array}\right], \qquad \widetilde{M} = \left[\begin{array}{cc|cc} \frac{39}{124} & 0 & 1 & -\frac{463}{2976} \\ \frac{184}{217} & -\frac{52}{93} & 1 & -\frac{463}{2232} \\ \hline -\frac{9}{7} & \frac{16}{7} & 1 & 0 \\ \frac{72}{7} & -\frac{96}{7} & 0 & -1 \end{array}\right] \tag{7.72}$$

with $c = [\frac{463}{1302} \quad \frac{727}{1736}]^{\intercal}$, $\widetilde{c} = [\frac{1009}{1736} \quad \frac{839}{1302}]^{\intercal}$, and

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \frac{463}{17856} \end{bmatrix}, \qquad D = \begin{bmatrix} \frac{16}{7} & 0 \\ 0 & -\frac{9}{7} \end{bmatrix}, \qquad \widetilde{D} = \begin{bmatrix} -\frac{9}{7} & 0 \\ 0 & \frac{16}{7} \end{bmatrix}.$$

Order 3 of convergence is achievable by involving three internal stages, thus we consider G-symplectic methods (2.4)-(2.5) with $s = 3$ and satisfying interchange symmetry. From Proposition 4.1, it follows that such methods satisfy (4.24) with

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ b_1(1-gx_1x_3) & 0 & 0 & 0 \\ b_1(1-gx_1x_2) & b_2(1-gx_2^2) & 0 & 0 \\ b_1(1-gx_1^2) & b_2(1-gx_1x_2) & b_3(1-gx_1x_3) & 0 \end{bmatrix},$$

$$\widetilde{A} = \begin{bmatrix} b_4(1-gx_1x_4) & 0 & 0 & 0 \\ b_4(1-gx_2x_4) & b_3(1-gx_2x_3) & 0 & 0 \\ b_4(1-gx_3x_4) & b_3(1-gx_3^2) & b_2(1-gx_2x_3) & 0 \\ b_4(1-gx_4^2) & b_3(1-gx_3x_4) & b_2(1-gx_2x_4) & b_1(1-gx_1x_4) \end{bmatrix}.$$

Through symbolic manipulations, we solve Equation (5.27) and order conditions (6.56)-(6.61) and obtain the method

$$M = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & -\frac{325}{448} \\ \frac{33}{64} & 0 & 0 & 1 & \frac{14625}{14336} \\ \frac{41}{48} & -\frac{1}{4} & 0 & 1 & \frac{325}{512} \\ \hline \frac{24}{17} & -\frac{128}{187} & \frac{3}{11} & 1 & 0 \\ \frac{224}{255} & -\frac{128}{187} & -\frac{32}{165} & 0 & -1 \end{array}\right], \quad \widetilde{M} = \left[\begin{array}{ccc|cc} \frac{19}{48} & 0 & 0 & 1 & -\frac{325}{512} \\ \frac{2319}{4928} & \frac{17}{1232} & 0 & 1 & -\frac{14625}{14336} \\ \frac{61}{462} & -\frac{1546}{1309} & \frac{209}{102} & 1 & \frac{325}{448} \\ \hline \frac{3}{11} & -\frac{128}{187} & \frac{24}{17} & 1 & 0 \\ \frac{32}{165} & \frac{128}{187} & -\frac{224}{255} & 0 & -1 \end{array}\right] \tag{7.73}$$

with $c = [0 \quad \frac{33}{64} \quad \frac{29}{48}]^{\intercal}$, $\widetilde{c} = [\frac{19}{48} \quad \frac{31}{64} \quad 1]^{\intercal}$ and

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \frac{14625}{14336} \end{bmatrix}.$$

It is worth observing that, according to the results in Section 4.1, a symplectic partioned Runge-Kutta of order 3 necessarily requires four internal stages. Here we only need to involve three stages, thus we save some function evaluations and gain the same accuracy with a lower computational effort.

