

Explicit two-step peer methods with reused stages[☆]

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Abstract

Two-step peer methods for the numerical solution of Initial Value Problems (IVP) combine the advantages of Runge-Kutta (RK) and multistep methods to obtain high stage order and provide in a natural way a dense output. In general, explicit s -stage peer methods require s evaluations of the vector field at each step. Nevertheless, Klinge and coworkers (BIT Numer Math, 2018) have shown that some methods use less function calls $s_e < s$, here called effective stages, by re-using $s_r = s - s_e$ previously computed stages (shifted stages) from the previous steps in the current one.

In this paper we propose a new approach, different from the one used by Klinge and coworkers, to re-use previously computed stages, that we call peer methods with reused stages, showing that methods with reused stages and s_e effective stages are equivalent to three-step peer methods with s_e stages. Then, we analyze all the families of methods with two effective stages, obtaining methods with $s = 3$ and orders 4 and 5 in which the free parameters of the families have been used to minimize the coefficient of the leading error term as well as to maximize the absolute stability interval. We have also studied one family of peer methods with $s = 4$ and three effective stages, obtaining a method with order 6, superconvergent of order 7, and optimized leading error term as well as absolute stability interval. Some numerical experiments show the performance of the obtained methods by comparing them with other previously obtained peer methods as well as other standard Runge-Kutta and multistep methods.

Keywords: Peer methods, two-step methods, IVP, stability, multi-step methods

2000 MSC: 65L05, 65L07

[☆]This work was supported by project PID2019-109045GB-C31

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1. Introduction

Peer two step methods [15] have proved to be efficient numerical integrators of IVPs

$$\frac{d}{dt}y(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^m. \quad (1)$$

Given approximations $Y_{n,j} \simeq y(t_{n,j})$ to the solution of (1) at points $t_{n,j} = t_n + c_j h$, $j = 1, \dots, s$, where h is the time step size, an s -stage two-step peer method computes new approximations

$$Y_{n+1,j} \simeq y(t_{n+1,j}), \quad f_{n+1,j} = f(t_{n+1,j}, Y_{n+1,j}), \quad j = 1, \dots, s,$$

to the solution of (1) and the vector field at the grid points $t_{n+1,j} = t_{n+1} + c_j h = t_n + h + c_j h$, $j = 1, \dots, s$ by means of the equations

$$Y_{n+1,j} = \sum_{k=1}^s a_{jk} Y_{n,k} + h \sum_{k=1}^s b_{jk} f_{n,k} + h \sum_{k=1}^s r_{jk} f_{n+1,k}, \quad j = 1, \dots, s, \quad (2)$$

where $\mathbf{A} = (a_{jk})$, $\mathbf{B} = (b_{jk})$, $\mathbf{R} = (r_{jk}) \in \mathbb{R}^{s \times s}$ are given real matrices that define the method.

If the matrix R is strictly lower triangular, then the method is explicit. In this paper we will consider only explicit methods.

Putting $\mathbf{e} = (1, \dots, 1)^T \in \mathbb{R}^s$, $\mathbf{c} = (c_1, \dots, c_s)^T$ and

$$\mathbf{Y}_k = \begin{pmatrix} Y_{k,1} \\ Y_{k,2} \\ \vdots \\ Y_{k,s} \end{pmatrix}, \quad f(t_k \mathbf{e} + h \mathbf{c}, \mathbf{Y}_k) = \begin{pmatrix} f(t_{k,1}, Y_{k,1}) \\ f(t_{k,2}, Y_{k,2}) \\ \vdots \\ f(t_{k,s}, Y_{k,s}) \end{pmatrix} \in (\mathbb{R}^m)^s, \quad (3)$$

equations (2) can be written in the matrix form

$$\begin{aligned} \mathbf{Y}_{n+1} &= (\mathbf{A} \otimes I_m) \mathbf{Y}_n + h (\mathbf{B} \otimes I_m) f(t_n \mathbf{e} + h \mathbf{c}, \mathbf{Y}_n) \\ &\quad + h (\mathbf{R} \otimes I_m) f(t_{n+1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n+1}), \end{aligned} \quad (4)$$

where \otimes denotes the standard Kronecker product and I_m is the unit matrix of order m . For our studies of order and stability it will be sufficient to consider the scalar case ($m = 1$) in which (4) becomes

$$\mathbf{Y}_{n+1} = \mathbf{A} \mathbf{Y}_n + h \mathbf{B} f(t_n \mathbf{e} + h \mathbf{c}, \mathbf{Y}_n) + h \mathbf{R} f(t_{n+1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n+1}). \quad (5)$$

