Numer Algor (2015) 70:607–624
DOI 10.1007/s11075-015-9964-y

ORIGINAL PAPER

The cohesiveness of G-symplectic methods

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Received: 27 October 2014 / Accepted: 13 January 2015 / Published online: 29 January 2015

Abstract General linear methods are multistage multivalue methods. This large family of numerical methods for ordinary differential equations, includes Runge–Kutta and linear multistep methods as special cases. G-symplectic general linear methods are multivalue methods which preserve a generalization of quadratic invariants. If Q is an invariant quadratic form then symplectic Runge–Kutta methods preserve this invariant. In the case of a G-symplectic general linear method, there exists a non-singular symmetric $r \times r$ matrix G such that $G \otimes Q$ is an invariant quadratic form for this method. Although the numerical results can be corrupted by parasitic behaviour, it is possible to overcome the effect of parasitic growth by imposing additional constraints on the method. For G-symmetric methods satisfying these additional conditions, numerical experiments give excellent results. A new concept known as "cohesiveness" is introduced in an attempt to explain this favourable numerical behaviour. It is shown that the deviation from perfect cohesiveness grows slowly as steps of the method are carried out.

Keywords Symplectic method · G-symplectic method · Parasitic growth · Underlying one-step method · Internal starting method · Cohesiveness

1 Introduction

Symplectic Runge–Kutta methods not only preserve symplectic behaviour for Hamiltonian problems but also preserve quadratic invariants for a variety of problems. Although general linear methods with more than a single input and output value cannot match this behaviour, they can imitate this performance to a certain extent.

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Specifically, the so-called G-symplectic methods which have zero parasitic growth factors, typically perform very well, using a variety of test problems. The purpose of this paper is to explain why this happens.

Symplectic Runge–Kutta methods were introduced by Sanz-Serna in [10] and are also the subject of a review paper [11] and a monograph [12]. Although G-symplectic methods were introduced in [2] and [3], it was not until [4] and [6] that methods were developed to overcome the deleterious effects of parasitism.

In Section 2 of the present paper, we will review the essential properties of general linear methods with special reference to G-symplectic methods. An example method, referred to as 4123A, is introduced to illustrate the computational and analytical constructs associated with this type of method. In Section 3 we will outline the behaviour of G-symplectic methods with zero parasitic growth factors, which have motivated the idea of cohesiveness that we would like to understand. In Section 4 the analytical tools, related to algebraic and B-series analysis, will be reviewed along with the ideas of the underlying one-step method. This leads to the formal definition of cohesiveness order. In Section 4.4 the main result will be presented; this establishes the slow growth of the deviation from cohesiveness. In Section 4.5 the analysis will be carried out in detail in the case of method 4123A. Finally in Section 5 the slow growth of deviation from cohesiveness is verified numerically.

2 Symplectic and G-symplectic methods

2.1 Standard problem

Let $X = \mathbb{R}^N$. We will consider numerical methods for a standard problem

$$y'(x) = f(y(x)), \qquad f : X \to X; \qquad y(x_0) = y_0 \in X. \tag{1}$$

It will be assumed that this problem has the property

$$[f(Y), QY] := [f(Y), Y]_Q = 0,$$

with the consequence that for y, satisfying (1), $[y(x), y(x)]_Q$ is constant.

We will study methods such that numerical approximations to $y(x)$ respect this invariance.

2.2 Symplectic Runge–Kutta methods

A Runge–Kutta method with tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathsf{T}} \end{array}$$

is *symplectic* (or *canonical*) if

$$M := \operatorname{diag}(b)A + A^{\mathsf{T}} \operatorname{diag}(b) - bb^{\mathsf{T}} = 0.$$

If the sequence of approximations generated by a canonical Runge–Kutta method is $y_0, y_1, y_2, \ldots$, then $[y_n, y_n]_Q$ is also invariant. This follows from

Theorem 1 (**Basic identity: Runge–Kutta case**) *Denote the stage values in step number n of a Runge–Kutta by Y and the stage derivatives by F. Then*

$$\sum_{i,j=1}^{s} m_{ij}[hF_i, hF_j]_Q = 2\sum_{i=1}^{s} b_i[hF_i, Y_i]_Q + [y_{n-1}, y_{n-1}]_Q - [y_n, y_n]_Q. \quad (2)$$

Proof The right-hand side of (2) is equal to

$$\sum_{i=1}^{s} b_i[hF_i, Y_i - y_{n-1}]_Q + \sum_{j=1}^{s} b_j[Y_j - y_{n-1}, hF_j]_Q - [y_n - y_{n-1}, y_n - y_{n-1}]_Q$$
$$= \sum_{i,j=1}^{s} (b_i a_{ij} + b_j a_{ji} - b_i b_j)[hF_i, hF_j]_Q.$$

□

2.3 General linear methods

Because general linear methods are multivalue, we need a notation for the collection of quantities imported at the start of step number n and for the quantities exported at the end of this step. These will be denoted by $y^{[n-1]}$ and $y^{[n]}$ respectively, each made up from r subvectors in X denoted as $y_i^{[n-1]}$ and $y_i^{[n]}$, where $i = 1, 2, \ldots, r$. As for a Runge–Kutta method, the stages will be denoted by Y_i, $i = 1, 2, \ldots, s$, which together comprise the vector Y. Similarly, F will denote the vector of stage derivatives made up from subvectors $F_i = f(Y_i)$, $i = 1, 2, \ldots, s$. These quantities are interconnected using four matrices A, U, B, V which together constitute the $(s + r) \times (s + r)$ partitioned matrix

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix}.$$

The connections between $y^{[n-1]}$, Y, F and $y^{[n]}$ can now be written

$$Y_i = h\sum_{j=1}^{s} a_{ij}F_j + \sum_{j=1}^{r} u_{ij}y_j^{[n-1]}, \quad i = 1, 2, \ldots, s,$$
$$y_i^{[n]} = h\sum_{j=1}^{s} b_{ij}F_j + \sum_{j=1}^{r} v_{ij}y_j^{[n-1]} \quad i = 1, 2, \ldots, r. \quad (3)$$

or, in compact form,

$$Y = (A \otimes I_N)F + (U \otimes I_N)y^{[n-1]}, \quad (4)$$
$$y^{[n]} = (B \otimes I_N)F + (V \otimes I_N)y^{[n-1]}. \quad (5)$$

It will be assumed throughout this paper that the implicit equation system (4) is well posed. This can be assured by requiring f to satisfy a local Lipschitz condition and assuming that h is sufficiently small. Under this assumption, the Y_i can be defined by functional iteration. In addition to $F_i = f(Y_i)$ evaluated at each stage, we will make use of $J_i^{[n]}$, equal to the Jacobian of f evaluated at Y_i found in step number n. The Jacobian will also be assumed to satisfy a local Lipschitz condition with constant L so that $\|J_i^{[n]} - J_j^{[n]}\| \le L\|Y_i - Y_j\|$. It follows that

$$\|J_i^{[n]} - J_j^{[n]}\| = O(h). \tag{6}$$

Furthermore, because two successive steps can be written as a single step of the composed method

$$\left[\begin{array}{cc|c} A & 0 & U \\ VA & A & VU \\ \hline VB & B & V^2 \end{array}\right],$$

we can also assume that

$$\|J_i^{[n+1]} - J_j^{[n]}\| = O(h). \tag{7}$$

2.4 Starting and finishing methods

Even though the process of computing $y^{[n]}$ from input values $y^{[n-1]}$ is completely specified by the four matrices (A, U, B, V), the sequence $y^{[0]}$, $y^{[1]}$, ... has to be initiated somehow. Given the initial value y_0 in (1), the r components $y_i^{[0]}$ need to be computed. This can be done by introducing a Runge–Kutta method with multiple outputs or, what is equivalent, a collection of r Runge–Kutta methods.