7.1. Starting method

To obtain a starting method pair for the method (7.72), use the information in Table 1 and the values of the coefficients in the method, to find

$$\begin{aligned} \widehat{\xi}_1 &= \widehat{b}^\top \mathbf{1} - \widehat{\xi}_1 = \tfrac{24}{7} - \widehat{\xi}_1, \\ \widehat{\xi}_1 + \widehat{\xi}_2 &= \widehat{b}^\top \widetilde{c} - \widehat{\xi}_2 = \tfrac{2040}{1519} - \widehat{\xi}_2, \\ \widetilde{\xi}_1 &= \widetilde{b}^\top \mathbf{1} - \widetilde{\xi}_1 = -\tfrac{24}{7} - \widetilde{\xi}_1, \\ \widetilde{\xi}_1 + \widetilde{\xi}_2 &= \widetilde{b}^\top \widehat{c} - \widetilde{\xi}_2 = -\tfrac{3168}{1519} - \widetilde{\xi}_2. \end{aligned}$$

Solve these to give

$$\widehat{\xi}_1 = -\widetilde{\xi}_1 = \frac{12}{7}, \qquad \widehat{\xi}_2 = \widetilde{\xi}_2 = -\frac{282}{1519}.$$

Practical starting algorithms can now be found from

$$\begin{aligned} \widehat{y}_1^{[0]} &= \widehat{y}_0, \\ \widehat{y}_2^{[0]} &= \tfrac{12}{7} h \widehat{f}\big(\widetilde{y}_0 - \tfrac{47}{434} h \widetilde{f}(\widehat{y}_0)\big), \\ \widetilde{y}_1^{[0]} &= \widetilde{y}_0, \\ \widetilde{y}_2^{[0]} &= -\tfrac{12}{7} h \widetilde{f}\big(\widehat{y}_0 + \tfrac{47}{434} h \widehat{f}(\widetilde{y}_0)\big). \end{aligned}$$

Similarly, to make the method (7.73) available as a practical algorithm, we will construct a starting method. The first step will be to find the B-series coefficients $\widehat{\xi}(t)$, $\widetilde{\xi}(t)$, for trees up to order 3. To simplify the notation we will write $\widehat{\xi}_1 = \widehat{\xi}(\tau)$, $\widehat{\xi}_2 = \widehat{\xi}([\tau])$, $\widehat{\xi}_3 = \widehat{\xi}([\tau^2])$, $\widehat{\xi}_4 = \widehat{\xi}([[\tau]])$.and similarly for $\widetilde{\xi}_i$, $i = 1,2,3,4$. Taking account of the special properties of the method pair, $\widehat{b}^\intercal \widehat{x} = \widetilde{b}^\intercal \widetilde{x} = 0$, we can find a simple expression for $(\widehat{\eta} D)_i$ and $(\widetilde{\eta} D)_i$, for $i = 4$, which we add to known expressions for $i = 1,2,3$:

$$\begin{aligned} (\widehat{\eta}D)_1 &= \mathbf{1}, & (\widetilde{\eta}D)_1 &= \mathbf{1}, \\ (\widehat{\eta}D)_2 &= \widetilde{c}, & (\widetilde{\eta}D)_2 &= \widehat{c}, \\ (\widehat{\eta}D)_3 &= \widetilde{c}^2, & (\widetilde{\eta}D)_3 &= \widehat{c}^2, \\ (\widehat{\eta}D)_4 &= \widetilde{A}\widehat{c} - \tfrac{1}{2} g\big(\widehat{b}^\intercal \mathbf{d}(\widehat{x})\widehat{c}\big)\widehat{x}, & (\widetilde{\eta}D)_4 &= \widehat{A}\widetilde{c} - \tfrac{1}{2} g\big(\widehat{b}^\intercal \mathbf{d}(\widetilde{x})\widetilde{c}\big)\widetilde{x}. \end{aligned}$$

Substitute into (6.41)–(6.44), and the corresponding equations for the $\widetilde{\xi}(t)$, and we find for the method (7.73), the values

$$\begin{aligned} \widehat{\xi}_1 &= \widetilde{\xi}_1 = 0, \\ \widehat{\xi}_2 &= \widetilde{\xi}_2 = -\tfrac{4}{45}, \\ -\widehat{\xi}_3 &= \widetilde{\xi}_3 = \tfrac{169}{8640}, \\ -\widehat{\xi}_4 &= \widetilde{\xi}_4 = \tfrac{41}{2160} \end{aligned}$$