In general, two-step s -stage peer methods require s derivative function calls per step. Nevertheless, Horváth and coworkers [11] and Klinge and coworkers [12] have shown that if the matrices \mathbf{A} , \mathbf{B} and \mathbf{R} have a special structure, it is possible to employ less function calls by re-using previously computed stages from the previous steps in the current one, in a similar way as Runge-Kutta schemes do with “first-same-as-last” (FSAL) technique [6]. In fact, in their approach, a method with s_r shifted stages uses one stage of previous s_r steps

in the current step. They call them peer methods with shifted stages. With this approach, these authors obtain methods with 4 stages but only 2 effective stages and s -stage peer methods with $s = 5, \dots, 8$ in which three stages are reused and only $s - 3$ evaluations of the vector field are required. It is worth to remark that after the introduction of peer methods (4) in 2004 by Schmitt and Weiner [13] there has been a constant flow of publications dealing not only with theoretical properties such as accuracy and stability of different families of these type of methods but also with the implementation comparing with classical IVPs solvers for different types of problems. A complete list of publications of peer type methods that includes more than 70 papers can be found in <https://www.mathematik.uni-marburg.de/~schmitt/peer/>.

In particular, the recent paper of Abdi *et al* [1] considers a family of s -stage Explicit Two-Step Peer (ETSPeer) methods with $s = 1, 2, 3, 4$ stages and order $p = s$ that are optimally zero-stable (the matrix \mathbf{A} of (4) has the form $\mathbf{A} = \mathbf{e} \mathbf{b}^T$ with $\mathbf{b} \in \mathbb{R}^s$) and further the eigenvalues $w_{s,j}$, $j = 1, \dots, s$ of the stability matrix of (4), $\mathbf{M}(z) = (I - z \mathbf{R})^{-1} (\mathbf{A} + z \mathbf{B})$ are all zero except $w_{s,1} = \sum_{j=0}^s (z^j)/(j!)$. Clearly this implies that stability region of the s -stage method is the same as the s -stage Runge-Kutta method with order s . Moreover to deal with variable step-size the elements of matrices \mathbf{A} and \mathbf{R} are constant whereas those of \mathbf{B} depend on the step-size ratio $\sigma_n = (h_{n+1})/(h_n)$ between two consecutive steps. These methods have been used to develop a variable-order variable-step code and numerical experiments show their efficiency when compared with others standard ODE codes for solving non-stiff IVPs.

Another recent contribution in the class of ETSPeer methods due to D. Conte and co workers [4], [5], is the development of methods where the coefficients depend on the Jacobian $f_y(t, y)$ of the function $f(t, y)$ at suitable points. Here the introduction of this dependence allows the authors to obtain methods with stability properties in all stages similar to linearly implicit methods and therefore are suitable for solving stiff systems. A detailed derivation of methods and numerical experiments can be seen in [4].

In this paper we consider peer methods in which s_r stages of the previous step are used in the current step, what we call s -stage peer methods with s_r reused stages and $s_e = s - s_r$ effective stages. Then we show that these methods are equivalent to three-step peer methods with s_e stages. Next we obtain families of methods with $s = 3$ and $s_e = 2$ with orders 4 and 5. We also develop a family of peer methods with $s = 4$ and $s_e = 2$ with order 5, superconvergent of order 6, and a family of methods with $s = 4$ and $s_e = 3$ with order 6 and superconvergence of order 7. The free parameters of the families are used to minimize the coefficient of the leading error term as well as to maximize the absolute stability interval.

The paper is organized as follows: In section 2 we give a review of peer methods and their accuracy and stability properties. In section 3 we define the relevant properties for our study relative to the peer methods with reused stages, proving that they are equivalent to three-step peer methods. In section 4 we study peer methods with two effective stages and develop families of methods

with orders 4 and 5. In section 5 we develop a family of peer methods with three effective stages and order 6. In section 6 we present some numerical experiments to show the performance of the new methods. Finally, we give some conclusions and future developments.