Write this starting process in the form of a mapping $\mathcal{S}_h : X \to X^r$ so that

$$y^{[0]} = \mathcal{S}_h y_0.$$

For many methods, a suitable starting method will have one component equal to the identity mapping id. In this case it will be possible to use this component of $y^{[n]}$ to give an approximation to $y(x_n)$.

However, in other cases we will need to introduce a "finishing process" $\mathcal{F}_h : X^r \to X$ with the property that $\mathcal{F}_h \circ \mathcal{S}_h = \mathrm{id}$ and use the approximation

$$y(x_n) \approx \mathcal{F}_h y^{[n]}$$

to obtain usable numerical results.

2.5 G-symplectic processes

The following condition is a generalization of the canonical property for Runge–Kutta methods

Definition 1 Let M denote the matrix

$$M = \begin{bmatrix} DA + A^{\mathsf{T}}D - B^*GB & DU - B^*GV \\ U^*D - V^*GB & G - V^*GV \end{bmatrix}, \tag{8}$$

where D is a real diagonal matrix and G is a non-singular Hermitian matrix. A general linear method (A, U, B, V) is G-symplectic if $M = 0$.

Note that A is necessarily a real matrix and hence $A^{\intercal}$ is an appropriate notation for the transpose of A in (8). On the other hand, as we will see in Section 2.6, the coefficient matrices U, B and V can possibly have non-real elements, depending on the choice of basis, and the notations B^*, U^* and V^* are appropriate.

Our aim is to study the behaviour of quantities like

$$\left[y_i^{[n]}, y_j^{[n]}\right]_Q := \left\langle y_i^{[n]}, Qy_j^{[n]}\right\rangle,$$

where Q is an $N \times N$ symmetric matrix. Note that the notation $[\cdot, \cdot]_Q$ is adopted rather than $\langle \cdot, \cdot \rangle_Q$ because Q need not have any positivity property and hence a notation suggesting inner-products would be misleading.

Given the $r \times r$ Hermitian matrix G, it is more useful to consider

$$\left[y^{[n]}, y^{[n]}\right]_{G\otimes Q} := \sum_{i,j=1}^{r} g_{ij} \left[y_i^{[n]}, y_j^{[n]}\right]_Q.$$

Given the real $s \times s$ diagonal matrix D, we also need a similar quadratic form on X^s denoted by $[\cdot, \cdot]_{D\otimes Q}$. Finally, using the $(s + r) \times (s + r)$ matrix M, define

$$[\mathbf{v}, \mathbf{v}]_{M\otimes Q} := \sum_{i,j=1}^{s+r} m_{ij}[v_i, v_j]_Q.$$

Theorem 2 (Basic identity: general linear case) *Let*

$$\mathbf{v} = \begin{bmatrix} hF \\ y^{[0]} \end{bmatrix},$$

then

$$[\mathbf{v}, \mathbf{v}]_{M\otimes Q} = [hF, Y]_{D\otimes Q} + [Y, hF]_{D\otimes Q} + \left[y^{[0]}, y^{[0]}\right]_{G\otimes Q} - \left[y^{[1]}, y^{[1]}\right]_{G\otimes Q}.$$

Proof This follows from the decomposition of M:

$$M = \begin{bmatrix} D \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} A & U \end{bmatrix} + \begin{bmatrix} A^{\intercal} \\ U^* \end{bmatrix} \begin{bmatrix} D & \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & G \end{bmatrix} - \begin{bmatrix} B^* \\ V^* \end{bmatrix} G \begin{bmatrix} B & V \end{bmatrix}.$$

□

If $M = 0$ and the term $[hF, Y]_{D\otimes Q}$ is zero then it follows from the basic identity that $\left[y^{[1]}, y^{[1]}\right]_{G\otimes Q} = \left[y^{[0]}, y^{[0]}\right]_{G\otimes Q}$ and in general that

$$\left[y^{[n]}, y^{[n]}\right]_{G\otimes Q} = \left[y^{[n-1]}, y^{[n-1]}\right]_{G\otimes Q}.$$

2.6 Partitioned diagonal form

In this paper we consider only general linear methods with the property that V has r distinct eigenvalues.

If T is a non-singular $r \times r$ matrix, then a change of basis

$$\begin{aligned} 2y^{[n-1]} &\mapsto (T * \otimes I_N) y^{[n-1]} =: \widetilde{y}^{[n-1]}, \\ y^{[n]} &\mapsto (T^* \otimes I_N) y^{[n]} \quad =: \widetilde{y}^{[n]} \end{aligned}$$

enables (4) and (5) to be written in the transformed form

$$Y = (A \otimes I_N)F + (\widetilde{U} \otimes I_N)\widetilde{y}^{[n-1]}, \tag{9}$$

$$\widetilde{y}^{[n]} = (\widetilde{B} \otimes I_N)F + (\widetilde{V} \otimes I_N)\widetilde{y}^{[n-1]}, \tag{10}$$

where the transformed coefficient matrices are

$$\begin{bmatrix} A & \widetilde{U} \\ \widetilde{B} & \widetilde{V} \end{bmatrix} = \begin{bmatrix} A & UT \\ T^*B & T^*VT \end{bmatrix}.$$

The G-stability condition (8) transforms to $\widetilde{M} = 0$, where

$$\widetilde{M} = \begin{bmatrix} I_s & 0 \\ 0 & T^* \end{bmatrix} M \begin{bmatrix} I_s & 0 \\ 0 & T \end{bmatrix} = \begin{bmatrix} DA + A^{\mathsf{T}}D - \widetilde{B}^*\widetilde{G}\widetilde{B} & D\widetilde{U} - \widetilde{B}^*\widetilde{G}\widetilde{V} \\ \widetilde{U}^*D - \widetilde{V}^*\widetilde{G}\widetilde{B} & \widetilde{G} - \widetilde{V}^*\widetilde{G}\widetilde{V} \end{bmatrix},$$

with $\widetilde{G} = T * GT$.

Because V has r distinct eigenvalues, it is always possible to choose T so that $\widetilde{V}$ is diagonal. For the method to be consistent [3], one of the eigenvalues of $\widetilde{V}$ must equal 1 and we will conventionally choose T so that this appears as the first diagonal element of $\widetilde{V}$. Also by consistency we can scale the coefficients so that $e_1^{\mathsf{T}}\widetilde{U} = \mathbf{1}$. If T is chosen to achieve these aims, we will refer to the transformed method with coefficient matrices $(A, \widetilde{U}, \widetilde{B}, \widetilde{V})$ as being in "diagonal form". Write $V = \mathrm{diag}(1, z_2, z_3, \ldots, z_r)$.