For the remainder of this subsection, the notations $(\widehat{A},\widehat{b},\widehat{c})$ and $(\widetilde{A},\widetilde{b},\widetilde{c})$ will refer to tableaux for a Runge–Kutta pair used to compute starting approximations for the second inputs to the general linear method under consideration. That is, the inputs are found from

$$\begin{aligned} \widehat{y}_1^{[0]} &= \widehat{y}_0, & \widetilde{y}_1^{[0]} &= \widetilde{y}_0, \\ \widehat{Y} &= \widehat{y}_0 + h\widehat{A}\widehat{F}, & \widetilde{Y} &= \widetilde{y}_0 + h\widetilde{A}\widetilde{F}, \\ \widehat{y}_2^{[0]} &= h\widehat{b}^{\intercal}\widehat{F}, & \widetilde{y}_2^{[0]} &= h\widetilde{b}^{\intercal}\widetilde{F}, \end{aligned}$$

where $\widehat{F}_i = \widehat{f}(\widetilde{Y}_i)$, $\widetilde{F}_i = \widetilde{f}(\widehat{Y}_i)$, $i = 1,2,\ldots,s$.

To ensure that the general linear method pair has order 3 relative to the proposed starting procedure, we need to choose the starting Runge–Kutta pair to satisfy

$$\begin{aligned} \widehat{b}\mathbf{1} &= \widehat{\xi}_1, & \widetilde{b}\mathbf{1} &= \widetilde{\xi}_1, \\ \widehat{b}\widetilde{c} &= \widehat{\xi}_2, & \widetilde{b}\widehat{c} &= \widetilde{\xi}_2, \\ \widehat{b}\widetilde{c}^2 &= \widehat{\xi}_3, & \widetilde{b}\widehat{c}^2 &= \widetilde{\xi}_3, \\ \widehat{b}\widetilde{A}\widehat{c} &= \widehat{\xi}_4, & \widetilde{b}\widehat{A}\widetilde{c} &= \widetilde{\xi}_4. \end{aligned}$$

A possible solution to these equations with $s = 3$ is the method pair

$$\begin{array}{c|ccc} 0 & & & \\ \frac{53}{256} & \frac{53}{256} & & \\ -\frac{53}{256} & 0 & -\frac{53}{256} & \\ \hline & \frac{173056}{379215} & -\frac{1024}{75843} & -\frac{167936}{379215} \end{array}\;, \qquad \begin{array}{c|ccc} 0 & & & \\ -\frac{53}{256} & -\frac{53}{256} & & \\ \frac{53}{256} & 0 & \frac{53}{256} & \\ \hline & -\frac{173056}{379215} & \frac{1024}{75843} & \frac{167936}{379215} \end{array}$$

and simulations presented in the next section will use this starting procedure.

8. Numerical experiments

We present in this section some numerical results obtained by applying the order 3 partitioned GLM (7.73). We first apply this method to the simple pendulum problem

$$\begin{aligned} \dot{p}(t) &= -\sin(q(t)), \\ \dot{q}(t) &= p(t), \\ p(0) &= 0, \\ q(0) &= 2.3, \end{aligned} \tag{8.74}$$

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

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

is separable and preserved along the time. In this particular example, the Hamiltonian is the total energy associated to the dynamical system and we aim to preserve it over a long time interval of integration. This would not be possible in general by using G-symplectic partitioned GLMs because, when they are applied to this problem, they suffer from parasitic behaviour. However, the methods presented in Section 7 are free of parasitism, since they satisfy condition (5.27). The absence of parasitism is also advisable from the numerical evidence: in fact, the implemented methods are able to realize a very accurate conservation of the total energy of the system, within round-off error. In our implementation, in order to control the propagation of the round-off error, we have always used compensated summations. Figures 2 and 3 show the patterns of the Hamiltonian deviations in each step of the integration carried out by applying one million steps of methods (7.72) and (7.73), respectively.