2. Quick review of two-step peer methods

Let $y(t)$ be a real valued function sufficiently smooth. For the method (5) the linear s -dim valued vector-valued linear operator $\mathcal{L}[y(t); h]$ defined by

$$\mathcal{L}[y(t); h] \equiv \mathbf{Y}(t+h) - \mathbf{A} \mathbf{Y}(t) - h \mathbf{B} \mathbf{Y}'(t) - h \mathbf{R} \mathbf{Y}'(t+h), \quad (6)$$

with $\mathbf{Y}(t) = y(\mathbf{t}\mathbf{e} + h\mathbf{c}) \equiv (y(t+c_1h), \dots, y(t+c_sh))^T$ allows us to define the order of consistency of the method. Note that for simplicity we are considering that $y(t)$ is a scalar function. The extension to the non-scalar general case is straightforward.

Definition 1. *The method (4) or (5) has order of consistency p if*

$$\mathcal{L}[y(t); h] = \mathcal{O}(h^{p+1}), \quad (h \rightarrow 0), \quad (7)$$

for all $y(t)$ sufficiently smooth.

If the method has order p , the consistency error constant vector $\mathbf{C}_{p+1} \neq \mathbf{0}$ is defined by

$$\mathcal{L}[t^{p+1}; h] = \mathbf{C}_{p+1} y^{(p+1)}(t) h^{p+1} \neq \mathbf{0}. \quad (8)$$

As it has been pointed out in [13], [15] the method (4) is zero-stable if and only if the matrix \mathbf{A} has the eigenvalue $\lambda_1(\mathbf{A}) = 1$ and the remaining eigenvalues $\lambda_j(\mathbf{A}), j = 2, \dots, s$ have modulus ≤ 1 and those of modulus one correspond to simple elementary divisors. Hence, a safe stability requirement is to choose \mathbf{A} so that

$$\lambda_1(\mathbf{A}) = 1, \quad \lambda_j(\mathbf{A}) = 0, \quad j = 2, \dots, s, \quad (9)$$

because these conditions ensure the zero stability ([9], pp. 293). This is usually called optimal zero stability. Remark that $\lambda_1(\mathbf{A}) = 1$ is a consequence of the preconsistency condition $\mathcal{L}[1; h] = 0$ which reduces to $\mathbf{A}\mathbf{e} = \mathbf{e}$.

A zero-stable method which is consistent of order p is convergent of order p (see e.g. [15]).

When fixed step size is used, Skeel [14] showed that some methods that satisfy an additional condition can increase their order of convergence. This property is called superconvergence. Weiner and coworkers [16] proved that optimal zero stable peer methods of order p satisfying

$$\boldsymbol{\nu}^T \mathbf{C}_{p+1} = 0, \quad \text{with } \boldsymbol{\nu} \in \mathbb{R}^s \text{ defined by } \lim_{n \rightarrow \infty} \mathbf{A}^n = \mathbf{e} \boldsymbol{\nu}^T, \quad (10)$$

are superconvergent and have at least, when implemented with fixed step size, order $p+1$.

The linear absolute stability of the methods (5) is studied by applying them to the scalar test equation $y' = \lambda y$, where λ is a complex constant. Putting $z = \lambda h$, (5) becomes

$$\mathbf{Y}_1 = (I - z\mathbf{R})^{-1} (\mathbf{A} + z\mathbf{B}) \mathbf{Y}_0 \equiv \mathbf{M}(z)\mathbf{Y}_0.$$

Then the stability region S is the set of all $z \in \mathbb{C}$ such that all eigenvalues of $\mathbf{M}(z)$ satisfy $|\lambda_j(\mathbf{M}(z))| \leq 1$ and those with $|\lambda_j(\mathbf{M}(z))| = 1$ correspond to simple divisors in its Jordan's canonical form. In particular, the absolute stability interval is defined as the intersection of the stability region with the negative real axis.

3. Two-step peer methods with reused stages

According to [12], a peer method (5) is said to have s_r shifted stages (therefore $s_e = s - s_r$ effective stages) if

$$c_j = c_{j+1} - 1, \text{ and } Y_{n+1,j} = Y_{n,j+1}, \text{ for } j = 1, \dots, s_r.$$

These conditions imply that

$$Y_{n+1,1} = Y_{n,2} = \dots = Y_{n-s_r+1,s_r+1}$$

and therefore the stage value Y_{n-s_r+1,s_r+1} is reused along s_r consecutive steps. Accordingly, the nodes c_j , $s_r \geq j \geq 1$, take the values $c_j = c_{s_r+1} - s_r + j$.