For the remainder of the paper we will assume that the method (A, U, B, V) is already in diagonal form and, accordingly, we will no longer use the notation $(A, \widetilde{U}, \widetilde{B}, \widetilde{V})$.

From the condition $G = V^*GV$ we deduce

$$g_{ij}(1 - \overline{z}_i z_j) = 0, \qquad i, j = 1, 2, \ldots, r$$

and it follows that $|z_i| = 1, i = 1, 2, \ldots, s$ and that G is a diagonal matrix. Without loss of generality, write $g_{11} = 1$

We will partition the method into its principal component and its non-principal components as follows:

$$\begin{aligned} V &= \mathrm{diag}(1, \widehat{V}), \qquad & U &= \left[1, \widehat{U}\right], \\ B &= \begin{bmatrix} b^{\mathsf{T}} \\ \widehat{B} \end{bmatrix}, & D &= \mathrm{diag}(b), & G &= \mathrm{diag}(1, \widehat{G}). \end{aligned}$$

with $\widehat{V}$ and $\widehat{G}$ diagonal matrices and all eigenvalues of V distinct and on the unit circle. Our next aim is to partition the method into its principal component and its non-principal components.

Write $\mathbf{p}^{\mathsf{T}}$ and $\mathbf{q}^{\mathsf{T}}$ as linear mappings:

$$\mathbf{p}^{\mathsf{T}} : \mathbb{R}^r \to \mathbb{R}, \qquad \mathbf{p}^{\mathsf{T}} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} \mapsto x_1,$$

$$\mathbf{q}^{\mathsf{T}} : \mathbb{R}^r \to \mathbb{R}^{r-1}, \quad \mathbf{q}^{\mathsf{T}} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} \mapsto \begin{bmatrix} x_2 \\ \vdots \\ x_r \end{bmatrix}.$$

As matrices, we recognise $\mathbf{p}^{\mathsf{T}}$ and $\mathbf{q}^{\mathsf{T}}$ as the first and remaining rows of the $r \times r$ identity matrix. We note the obvious identity

$$\mathbf{p}\mathbf{p}^{\mathsf{T}} + \mathbf{q}\mathbf{q}^{\mathsf{T}} = I.$$

These operators will be used to construct various submatrices:

$$\begin{aligned} U\mathbf{p} &= \mathbf{1}, & U\mathbf{q} &= \widehat{U}, & \mathbf{p}^{\mathsf{T}}B &= b^{\mathsf{T}}, & \mathbf{q}^{\mathsf{T}}B &= \widehat{B}, \\ \mathbf{p}^{\mathsf{T}}V\mathbf{p} &= 1, & \mathbf{q}^{\mathsf{T}}V\mathbf{q} &= \widehat{V}, & \mathbf{p}^{\mathsf{T}}V\mathbf{q} &= \mathbf{0}, & \mathbf{q}^{\mathsf{T}}V\mathbf{p} &= \mathbf{0}^{\mathsf{T}}, \\ \mathbf{p}^{\mathsf{T}}G\mathbf{p} &= 1, & \mathbf{q}^{\mathsf{T}}G\mathbf{q} &= \widehat{G}, & \mathbf{p}^{\mathsf{T}}G\mathbf{q} &= \mathbf{0}, & \mathbf{q}^{\mathsf{T}}G\mathbf{p} &= 0^{\mathsf{T}}. \end{aligned}$$

The inverse operation of breaking a vector into $\mathbf{p}$ and $\mathbf{q}$ components will be written as $[\cdot, \cdot]$. For example, $y^{[n]} = [\mathbf{p}^{\mathsf{T}}y^{[n]}, \mathbf{q}^{\mathsf{T}}y^{[n]}]$, where for convenience we will write $\mathbf{p}$, $\mathbf{q}$, $\mathbf{p}^{\mathsf{T}}$ and $\mathbf{q}^{\mathsf{T}}$ interchangeably with $\mathbf{p} \otimes I_N$, $\mathbf{q} \otimes I_N$, $\mathbf{p}^{\mathsf{T}} \otimes I_N$ and $\mathbf{q}^{\mathsf{T}} \otimes I_N$, respectively.

2.7 Parasitic growth factors

It was shown in [6] that parasitism can occur if the diagonal elements of $\mathbf{q}^{\mathsf{T}}BU\mathbf{q}$ are non-zero. When parasitism occurs the growth factors are $(\mathbf{q}^{\mathsf{T}}V\mathbf{q})^{-1}\mathbf{q}^{\mathsf{T}}BU\mathbf{q}$. It was shown in [6], how to overcome parasitism either through cancellation over successive steps or by the construction of methods in which the growth factors are identically zero.

In this paper, it will be assumed that we are dealing only with methods constructed in this way.

2.8 An example method

The following method, referred to in [5] as method 4123A, is defined by the matrices

$$\left[\begin{array}{cc} A & U \\ B & V \end{array}\right] = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 1 \\ \frac{2}{3} & 0 & 0 & 1 & -1 \\ \frac{2}{5} & -\frac{3}{10} & \frac{1}{2} & 1 & -\frac{1}{5} \\ \hline \frac{1}{3} & -\frac{3}{8} & \frac{25}{24} & 1 & 0 \\ \frac{1}{3} & \frac{3}{8} & -\frac{5}{24} & 0 & -1 \end{array}\right]. \tag{11}$$

The notation $p\overline{p}rs = 4123$ means that the order is $p = 4$, the "stage order" is $\overline{p} = 1$, $r = 2$ and $s = 3$. The method 4123A is one of a family of similar methods derived in [5].

With inputs $y_1^{[n-1]}$, $y_2^{[n-1]}$ to step number n, the first two stages are calculated from

$$Y_1 = y_1^{[n-1]} + y_2^{[n-1]}, \qquad F_1 = f(Y_1), \tag{12}$$

$$Y_2 = \tfrac{2}{3}hF_1 + y_1^{[n-1]} - y_2^{[n-1]}, \qquad F_2 = f(Y_2), \tag{13}$$

where the coefficients are taken from the first two rows of A and U. To find Y_3 and F_3, it is necessary to solve the equations

$$Y_3 - \tfrac{1}{2}hF_3 = \tfrac{2}{5}hF_1 - \tfrac{3}{10}hF_1 + y_1^{[n-1]} - \tfrac{1}{5}y_2^{[n-1]}, \qquad F_3 = hf(Y_3), \tag{14}$$

using the same solution techniques as for one of the stages of a diagonally-implicit Runge–Kutta method. Finally the output at the end of the step is given by

$$y_1^{[n]} = \tfrac{1}{3}hF_1 - \tfrac{3}{8}hF_2 + \tfrac{25}{24}hF_3 + y_1^{[n-1]}, \tag{15}$$

$$y_2^{[n]} = \tfrac{1}{3}hF_1 + \tfrac{3}{8}hF_2 - \tfrac{5}{24}hF_3 - y_2^{[n-1]}. \tag{16}$$

Using $D = \mathrm{diag}(\frac{1}{3}, -\frac{3}{8}, \frac{25}{24})$ and $G = \mathrm{diag}(1, -1)$, it is found that M given by (8) vanishes, showing that 4123A is G-symplectic. Evaluate the matrix product

$$BU = \begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix},$$

to show that the parasitic growth factor $e_2^{\mathsf{T}}BUe_2$ for this sample method is zero.