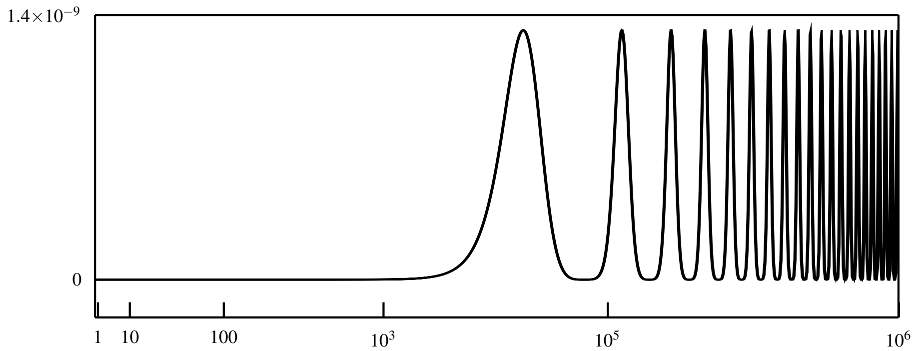


Figure 2: Hamiltonian deviation associated to 10^6 steps of (7.72) to problem (8.74), with $h = 10^{-4}$

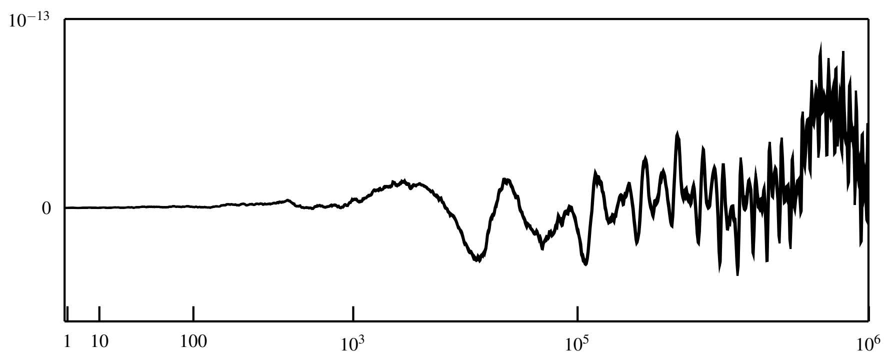


Figure 3: Hamiltonian deviation associated to 10^6 steps of (7.73) to problem (8.74), with $h = 10^{-4}$

We next consider the Heńon-Heiles problem

$$\begin{aligned} \dot{p}_1(t) &= -q_1(t)(1+2q_2(t)), \\ \dot{p}_2(t) &= -(q_2(t)+q_1^2(t)-q_2^2(t)), \\ \dot{q}_i(t) &= p_i(t), \quad i=1,2, \end{aligned} \tag{8.75}$$

with $q_1(0) = q_2(0) = p_2(0) = 0, p_1(0) = \sqrt{0.3185}$. whose Hamiltonian is

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

The behavoiur of the methods object of investigation is described in Figures 4 and 5, where the observed Hamiltonian deviations are plotted at each time step.

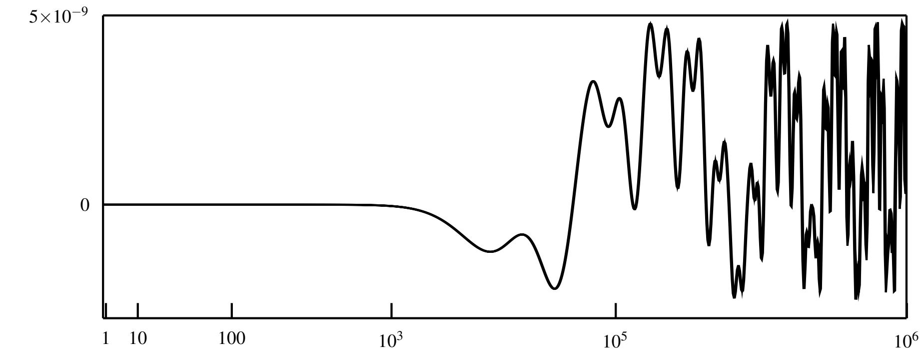


Figure 4: Hamiltonian deviation associated to 10^6 steps of (7.72) to problem (8.75), with $h = 10^{-4}$