Here, instead of using the information of the last s_r computed steps, we will consider only information of the last computed step, reusing s_r stages of the previous step as stages of the current step. Thus we give the following

Definition 2. *An explicit s -stage peer method (5) is said to have s_r reused stages (therefore $s_e = s - s_r$ effective stages) if there exist s_r pairs $(i_1, j_1) \dots, (i_{s_r}, j_{s_r})$ such that*

- $i_k \neq i_l, j_k \neq j_l$, for all $k \neq l$ and $i_k \neq j_l$ for all k, l .
- $c_{i_k} = c_{j_k} - 1$, $k = 1, \dots, s_r$.
- $Y_{n+1,i_k} = Y_{n,j_k}$, $k = 1, \dots, s_r$.

These conditions imply that the j_k -th stage value of the n -th step, Y_{n,j_k} , is reused only at the i_k -th stage of the $(n+1)$ -th step. Moreover the coefficients of the method satisfy

$$\begin{aligned} \mathbf{e}_{i_k}^T \mathbf{B} &= \mathbf{e}_{i_k}^T \mathbf{R} = (0, \dots, 0)^T, \quad k = 1, \dots, s_r, \\ \mathbf{e}_{i_k}^T \mathbf{A} &= \mathbf{e}_{j_k}^T, \quad c_{i_k} = c_{j_k} - 1, \quad k = 1, \dots, s_r. \end{aligned} \tag{11}$$

It is clear that the number of evaluations of the derivative function reduces to $s_e = s - s_r$ at each step. Moreover, the order conditions (7) are immediately satisfied for the components corresponding to the s_r reused stages.

Remark 1.

- From the condition $i_k \neq i_l, j_k \neq j_l$, for all $k \neq l, i_k \neq j_l$ for all k, l , we deduce that $s_r \leq s/2$ and consequently $s_r \leq s_e$.
- By reordering properly the stages, we can get an equivalent peer method where $i_1 = 1, \dots, i_{s_r} = s_r$, that is, the reused stages are the first s_r ones, and $j_k > s_r$ for $k = 1, \dots, s_e$. Moreover, we can assume, without lacking of generality, that $j_1 < j_2 < \dots < j_{s_e}$.

As an example, the three stage general method given by $\mathbf{c} = (c_2 - 1, c_2, c_3)^T$ and

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 0 & 0 & 0 \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}, \mathbf{R} = \begin{pmatrix} 0 & 0 & 0 \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix},$$

satisfies $\mathbf{e}_1^T \mathbf{B} = \mathbf{e}_1^T \mathbf{R} = (0, 0, 0)$ and $\mathbf{e}_1^T \mathbf{A} = \mathbf{e}_2$. It has one reused stage, $s_r = 1$, and two effective stages, $s_e = 2$. In this case, $i_1 = 1$ and $j_1 = 2$. In addition, since $Y_{1,1} = Y_{0,2}$, we can regroup the evaluations $f(t_1 + c_1 h, Y_{1,1})$ and $f(t_0 + c_2 h, Y_{0,2})$ in one term and rewrite the method with the matrices

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 0 & 0 & 0 \\ b_{21} & b_{22} + r_{21} & b_{23} \\ b_{31} & b_{32} + r_{31} & b_{33} \end{pmatrix}, \mathbf{R} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & r_{22} & r_{23} \\ 0 & r_{32} & r_{33} \end{pmatrix}.$$

We will then consider that a method with reused stages satisfies in addition

$$r_{ij} = 0 \text{ for } j \leq s_r \quad (12)$$

Theorem 1. *Any two-step peer method with s stages and s_r reused stages is equivalent to a three-step peer method with $s_e = s - s_r$ stages.*

PROOF. A three-step peer method can be written as

$$\mathbf{Y}_{n+1} = A_0 \mathbf{Y}_{n-1} + \mathbf{A}_1 \mathbf{Y}_n + h \mathbf{B}_0 f(t_{n-1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n-1}) + h \mathbf{B}_1 f(t_n \mathbf{e} + h \mathbf{c}, \mathbf{Y}_n) + h \mathbf{R}_2 f(t_{n+1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n+1}). \quad (13)$$

where \mathbf{Y}_{n-1} and \mathbf{Y}_n are approximations at two previous steps. Denoting

$$\begin{aligned} \mathbf{Z}_n &= (\mathbf{Y}_{n-1}, \mathbf{Y}_n)^T, \\ \mathbf{Z}_{n+1} &= (\mathbf{Y}_n, \mathbf{Y}_{n+1})^T, \\ \bar{\mathbf{c}} &= (\mathbf{c}, \mathbf{e} + \mathbf{c})^T, \\ f(t_n \mathbf{e} + h \bar{\mathbf{c}}, \mathbf{Z}_n) &= (f(t_{n-1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n-1}), f(t_n \mathbf{e} + h \mathbf{c}, \mathbf{Y}_n))^T, \\ f(t_{n+1} \mathbf{e} + h \bar{\mathbf{c}}, \mathbf{Z}_{n+1}) &= (f(t_n \mathbf{e} + h \mathbf{c}, \mathbf{Y}_n), f(t_{n+1} \mathbf{e} + h \mathbf{c}, \mathbf{Y}_{n+1}))^T, \end{aligned} \quad (14)$$