A full discussion of starting methods will be presented in Section 4 but, as an introduction, we will look at the consequences of using starting values

$$y_1^{[0]} = y_0, \qquad y_2^{[0]} = \theta hf(y_0) = \theta hy'(x_0), \tag{17}$$

where θ is a constant to be determined. If such a simple starting method is to be used, it should at least be possible after a single step to obtain results consistent with the flow of the problem. That is, we would hope to obtain, after a single step

$$y_1^{[1]} = y_0 + hy'(x_0) + O(h^2), \qquad y_2^{[1]} = \theta hf(y_0) + O(h^2), \tag{18}$$

The stage values, found from (12), (13), (14) are each equal to $y(x_0) + O(h)$ and the corresponding stage derivatives, F_1, F_2, F_3, are each equal to $y'(x_0) + O(h)$. Substitute into (15) and (16) and we find

$$y(x_0) + hy'(x_0) = \left(\tfrac{1}{3} - \tfrac{3}{8} + \tfrac{25}{24}\right)hy'(x_0) + y(x_0) + O(h^2), \tag{19}$$

$$\theta hy'(x_0) = \left(\tfrac{1}{3} + \tfrac{3}{8} - \tfrac{5}{24}\right)hy'(x_0) - \theta hy'(x_0) + O(h^2). \tag{20}$$

It can be verified that (19) is always satisfied and that (20) is satisfied when $\theta = \frac{1}{4}$. We will see in Section 4, that we need more sophisticated starting values for $y_1^{[0]}$ and $y_2^{[0]}$ than y_0 and $\frac{1}{4}hf(y_0)$ respectively, but we know at least that we should use

$$y_2^{[0]} = \tfrac{1}{4}hy'(x_0) + O(h^2). \tag{21}$$

3 Experimental behaviour of G-symplectic methods

Because we are dealing only with methods in partitioned diagonal form, the preconsistency vector will be $\mathbf{p} = e_1$

For problems possessing quadratic invariants, the G-symplectic conditions imply that a *quadratic combination* of the r quantities $y_1^{[n]}, y_2^{[n]}, \ldots, y_r^{[n]}$, is conserved. But this is not the same as conserving the principal component even though experimental evidence supports the belief that the principal component is *approximately* conserved.

What we might have expected is that the r quantities wander away from their exact values with no special relationship to each other. But they seem to stay together better than this. The aim now is to express these intuitive ideas more precisely.

Let $\mathcal{S}_h$ denote the starting method then the global truncation error can be written as

$$\mathcal{S}_h y(x_n) - y^{[n]}$$

We would expect each of the r components of this error to grow like

$$nh^{p+1} = (x_n - x_0)h^p,$$

But it looks as though

$$\delta_n = (\mathbf{q}^{\mathsf{T}}\mathcal{S}_h \circ (\mathbf{p}^{\mathsf{T}}\mathcal{S}_h)^{-1})\mathbf{p}^{\mathsf{T}}y^{[n]} - \mathbf{q}^{\mathsf{T}}y^{[n]} \tag{22}$$

grows more slowly. We will write

$$\mathcal{R}_h := \mathbf{q}^{\mathsf{T}}\mathcal{S}_h \circ (\mathbf{p}^{\mathsf{T}}\mathcal{S}_h)^{-1}.$$

The relationship between various components in (22) is illustrated in Fig. 1.

The advantages of the slow growth of (22) will be illustrated in the case of the method 4123A, where $\mathbf{p} = e_1$, $\mathbf{q} = e_2$ and where

$$\left[y^{[n]}, y^{[n]}\right]_{G\otimes Q]} = \left[y_1^{[n]}, y_1^{[n]}\right]_Q - \left[y_2^{[n]}, y_2^{[n]}\right]_Q. \tag{23}$$

Assume the starting method satisfies (21). Then for $n = 0$, (23) is approximately equal to

$$[y(x_0), y(x_0)]_Q - \tfrac{1}{16}h^2[y'(x_0), y'(x_0)]_Q \tag{24}$$

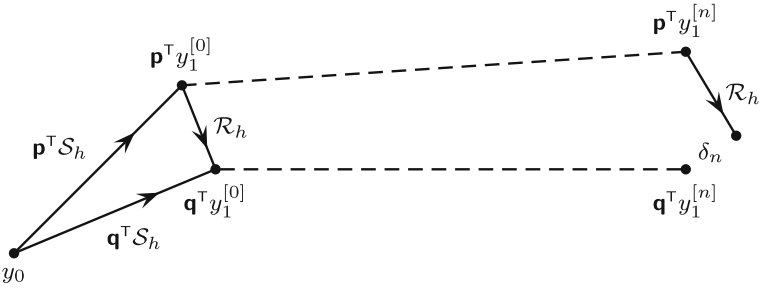


Fig. 1 The development of (22) from the starting process to the completion of n steps

and, for h small, the first term would be expected to be dominant. After n steps have been carried out, the value of (24) will be replaced by

$$[y(x_n), y(x_n)]_Q - \tfrac{1}{16}h^2[y'(x_n), y'(x_n)]_Q, \tag{25}$$

approximately. Even though $y_1^{[n]}$ may have drifted away from $y(x_n)$, because of the normal growth of truncation errors, the slow growth of (22), suggests that (25) is still valid as long as $y(x_n)$ and $y'(x_n)$ are replaced by the local values of these functions.

Why (22) grows slowly, is the question addressed in this paper.

4 Analysis of methods

4.1 Order conditions and the underlying one-step method

The conditions for order p are that, given a suitable starting method $\mathcal{S}_h$,

$$\mathcal{M}_h \circ \mathcal{S}_h = \mathcal{S}_h \circ \mathcal{E}_h + O(h^{p+1}), \tag{26}$$

where $\mathcal{M}_h$ is the action of the general linear method and $\mathcal{E}_h$ is the action of the exact solution. These relations can be represented in Fig. 2. To convert this abstract diagram into a practical scheme for analysing order properties we make use of the algebraic theory introduced in [1] and reformulated under the name of B-series in [7]. There are alternative normalisations in the literature but in this paper we will use the conventions established in [2] and [3].

A B-series is a Taylor expansion of the form

$$B(a, y_0) = a(\emptyset)y_0 + \sum_{t\in T} \frac{h^{|t|}a(t)}{\sigma(t)}F(t)(y_0), \tag{27}$$

where T is the set of all rooted trees and $\emptyset$ is the empty tree.

