Applied Numerical Mathematics 117 (2017) 69–86

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Partitioned general linear methods for separable Hamiltonian problems

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ARTICLE INFO

Article history:
Received 25 January 2017
Accepted 1 February 2017
Available online 7 February 2017

Keywords:
Separable Hamiltonian problems
Multivalue numerical methods
G-symplecticity
Symmetric methods
Parasitic components

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.

1. Introduction

G-symplectic general linear methods [2–5,7,8,10–12,14] 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

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

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

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

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http://dx.doi.org/10.1016/j.apnum.2017.02.001
0168-9274/

and it follows that

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

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

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

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

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

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

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.