the above expression (13) can be rewritten as

$$\mathbf{Z}_{n+1} = \bar{\mathbf{A}}\mathbf{Z}_n + h\bar{\mathbf{B}}f(t_n\mathbf{e} + h\bar{\mathbf{c}}, \mathbf{Z}_n) + h\bar{\mathbf{R}}f(t_{n+1}\mathbf{e} + h\bar{\mathbf{c}}, \mathbf{Z}_{n+1}), \quad (15)$$

where

$$\bar{\mathbf{A}} = \begin{pmatrix} 0 & I \\ \mathbf{A}_0 & \mathbf{A}_1 \end{pmatrix}, \quad \bar{\mathbf{B}} = \begin{pmatrix} 0 & 0 \\ \mathbf{B}_0 & \mathbf{B}_1 \end{pmatrix}, \quad \bar{\mathbf{R}} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{R}_2 \end{pmatrix}. \quad (16)$$

Conversely, any s -stage two-step peer method with such an structure can be equivalently written as a three-step peer method with $s/2$ stages.

We will show that a peer method with s_e effective stages satisfying (11) and (12) can be written in the above form with $2s_e$ stages and consequently, it is equivalent to a three-step peer method.

If $s_r = s_e = s/2$, by reordering adequately the first $s/2$ stages, the matrices \mathbf{A} , \mathbf{B} , \mathbf{R} have already the structure in (16) and the vector \mathbf{c} has the form of $\bar{\mathbf{c}}$ in (14). The method is equivalent to a method (15), (16).

If $s_r < s_e$, we can add $s_e - s_r$ stages by adding $s_e - s_r$ zero rows to \mathbf{B} and \mathbf{R} and the same zero columns. For the matrix \mathbf{A} we add $s_e - s_r$ zero rows, except the diagonal element set to 1, and the same zero columns, so that the new matrices have the form (15),(16). Thus, for the above example, the method is equivalent to the scheme with

$$\bar{\mathbf{A}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ a_{21} & 0 & a_{22} & a_{23} \\ a_{31} & 0 & a_{32} & a_{33} \end{pmatrix}, \quad \bar{\mathbf{B}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ b_{21} & 0 & b_{22} & b_{23} + r_{21} \\ b_{31} & 0 & b_{32} & b_{33} + r_{31} \end{pmatrix}, \quad \bar{\mathbf{R}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & r_{22} & r_{23} \\ 0 & 0 & r_{32} & r_{33} \end{pmatrix},$$

and $\bar{\mathbf{c}} = (c_2 - 1, c_3 - 1, c_2, c_3)^T$. This method is equivalent to a three-step peer method.

Remark 2. Note that all peer methods with s_e effective stages have a similar computational cost because they require the same number of evaluations of the vector field per step. However, the number of total stages s affects the number of vectors that must be saved at each step, that is, greater number of stages s implies greater storage requirements and more arithmetic operations.

Remark 3. In this paper we are considering methods that reuse some of the stages of just the previous step. Stages of k previous steps can be used in the current step, as it was done in [12]. In such a case, the peer method with s_e effective stages will be equivalent to a k -step peer method with s_e stages.

Remark 4. In the case of variable step-size, if we are advancing from t_n to t_{n+1} with step size $h_n \neq h_{n-1}$ we require the values $Y_{n,i} \simeq y(t_n + c_i h_n)$ for $i = 1, \dots, s_r$. However, from the previous step we have the values $Y_{n-1,j} \simeq y(t_{n-1} + c_j h_{n-1})$, $j > s_r$, which are not exactly the same because $t_n + c_i h_n = t_{n-1} + h_{n-1} + (c_j - 1)h_n \neq t_{n-1} + c_j h_{n-1}$. This is solved in [12] by taking variable nodes c_j in such a way that $c_j h_{n-1} = h_{n-1} + c_i h_n$. The formulation as a three-step peer method can have some advantage. Thus, we can keep

the nodes constant and get approximations $\widehat{Y}_{n,i} \simeq y(t_n + c_i h_n)$ of order p by interpolating the previous known values $Y_{n,i}, f_{n,i}$. Recall that all the stages have the same order p . This approach is similar to the interpolatory technique in variable step multistep methods [8, 10]. Another possibility is to state the order conditions for the three-step peer method in terms of the step-size ratio $r_n = h_n/h_{n-1}$ and compute the coefficients of the method as functions of r_n , similarly to the variable coefficients technique in multistep methods [2]. This approach is equivalent to the one proposed in [12].