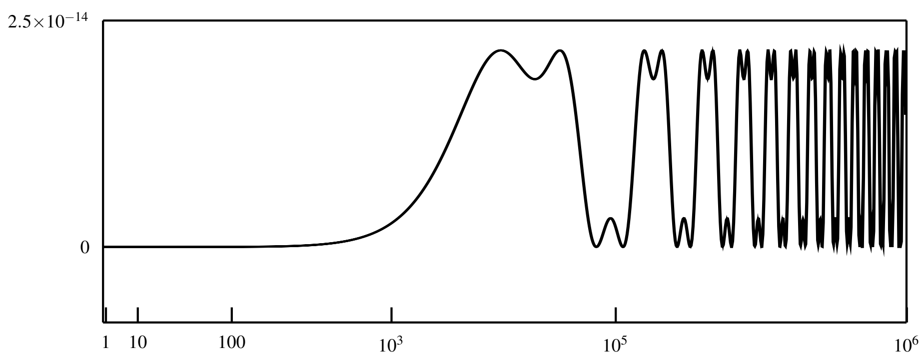


Figure 5: Hamiltonian deviation associated to 10^6 steps of (7.73) to problem (8.75), with $h = 10^{-4}$

We finally focus our attention on the Kepler problem

$$\begin{aligned} \dot{p}_i(t) &= -\frac{q_i(t)}{(q_1(t)^2 + q_2(t)^2)^{3/2}}, \\ \dot{q}_i(t) &= p_i(t), \quad i = 1, 2, \end{aligned} \tag{8.76}$$

with $q_1(0) = 1 - e$, $q_2(0) = p_1(0) = 0$, $p_2(0) = \sqrt{\frac{1+e}{1-e}}$, being $0 \le e < 1$ the eccentricity of the elliptic orbits described by the motion of a planet revolving around sun. The Hamiltonian of this problem is

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

The observed Hamiltonian deviations when methods (7.72) and (7.73) are applied to this problem are reported in Figures 6 and 7. As the angular momentum is preserved by the continous problem, our method is also able to accurately preserve it, as shown in Figures 8 and 9.

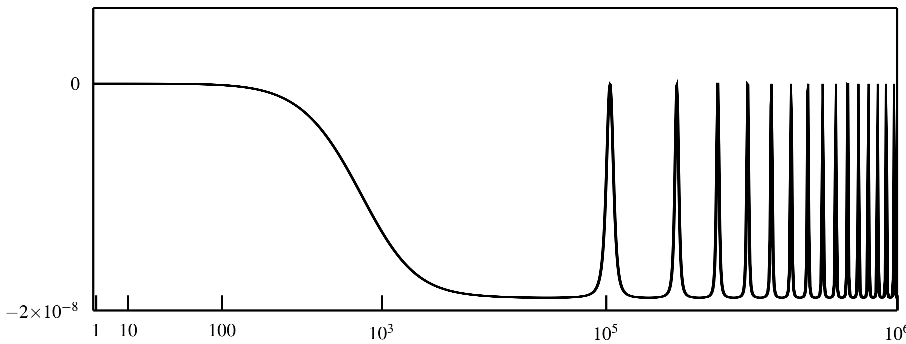


Figure 6: Hamiltonian deviation associated to 10^6 steps of (7.72) to problem (8.76), with $e = 1/2$ and stepsize $h = 10^{-4}$

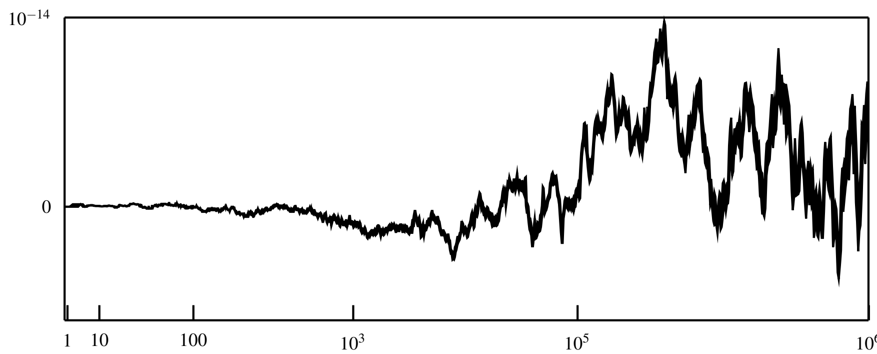


Figure 7: Hamiltonian deviation associated to 10^6 steps of (7.73) to problem (8.76), with $h = 10^{-4}$

9. Conclusions

In the numerical integration of separable Hamiltonian problems, partitioned Runge–Kutta methods play an important role. In this paper we have considered the more general class of partitioned G-symplectic general linear methods.