The notation is explained in [2] and [3] and examples for trees up to order 4, are shown in Fig. 3. In this table $\mathbf{f}$, $\mathbf{f}'$, $\mathbf{f}''\ldots$ denote $f(y_0)$, $f'(y_0)$, $f''(y_0)$, $\ldots$. The function $|t|$ is "the order of t", $\sigma(t)$ is the symmetry of t and $F(t)y_0$ is the elementary

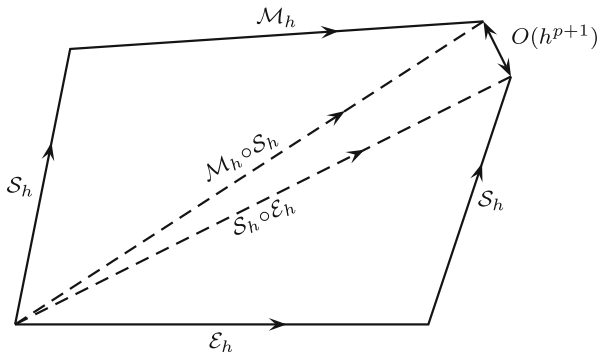


Fig. 2 Conditions for order p

t	$\emptyset$	•							
$\lvert t\rvert$	0	1	2	3	3	4	4	4	4
$\sigma(t)$	1	1	1	2	1	6	1	2	1
$F(t)y_0$	y_0	$\mathbf{f}$	$\mathbf{f}'\mathbf{f}$	$\mathbf{f}''(f,f)$	$\mathbf{f}'\mathbf{f}'\mathbf{f}$	$\mathbf{f}^{(3)}(\mathbf{f},\mathbf{f},\mathbf{f})$	$\mathbf{f}''(\mathbf{f},\mathbf{f}'\mathbf{f})$	$\mathbf{f}'(\mathbf{f}''(\mathbf{f}.\mathbf{f}))$	$\mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}$
$\mathbf{E}(t)$	1	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{12}$	$\frac{1}{24}$
$\mathbf{D}(t)$	0	1	0	0	0	0	0	0	0

Fig. 3 Examples of tree functions up to order 4

differential evaluated at y_0. Sample values of $\mathbf{E}(t)$ and $\mathbf{D}(t)$ are also shown in Fig. 3. The significance of these are given by the formulae

$$\begin{aligned} B(\mathbf{E}, y(x_0)) &= y(x_0 + h), \\ B(\mathbf{D}, y_0) &= hf(y_0) \end{aligned}$$

Using the composition rule for B-series, the order conditions can be found from

$$\begin{aligned} y^{[0]} &= B(\xi, y_0), \\ \eta &= A(\eta\mathbf{D}) + U\xi, \\ \mathbf{E}\xi &= B(\eta\mathbf{D}) + V\xi, \end{aligned} \tag{28}$$

where (28) must hold for all trees such that $|t| \le p$.

The underlying one-step method, introduced by Stoffer [13], following the work of Kirchgraber [8], is an idealised method $\widehat{\mathcal{E}}_h$ which enables (26) to be replaced by

$$\mathcal{M}_h \circ \widehat{\mathcal{S}}_h = \widehat{\mathcal{S}}_h \circ \widehat{\mathcal{E}}_h, \tag{29}$$

where $\mathcal{S}_h$ is replaced by an idealised starting method $\widehat{\mathcal{S}}_h$. The modified order diagram is given in Fig. 4.

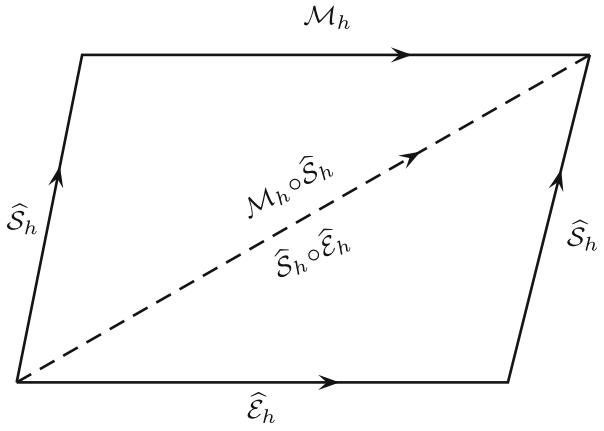


Fig. 4 Underlying one-step method

The B-series equivalent of this diagram becomes

$$\begin{aligned} y^{[0]} &= B(\widehat{\xi}, y_0), \\ \eta &= A(\eta \mathbf{D}) + U\widehat{\xi}, \qquad (30) \\ \widehat{\mathbf{E}}\widehat{\xi} &= B(\eta \mathbf{D}) + V\widehat{\xi}, \qquad (31) \end{aligned}$$

where (31) now holds for all rooted trees. Formal series can be found recursively for $\widehat{\mathbf{E}}$ and for the modified $\widehat{\xi}$.

4.2 Cohesiveness and deviation

Let $\widehat{\mathcal{R}}_h = (\mathbf{q}^{\mathsf{T}}\widehat{\mathcal{S}}_h) \circ (\mathbf{p}^{\mathsf{T}}\widehat{\mathcal{S}}_h)^{-1}$. Define the "deviation operator" Δ_h by the formula

$$\Delta_h = \mathbf{q}^{\mathsf{T}} - \widehat{\mathcal{R}}_h \mathbf{p}^{\mathsf{T}},$$

so that the deviation in step number n is given by

$$\delta_n = \Delta_h y^{[n]}.$$

Theorem 3 *If $\delta_{n-1} = 0$, then $\delta_n = 0$.*

Proof Let $y_0, y_1, \ldots$ denote the sequence of approximations generated by the underlying one step method so that $\widehat{\mathcal{S}}_h y_n = y^{[n]}$.

Hence,

$$(\mathbf{q}^{\mathsf{T}}\widehat{\mathcal{S}}_h) \circ (\mathbf{p}^{\mathsf{T}}\widehat{\mathcal{S}}_h)^{-1}\mathbf{p}^{\mathsf{T}} y^{[n]} = (\mathbf{q}^{\mathsf{T}}\widehat{S}\widehat{S}_h) \circ (\mathbf{p}^{\mathsf{T}}\widehat{\mathcal{S}}_h)^{-1}\mathbf{p}^{\mathsf{T}}\widehat{\mathcal{S}}_h y_n = \mathbf{q}^{\mathsf{T}}\widehat{\mathcal{S}}_h y_n,$$

so that $\delta_n = 0$. □

In practice, δ_0 will depend on the starting method $\mathcal{S}_h$, used to determine $y^{[0]}$. For acceptable accuracy, $\mathcal{S}_h$ should be chosen to be an order p approximation to $\widehat{\mathcal{S}}_h$ but, we can construct starting methods satisfying the following definition for any $q \geq p$.

Definition 2 A starting method S_h has cohesiveness order q if

$$\mathcal{R}_h = \widehat{\mathcal{R}}_h + O(h^{q+1}) \qquad (32)$$

or equivalently if

$$\xi(t) = \widehat{\xi}(t), \qquad |t| \leq q.$$

for an arbitrary high integer q. We will show how to do this in Section 4.3.

This will be followed by Section 4.4, where we show that the growth of deviation takes place at a moderate rate.