In the next sections we will develop peer methods with 3 and 4 stages having one or two reused stages, assuming fixed step-size. A first point is the construction of the transition matrices \mathbf{A} with the preconsistency condition and such that the method is optimally 0-stable. Then \mathbf{A} must satisfy $\mathbf{A}\mathbf{e} = \mathbf{e}$ and $s - 1$ eigenvalues of \mathbf{A} must vanish. If an s -stage method has s_r reused stages and $s_e = s - s_r$ effective stages, its matrix \mathbf{A} has its s_r first rows constant. Then there are in principle $s \times s_e$ free parameters in \mathbf{A} . The preconsistency condition $\mathbf{A}\mathbf{e} = \mathbf{e}$ imposes s_e linear relations between the coefficients of \mathbf{A} and implies that one eigenvalue of \mathbf{A} is 1. The condition that the other $s - 1$ eigenvalues of \mathbf{A} must be zero imposes, through the characteristic polynomial of \mathbf{A} , $s - 1$ additional relations. In conclusion, it is expected that the number of free parameters of \mathbf{A} is $s \times s_e - s_e - (s - 1) = (s - 1)(s_e - 1)$. The point here is that when either s or s_e are not small it turns out a complicated task to give an explicit expression of the elements of \mathbf{A} in terms of a set of $(s - 1)(s_e - 1)$ free parameters because as remarked above for an optimally stable matrix A some relations between the a_{ij} are non linear algebraic equations. Note that in [12] the matrix A is assumed to be upper triangular, with diagonal elements $0, \dots, 0, 1$, and consequently there are $(s_e - 1)(s_e - 2)/2$ free parameters. Here we are assuming a general matrix, \mathbf{A} , which gives more available parameters but at the price of solving some complicate nonlinear conditions.

The free parameters will be selected having in mind the following conditions:

- Take $c_s = 1$ so that the last stage $Y_{n,s}$ gives an approximation to the solution $y(t_n + h)$ at the grid point $t_n + h$.
- Make the norm of the coefficient \mathbf{C}_{p+1} of the leading term (8) of the local error as small as possible.
- Make the absolute stability interval as large as possible.
- Have superconvergence if possible.

4. Peer methods with two effective stages

There are three possibilities of two-step peer methods with two effective stages, $s_e = 2$, that are equivalent to a three-step peer method with two stages: two with three stages

- $s = 3$ with $\mathbf{c} = (c_1 = c_2 - 1, c_2, 1)^T$ and $Y_{1,1} = Y_{0,2}$. In this case $\mathbf{e}_1^T \mathbf{A} = \mathbf{e}_2^T$ and therefore $a_{11} = 0, a_{12} = 1, a_{13} = 0$.

- $s = 3$ with $\mathbf{c} = (0, c_2, 1)^T$ and $Y_{1,1} = Y_{0,3}$. Then $\mathbf{e}_1^T \mathbf{A} = \mathbf{e}_3^T$ and $a_{11} = 0, a_{12} = 0, a_{13} = 1$.

and one with four stages

- $s = 4$ with $\mathbf{c} = (c_1 = c_3 - 1, 0, c_3, 1)^T$ and $Y_{1,1} = Y_{0,3}$ and $Y_{1,2} = Y_{0,4}$. Then $\mathbf{e}_1^T \mathbf{A} = \mathbf{e}_3^T, \mathbf{e}_2^T \mathbf{A} = \mathbf{e}_4^T$ and $a_{11} = 0, a_{12} = 0, a_{13} = 1, a_{14} = 0, a_{21} = 0, a_{22} = 0, a_{23} = 0, a_{24} = 1$.

Methods with $s_e = 2$ and $s > 4$ have $s_r = s - s_e > s_e$ reused stages and therefore they are equivalent to methods with $s = 3, 4$.