It is typical of multivalue methods that parasitism can destroy the quality of long-term integrations. We will attempt to overcome this difficulty by requiring parasitism growth rates to be zero. For efficient implementation we will also impose the constraint that the coefficient matrices relating stages and stage derivatives have a triangular structure designed to make the methods effectively explicit.

Using a special structure interrelating the two components of a method pair, we have found order conditions up to $p = 4$. From these, practical methods can be con-

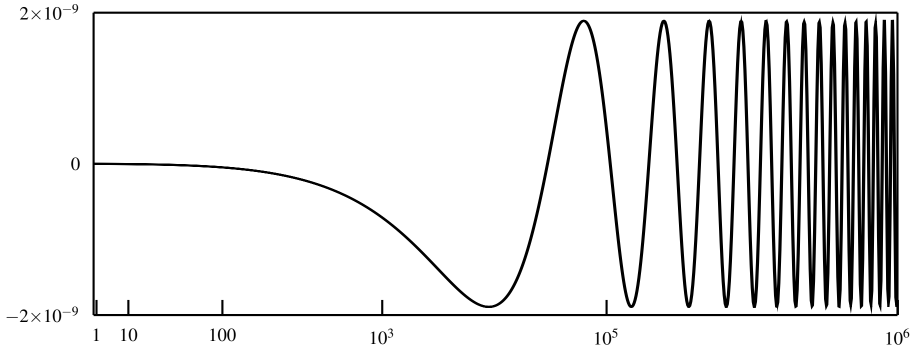


Figure 8: Deviation of the angular momentum associated to 10^6 steps of (7.72) to problem (8.76), with $e = 0$ and stepsize $h = 10^{-4}$

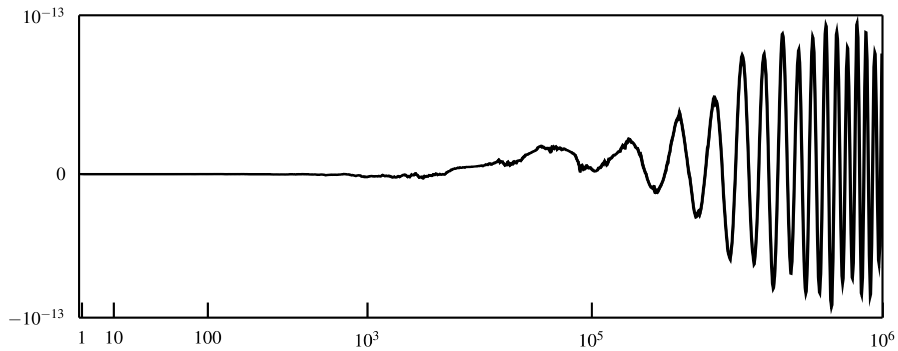


Figure 9: Deviation of the angular momentum associated to 10^6 steps of (7.73) to problem (8.76), with $h = 10^{-4}$

structed. As a consequence we have constructed a family of partitioned pairs with $p = 3$ and these are presented in the paper.

Although these are 2-value methods, they apparently preserve invariance properties just as well as for Runge-Kutta methods, and they have cost advantages. Simulations on selected problems verify the ability of these methods to closely conserve invariants and symplectic behaviour over an extended number of steps.

The concepts of conformability and weak conformability, introduced in [7], provide simplifications and insights into the order conditions for non-partitioned methods. An early application [8] has enabled a method of order eight to be constructed. It is anticipated that conformability can also be applied to partitioned methods and this will be the subject of future research.