4.3 Construction of starters with high cohesiveness order

Write the composition rule for two B-series, $B(\alpha, y_0) = y_0 + O(h)$ and $B(\beta, y_0) = \beta(\emptyset)y_0 + O(h)$ in the form

$$(\alpha\beta)(t) = \beta(\emptyset)\alpha(t) + \beta(t) + \sum_{u<t} C(t, u, \alpha)\beta(u),$$

where $u < t$ means that u is a proper sub-tree of t and shares the same root. We now consider the mapping $\widehat{\mathcal{R}}_h = (\mathbf{q}^\intercal \widehat{\mathcal{S}}) \circ (\mathbf{p}^\intercal \widehat{\mathcal{S}})^{-1}$ with B-series defined by $\widehat{\zeta} = (\mathbf{p}^\intercal \widehat{\xi})^{-1}(\mathbf{q}^\intercal \widehat{\xi})$.

Theorem 4 *$\widehat{\zeta}$ is defined by the equations*

$$\eta(\emptyset) = 1, \tag{33}$$

$$\eta(t) = A(\eta \mathbf{D})(t) + (U\mathbf{q})\widehat{\zeta}(t), \qquad |t| \geq 1, \tag{34}$$

$$\widehat{\zeta}(t) = (I - \mathbf{q}^\intercal V \mathbf{q})^{-1}\big(\mathbf{q}^\intercal B(\eta \mathbf{D})(t) - \sum_{u<t} C\big(t, u, b^\intercal(\eta \mathbf{D})\big)\widehat{\zeta}(u)\big), \tag{35}$$

Proof In (30), (31), substitute $(\mathbf{p}^\intercal \widehat{\xi})\eta$ in place of η and break (31) into $\mathbf{p}$ and $\mathbf{q}$ components. The results are

$$(\mathbf{p}^\intercal \widehat{\xi})\eta = A(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + U\widehat{\xi} \qquad = A(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + 1\mathbf{p}^\intercal \widehat{\xi} + U\mathbf{q}\mathbf{p}^\intercal \widehat{\xi}\zeta, \tag{36}$$

$$\widehat{\mathbf{E}}\mathbf{p}^\intercal \widehat{\xi} = \mathbf{p}^\intercal B(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + \mathbf{p}^\intercal V \widehat{\xi} = \mathbf{p}^\intercal B(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + \mathbf{p}^\intercal \widehat{\xi}. \tag{37}$$

$$\widehat{\mathbf{E}}\mathbf{q}^\intercal \widehat{\xi} = \mathbf{q}^\intercal B(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + \mathbf{q}^\intercal V \widehat{\xi} = \mathbf{q}^\intercal B(\mathbf{p}^\intercal \widehat{\xi})\eta \mathbf{D} + (\mathbf{q}^\intercal V \mathbf{q})\widehat{\xi}\zeta. \tag{38}$$

Multiply each of (36), (37), (38) by $(\mathbf{p}^\intercal \widehat{\xi})^{-1}$ and write $\widetilde{\mathbf{E}} = (\mathbf{p}^\intercal \widehat{\xi})^{-1}\widetilde{\mathbf{E}}(\mathbf{p}^\intercal \widehat{\xi})$. These give the results

$$\eta = A(\eta \mathbf{D}) + 1 + U\mathbf{q}\zeta, \tag{39}$$

$$\widetilde{\mathbf{E}} = \mathbf{p}^\intercal B(\eta \mathbf{D}) + 1, \tag{40}$$

$$\widetilde{\mathbf{E}}\zeta = \mathbf{q}^\intercal B(\eta \mathbf{D}) + \mathbf{q}^\intercal V \mathbf{q}\zeta. \tag{41}$$

The (39) is equivalent to (33) and (34). Substitute $\widetilde{\mathbf{E}}$ given by (40) into (41) and the result is

$$(\mathbf{p}^\intercal B(\eta \mathbf{D}) + 1)\zeta = \mathbf{q}^\intercal B(\eta \mathbf{D}) + \mathbf{q}^\intercal V \mathbf{q}\zeta.$$

Use the product rule on the left-hand side and (35) follows. □

In a practical starting method $\mathcal{R}_h$ is an approximation to $\widetilde{\mathcal{R}}_h$ and in the corresponding B-series, ζ is an approximation to $\widehat{\zeta}$. Suppose the order of this approximation is q. The difficulty of constructing a suitable multi-output Runge–Kutta method $\mathcal{R}_h$ increases sharply as q increases and we will discuss an algorithm for enhancing this order iteratively. This iterative scheme is reminiscent of the algorithm presented in [9].

Theorem 5 *If $\mathcal{R}_h$ has cohesiveness order q, then the following internal starting method has cohesiveness order $q + 1$:*

$$y_0 \mapsto \mathcal{R}_h y_0 + (I - \mathbf{q}^\intercal V \mathbf{q})^{-1}(\mathbf{q}^\intercal - \mathcal{R}_h \mathbf{p}^\intercal)\mathcal{M}_h[y_0, \mathcal{R}_h y_0]. \tag{42}$$

Proof Write $(\mathbf{q}^\mathsf{T} - \mathcal{R}_h\mathbf{p}^\mathsf{T})\mathcal{M}_h[y_0, \mathcal{R}_h y_0]$, to within $O(h^{q+3})$, as the sum of three terms as follows:

$$(\mathbf{q}^\mathsf{T} - \mathcal{R}_h\mathbf{p}^\mathsf{T})\mathcal{M}_h[y_0, \mathcal{R}_h y_0] =$$
$$(\mathbf{q}^\mathsf{T} - \widehat{\mathcal{R}}_h\mathbf{p}^\mathsf{T})\mathcal{M}_h[y_0, \widehat{\mathcal{R}}_h y_0] \quad (43)$$
$$+\mathbf{q}^\mathsf{T}(\mathcal{M}_h[y_0, \mathcal{R}_h y_0] - \mathcal{M}_h[y_0, \widehat{\mathcal{R}}_h y_0]) \quad (44)$$
$$+(\widehat{\mathcal{R}}_h\mathbf{p}^\mathsf{T} - \mathcal{R}_h\mathbf{p}^\mathsf{T})\mathcal{M}_h[y_0, \widehat{\mathcal{R}}_h y_0] \quad (45)$$

The first term (43) is zero; whereas (44) equals $\mathbf{q}^\mathsf{T}V\mathbf{q}(\mathcal{R}_h y_0 - \widehat{\mathcal{R}}_h y_0) + O(h^{q+3})$ and (45) equals $\widehat{\mathcal{R}}_h y_0 - \mathcal{R}_h y_0) + O(h^{q+3})$. Combining the terms to within $O(h^{q+3})$ we evaluate the right-hand side of (42):

$$\mathcal{R}_h y_0 + (I - \mathbf{q}^\mathsf{T}V\mathbf{q})^{-1}(\mathbf{q}^\mathsf{T} - \mathcal{R}_h\mathbf{p}^\mathsf{T})\mathcal{M}_h[y_0, \mathcal{R}_h y_0] = \mathcal{R}_h y_0 + (\widehat{\mathcal{R}}_h y_0 - \mathcal{R}_h y_0) = \widehat{\mathcal{R}}_h y_0.$$

□

4.4 Slow growth of $\Delta_h y^{[n]}$

Our aim now will be to understand how a small perturbation in $\Delta_h y^{[0]}$ will affect later values.