4.1. Case $\mathbf{c} = (c_2 - 1, c_2, 1)^T$

Imposing the preconsistency condition $\mathbf{A}\mathbf{e} = \mathbf{e}$ and that the matrix \mathbf{A} has eigenvalues $1, 0, 0$ (optimal zero stability) we have two possibilities for the matrix \mathbf{A} . If $a_{32} = 1$ the matrix \mathbf{A} has the form

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ a_{21} & 1 & -a_{21} \\ 0 & 1 & 0 \end{pmatrix}, \quad (17)$$

and there is one free parameter a_{21} . If $a_{32} \neq 1$, \mathbf{A} has the form

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ a_{31} + \frac{a_{31}^2}{a_{32} - 1} & a_{31} + a_{32} & -\frac{(a_{32} + a_{31} - 1)^2}{a_{32} - 1} \\ a_{31} & a_{32} & 1 - a_{31} - a_{32} \end{pmatrix}, \quad (18)$$

and we have two free parameters a_{31} and $a_{32} \neq 1$.

Next we study the maximum order attainable for these transition matrices.

4.1.1. Case $a_{32} = 1$

In case of the matrix \mathbf{A} given by (17) we have 9 free parameters: $c_2, a_{21}, b_{21}, b_{22}, b_{23}, b_{31}, b_{32}, b_{33}$ and r_{32} . With them we can attain order 4. In fact, expanding (6) around the point $t + (c_2 - 1)h$ we get the following order conditions for the second stage (recall that we are assuming the conditions (12) and consequently $r_{21} = 0$)

$$\begin{cases} (2 - c_2)a_{21} - b_{21} - b_{22} - b_{23} + 1 = 0, \\ (2 - c_2)^2 a_{21} - 2b_{22} - 2(c_2 + 1)b_{23} + 3 = 0, \\ (2 - c_2)^3 a_{21} - 3b_{22} - 3(c_2 + 1)^2 b_{23} + 7 = 0, \\ (2 - c_2)^4 a_{21} - 4b_{22} - 4(c_2 + 1)^3 b_{23} + 15 = 0, \end{cases}$$

from where we can obtain b_{21}, b_{22}, b_{23} and a_{21} . We have a linear system in these parameters whose matrix of coefficients has a non zero determinant if $c_2 \neq 0, 1, 2$. Then, we have a unique solution in terms of c_2 .

Analogously, for the third stage, b_{31} , b_{32} , b_{33} and r_{32} can be obtained in terms of c_2 from the orderconditions,

$$\begin{cases} -c_2 - b_{31} - b_{32} - b_{33} = 0, \\ (1 - c_2)^2 + 4c_2 - 2b_{32} - 2(2 - c_2)b_{33} - 4r_{32} + 3 = 0, \\ (3 - c_2)^3 - 3b_{32} - 3(2 - c_2)^2b_{33} - 12r_{32} - 1 = 0, \\ (3 - c_2)^4 - 4b_{42} - 4(2 - c_2)^3b_{33} - 32r_{32} - 1 = 0, \end{cases}$$

that form a linear system whose coefficient matrix is non-singular again if $c_2 \neq 0, 1, 2$. Then, the method with order ≥ 4 is determined by the non-zero parameters

$$\begin{aligned} a_{21} &= \frac{3 - 10c_2}{c_2(2 - c_2)^3}, & r_{32} &= \frac{(2 - c_2)^2(-c_2^2 + 2c_2 + 6)}{24c_2}, \\ b_{21} &= -\frac{c_2^3 + c_2^2 + 3c_2 - 1}{2c_2(2 - c_2)^2}, & b_{22} &= \frac{(1 + c_2)(1 - 3c_2)}{2c_2(1 - c_2)}, \\ b_{23} &= \frac{5c_2^2 - 2c_2 + 1}{2c_2(1 - c_2)(2 - c_2)^2}, & b_{31} &= \frac{(2 - c_2)(c_2^2 - 6c_2 + 6)}{24}, \\ b_{32} &= \frac{(4 - c_2)(2 - c_2)(c_2^2 + 2c_2 - 2)}{12(1 - c_2)}, & b_{33} &= \frac{c_2^3 - 6c_2^2 + 10c_2 - 4}{4c_2(1 - c_2)}. \end{aligned}$$

The remaining parameter c_2 will be fixed by considering the Euclidean norm of the error constant vector and the real interval of absolute stability. For this method the norm of the error constant vector is

$$C_5 = \|\mathbf{C}_5\|_2 = \left(\frac{(5c_2^3 + c_2^2 + 3c_2 - 1)^2}{57600c_2^2} + \frac{(2 - c_2)^2(3c_2^3 - 3c_2^2 - 34c_2 + 26)^2}{2073600} \right)^{1/2}.$$

The error coefficient C_5 does not vanish for any value of c_2 and the method can not have order 5. The minimum value of C_5 is attained at $c_2 = 0.563$ and has the value $C_5(0.563) = 0.016814$.