References

[1] L. ABIA AND J. M. SANZ-SERNA, *Partitioned Runge-Kutta Methods for Separable Hamiltonian Problems*, Math. Comp. 60 (1993), no. 202, 617–634.

[2] J. C. BUTCHER, *General Linear Methods*, Acta Numer. 15 (2006), 157–256.

[3] J. C. BUTCHER, *Numerical methods for Ordinary Differential Equations*, Third Edition, Wiley, Chichester, 2016.

[4] J. C. BUTCHER, *The cohesiveness of G-symplectic methods*, Numer. Algorithms 70(3) (2015), 607–624.

[5] J. C. BUTCHER, Y. HABIB, A. T. HILL AND T. J. T. NORTON, *The control of parasitism in G-symplectic methods*, SIAM J. Numer. Anal. 52 (5) (2014), pp. 2440-2465 (2014).

[6] J. C. BUTCHER AND L. L. HEWITT, *The existence of symplectic general linear methods*, Numer. Algorithms 51 (2009), 77–84.

[7] J. C. BUTCHER AND G. IMRAN *Order conditions for G-symplectic methods*, BIT Numer. Math. 55 (4) (2015), 927–948.

[8] J. C. BUTCHER, G. IMRAN AND H. PODHAISKY *A G-symplectic method with order 6*, BIT Numer. Math., doi: 10.1007/s10543-016-0630-0 (2016).

[9] M. P. CALVO AND E. HAIRER, *Further reduction in the number of independent order conditions for symplectic, explicit Partitioned Runge-Kutta and Runge-Kutta-Nyström methods*, Appl. Numer. Math. 18 (1995), pp. 107–114.

[10] P. CHARTIER, E. FAOU AND A. MURUA, *An algebraic approach to invariant preserving integators: The case of quadratic and Hamiltonian invariants*, Numer. Math. 103 (20006), 575–590.

[11] R. D'AMBROSIO AND E. HAIRER, *Long-term stability of multi-value methods for ordinary differential equations*, J. Sci. Comput. 60(3), 627–640 (2014).

[12] R. D'AMBROSIO, G. DE MARTINO AND B. PATERNOSTER, *Numerical integration of Hamiltonian problems by G-symplectic methods*, Adv. Comput. Math. 40(2), 553–575 (2014).

[13] R. D'AMBROSIO, E. HAIRER AND C. J. ZBINDEN, *G-symplecticity implies conjugate-symplecticity of the underlying one-step method*, BIT Numer. Math. 53, 867–872 (2013).

[14] E. HAIRER, *Order Conditions for Numerical Methods for Partitioned Ordinary Differential Equations*, Numer. Math. 36 (1981), pp. 431-445.

[15] E. HAIRER, C. LUBICH AND G. WANNER, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations*, Second edition, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin, 2006.

[16] N. J. HIGHAM, *Accuracy and Stability of Numerical Algorithms, Second Edition*, SIAM, Philadelphia, 2002.

[17] L. JAY, *Symplectic partitioned Runge-Kutta methods for constrained Hamiltonian systems*, SIAM J. Numer. Anal. 33 (1996), no. 1, 368–387.

[18] F. M. LASAGNI, *Canonical Runge-Kutta methods*, Z. Angew. Math. Phys., 39 (1988), pp. 952-953.

[19] R. I. MCLACHLAN AND G. R. W. QUISPEL, *Geometric Integrators for ODEs*, J. Phys. A: Math. Gen. 39 (2006), no. 19, pp. 5251-5285.

[20] A. MURUA, *On order conditions for partitioned symplectic methods*, SIAM J. Numer. Anal. 34 (1997), no. 6, 2204-2211.

[21] J. M. SANZ-SERNA AND M. P CALVO, *Numerical Hamiltonian Problems*, Chapman & Hall, London, England, 1994.

[22] J. M. SANZ-SERNA AND L. ABIA, *Order conditions for canonical Runge-Kutta schemes*, SIAM J. Numer. Anal. 28, no. 4, 1081-1096 (1991).

[23] Y. B. SURIS, *Partitioned Runge-Kutta methods as phase volume preserving integrators*, Phys. Lett. A 220 (1996), no. 1-3, 63–69.