Theorem 6 *Let (A, U, B, V) be a G-symplectic method in partitioned diagonal form such that the eigenvalues of V are distinct and such that the diagonal elements of $\mathbf{q}^\mathsf{T}BU\mathbf{q}$ are zero. Let*

$$\begin{aligned} M_k &= \left(\mathbf{q}^\mathsf{T}V\mathbf{q} \otimes I + h(\mathbf{q}^T B \otimes I)\mathrm{diag}(I \otimes J_1^{[k]})(U\mathbf{q} \otimes I)\right) \\ &= \mathbf{q}^T V\mathbf{q} \otimes I + h(\mathbf{q}^T BU\mathbf{q} \otimes J_1^{[k]}), \end{aligned}$$

then

$$\|M_n M_{n-1} \cdots M_2 M_1\| = 1 + O(h + nh^2).$$

Proof For convenience we will write $\delta = \Delta_h y^{[k-1]}$ and we will calculate the Fréchet derivative of $\Delta_h y^{[k]}$ with respect to δ.

First,

$$Y \mapsto Y + (U\mathbf{q} \otimes I)\delta + O(\|\delta\|^2),$$

and second

$$hF \mapsto hF + h\mathrm{diag}(J_1^{[k]}, J_2^k, \ldots, J_s^{[k]})(U\mathbf{q} \otimes I)\delta + O(\|\delta\|^2).$$

This leads to

$$\Delta_h y^{[n]} \mapsto \left(\mathbf{q}^\mathsf{T}V\mathbf{q} \otimes I + h(\mathbf{q}^\mathsf{T}B \otimes I)\mathrm{diag}(J_1^{[k]}, J_2^k, \ldots, J_s^{[k]})(U\mathbf{q} \otimes I)\right)\delta + O(\|\delta\|^2),$$

so that the Fréchet derivative of δ_n with respect to δ_{n-1} is

$$\widetilde{M}_k := \mathbf{q}^\mathsf{T}V\mathbf{q} \otimes I + h(\mathbf{q}^\mathsf{T}B \otimes I)\mathrm{diag}(J_1^{[k]}, J_2^{[k]}, \ldots, J_s^{[k]})(U\mathbf{q} \otimes I).$$

It follows from (6) that $\widetilde{M}_k = M_k + O(h^2)$.

Define the $(r-1)\times(r-1)$ matrix K by the formula

$$e_i^{\mathsf{T}} K e_j = \begin{cases} \dfrac{1}{z_{j+1}-z_{i+1}} e_{i+1}^{\mathsf{T}} B U e_{j+1}, & i \neq j, \\ 0, & i = j, \end{cases}$$

so that

$$\mathbf{q}^{\mathsf{T}} B U \mathbf{q} = K \mathbf{q}^{\mathsf{T}} V \mathbf{q} - \mathbf{q}^{\mathsf{T}} V \mathbf{q} K$$

and

$$M_k = \mathbf{q}^{\mathsf{T}} V \mathbf{q} \otimes I + h(K \mathbf{q}^{\mathsf{T}} V \mathbf{q} - \mathbf{q}^{\mathsf{T}} V \mathbf{q} K) \otimes J_1^{[k]}.$$

Define the matrices

$$\begin{aligned} N_k &= (I \otimes I + hK \otimes J_1^{[k]})^{-1} M_k (I \otimes I + hK \otimes J_1^{[k]}), \quad k = 1, 2, \ldots, n, \\ P_k &= (I \otimes I + hK \otimes J_1^{[k]})^{-1} (I \otimes I + hK \otimes J_1^{[k-1]}), \quad k = 2, 3, \ldots, n. \end{aligned}$$

Hence, we can write

$$\begin{aligned} &M_n M_{n-1} \cdots M_2 M_1 \\ &\quad = (I \otimes I + hK \otimes J_1^{[n]}) N_n P_n N_{n-1} P_{n-1} \cdots P_2 N_1 (I \otimes I + hK \otimes J_1^{[1]})^{-1}. \end{aligned}$$

Calculate the norms of the factors

$$\begin{aligned} \|I \otimes I + hK \otimes J_1^{[n]}\| &= 1 + O(h), \\ \|N_k\| &= \|V \otimes I + O(h^2)\| \\ &= 1 + O(h^2), \\ \|P_k\| &= \|I \otimes I + hK \otimes \left(J_1^{[k]} - J_1^{[k-1]}\right)\| + O(h^2) \\ &= 1 + O(h^2), \\ \|(I \otimes I + hK \otimes J_1^{[1]}\|)^{-1} &= 1 + O(h). \end{aligned}$$

Hence, we have

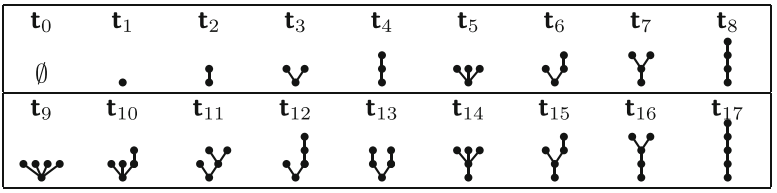
$$\|M_n M_{n-1} \cdots M_2 M_1\| = 1 + O(h + nh^2).$$

□

This slow rate of growth is a partial explanation of the excellent behaviour of G-symplectic methods which have zero parasitism growth factors. It is proposed to combine this result with the use of an internal starting method with order $q \geq p$ so that the cohesiveness after n steps is preserved to within $(1 + O(h + nh^2))O(h^{q+1})$.

4.5 Analysis of method 4123A

We will apply the results in this section to 4123A given by (11). We will number trees up to order 5 as follows.



For a B-series coefficient α we will write $\alpha_i = \alpha(\mathbf{t}_i)$. It was shown in [5] that the method (11) has order 4 relative to the starting value given by

$$\left[\begin{array}{ccccc}\mathbf{p}^{\mathsf{T}}\xi_0 & \mathbf{p}^{\mathsf{T}}\xi_1 & \mathbf{p}^{\mathsf{T}}\xi_2 & \mathbf{p}^{\mathsf{T}}\xi_3 & \mathbf{p}^{\mathsf{T}}\xi_4\end{array}\right] = \left[\begin{array}{ccccc}1 & 0 & -\frac{1}{32} & -\frac{7}{4320} & \frac{149}{8640}\end{array}\right], \tag{46}$$

$$\begin{aligned}&\left[\begin{array}{cccccccccc}\mathbf{q}^{\mathsf{T}}\xi_0 & \mathbf{q}^{\mathsf{T}}\xi_1 & \mathbf{q}^{\mathsf{T}}\xi_2 & \mathbf{q}^{\mathsf{T}}\xi_3 & \mathbf{q}^{\mathsf{T}}\xi_4 & \mathbf{q}^{\mathsf{T}}\xi_5 & \mathbf{q}^{\mathsf{T}}\xi_6 & \mathbf{q}^{\mathsf{T}}\xi_7 & \mathbf{q}^{\mathsf{T}}\xi_8\end{array}\right]\\ &\quad = \left[\begin{array}{ccccccccc}0 & \frac{1}{4} & -\frac{1}{16} & -\frac{49}{960} & -\frac{13}{384} & \frac{2543}{57600} & \frac{193}{7680} & \frac{619}{34560} & \frac{163}{69120}\end{array}\right].\end{aligned}$$

Using the algorithm described in Theorem 4, ζ can be evaluated to arbitrary accuracy. Up to order 5 the result is

$$\begin{aligned}&\left[\begin{array}{ccccc}\zeta_0 & \zeta_1 & \zeta_2 & \cdots & \zeta_{17}\end{array}\right]\\ &\quad = \left[\begin{array}{cccccccccccc}0 & \frac{1}{4} & -\frac{1}{16} & -\frac{49}{960} & -\frac{5}{192} & \frac{2543}{57600} & \frac{89}{3840} & \frac{211}{11520} & -\frac{1}{256} & \frac{212879}{3456000} & \frac{6937}{230400} & \frac{1037}{46080}\\ \frac{35}{3072} & \frac{287}{15360} & \frac{13003}{691200} & \frac{389}{46080} & \frac{277}{46080} & \frac{11}{3072}\end{array}\right].\end{aligned}$$

The starting method can be broken into two operations; first the computation of $\mathbf{p}^{\mathsf{T}}y^{[0]}$ using a Runge–Kutta method characterised by (46) and secondly the computation of $\mathbf{q}^{\mathsf{T}}y^{[0]}$ by applying a method approximating ζ, applied to $\mathbf{p}^{\mathsf{T}}y^{[0]}$.

A possible tableau for the computation of $\mathbf{p}^{\mathsf{T}}y^{[0]}$ is

$$\begin{array}{c|ccc}0 & & & \\ -\frac{7}{135} & -\frac{7}{135} & & \\ \frac{7}{135} & -\frac{1}{2} & \frac{149}{270} & \\ \hline & \frac{135}{224} & 0 & -\frac{135}{224}\end{array} \tag{47}$$

and this will be adopted in the simulations carried out in Section 5.

For the second component of the starting method, and for calculating the deviation function, we will make use of some of the following approximations to $\widehat{\mathcal{R}}_h$:

$\mathcal{R}_h^4$ A fourth order approximation to ζ, based on a four stage Runge–Kutta tableau:

$$\begin{array}{c|cccc} 0 & & & & \\ -\frac{13}{30} & -\frac{13}{30} & & & \\ -\frac{1}{10} & -\frac{67}{1170} & -\frac{5}{117} & & \\ -\frac{51}{100} & -\frac{1330607}{2366000} & -\frac{626773}{3380000} & \frac{432837}{1820000} & \\ \hline 0 & -\frac{1863}{1768} & \frac{4245}{4784} & \frac{855}{656} & -\frac{56875}{64124} \end{array},$$

where the zero in the last row signifies that the approximation is $y_0 \mapsto h \sum_j b_i F_i$ rather than $y_0 \mapsto y_0 + h \sum_j b_i F_i$ as in a standard Runge–Kutta method.

$\mathcal{R}_h^5$ A refinement to order 5 based on carrying out an iteration of (42) in Theorem 5 to $\mathcal{R}_h^4$.

$\mathcal{R}_h^6$ A refinement to order 6 based on carrying out an iteration of (42) in Theorem 5 to $\mathcal{R}_h^5$.

$\mathcal{R}_h^7$ A refinement to order 7 based on carrying out an iteration of (42) in Theorem 5 to $\mathcal{R}_h^6$.

5 Numerical simulations

Using method 4123A, a numerical solution was carried out for the Hénon–Heiles problem, defined from the Hamiltonian

$$\tfrac{1}{2}\left(p_1^2 + p_2^2 + q_1^2 + q_2^2\right) + q_1^2 q_2 - q_2^3/3,$$

with initial values $q_1 = q_2 = p_2 = 0$, $p_1 = \sqrt{0.3185}$. Figure 5 shows the deterioration of cohesiveness as 10^6 steps are taken with $h = 0.01$. Results are given for three cases: $q = 4, 5, 6$. The value of $\mathbf{p}^{\mathsf{T}} y^{[0]}$ was calculated as described in

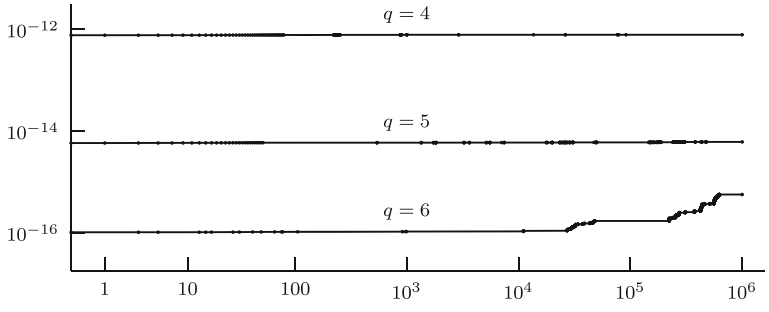


Fig. 5 Maximum deviation after n steps with $h = 0.01$ using starting methods of order $q = 4, 5, 6$

Section 4.5 using the tableau (47). Furthermore the second input was found from $\mathbf{q}^{\mathsf{T}} y^{[0]} = \mathcal{R}_h^q \mathbf{p}^{\mathsf{T}} y^{[0]}$. To calculate the deviation from cohesiveness the formula

$$\Delta_h y^{[n]} = \mathbf{q}^{\mathsf{T}} y^{[n]} - \widehat{\mathcal{R}}_h \mathbf{p}^{\mathsf{T}} y^{[n]}$$

would have to be evaluated. However, this is impossible because there is no algorithm know for $\widehat{\mathcal{R}}_h$ and in the calculations this is replaced by $\mathcal{R}_h^{q+1}$. In additional experiments not reported here, the use of $\mathcal{R}_h^{q+2}$ and even $\mathcal{R}_h^{q+3}$ were also used but this made almost no difference. In the figure the highest observed value of $\|\Delta_h y^{[k]}\|$ for $k = 1, 2, \ldots, n$ was plotted, with dots indicating where a jump has occurred.

For $q = 4$ and $q = 5$, the absence of significant growth in the deviation from cohesiveness is supportive of the theory in Section 4.4. No detailed explanation is offered for the relatively disappointing result for $q = 6$ but it is likely that round-off errors have played a part in the growth of deviation after such a large number of steps.

6 Conclusions

Cohesiveness was defined to describe the holding together of the multiple values generated as output from a step. Under appropriate assumptions the deviation from cohesiveness was shown to grow very slowly. This was confirmed by experiments.

Acknowledgments The author is grateful to Adrian Hill and Terry Norton for making their paper [9] available to me in advance of its publication. He expresses his thanks also to the anonymous referees whose comments have led to significant improvements to the paper. He also thanks the Marsden Fund for their support.

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