On the other hand, computing numerically the interval of absolute stability of the method we get that it attains its maximum value at $c_2 = 0.45$. As a compromise between minimizing the error coefficient and maximizing the stability interval, we propose to take $c_2 = 0.46$ for which $C_5 = 0.0191722$ and the stability interval is $[-0.85, 0]$.

The exact rational coefficients of the method for $c_2 = 23/50$ are

$$\begin{aligned} a_{21} &= \frac{-100000000}{10500259}, & r_{32} &= \frac{99435259}{6900000}, \\ b_{21} &= \frac{-86117}{272734}, & b_{22} &= \frac{-1387}{1242}, & b_{23} &= \frac{3556250}{3681909}, \\ b_{31} &= \frac{-167167}{3000000}, & b_{32} &= \frac{9862853}{13500000}, & b_{33} &= \frac{-71533}{124200}, \\ c_1 &= -27/50, & c_2 &= 23/50, & c_3 &= 1. \end{aligned} \tag{19}$$

Another option to select the parameter c_2 is to impose the superconvergence. This is accomplished if $\boldsymbol{\nu}^T \mathbf{C}_5 = 0$ with $\boldsymbol{\nu}^T = (a_{21}, 1, -a_{21})$. This condition is satisfied for $c_2 = 0.293865329707072$, that gives the stability interval $[-0.31263, 0]$, yielding the coefficients

$$\begin{aligned} a_{21} &= 1.0392457378907218849, & r_{32} &= 3.2205711960111734306, \\ b_{21} &= -0.10871679818314161401, & b_{22} &= 0.47234216956993994061, \\ b_{23} &= 0.66471606254708996838, & b_{31} &= -0.95609053754149465449, \\ b_{32} &= 2.2459253000123416179, & b_{33} &= -2.7599113569149019133, \\ c_1 &= -0.706134670292928, & c_2 &= 0.293865329707072, \\ c_3 &= 1. \end{aligned} \quad (20)$$

For $c_2 = 0.9626284454321548437$, we also obtain superconvergence but the stability interval $[-0.01167, 0]$ is very small.

4.1.2. Case $a_{32} \neq 1$

In the case of matrix A given by (18) we have 10 parameters $a_{31}, a_{32}, b_{ij}, r_{32}$ and c_2 . With them, we can get a method of order 5.

The order equations up to order 4 for the second stage

$$\left\{ \begin{aligned} \frac{(2-c_2)(a_{31}+a_{32}-1)^2}{a_{32}-1} - a_{31} - a_{32} - b_{21} - b_{22} - b_{23} + 2 &= 0, \\ \frac{(2-c_2)^2(a_{31}+a_{32}-1)^2}{a_{32}-1} - a_{31} - a_{32} - 2b_{22} - 2(2-c_2)b_{23} + 4 &= 0, \\ \frac{(2-c_2)^3(a_{31}+a_{32}-1)^2}{a_{32}-1} - a_{31} - a_{32} - 3b_{22} - 3(2-c_2)^2b_{23} + 8 &= 0, \\ \frac{(2-c_2)^4(a_{31}+a_{32}-1)^2}{a_{32}-1} - a_{31} - a_{32} - 4b_{22} - 4(2-c_2)^3b_{23} + 16 &= 0, \end{aligned} \right.$$

can be solved for $b_{23}, b_{21}, a_{31}, a_{32}$ as functions of b_{22} and c_2 whenever $c_2 \neq 0, 1, 2$.

The equations of order 4 for the third stage

$$\left\{ \begin{aligned} (2-c_2)a_{31} + (1-c_2)a_{32} - b_{31} - b_{32} - b_{33} + 1 &= 0, \\ 2(1-c_2) + (2-c_2)^2a_{31} + (1-c_2)(3+c_2)a_{32} - 2b_{32} + 2c_2b_{33} - 4r_{32} + 3 &= 0, \\ (3-c_2)^3 + (2-c_2)^3(a_{31}+a_{32}-1) - a_{32} - 3b_{32} - 3(2-c_2)^2b_{33} - 12r_{32} &= 0, \\ (3-c_2)^4 + (2-c_2)^4(a_{31}+a_{32}-1) - a_{32} - 4b_{32} - 4(2-c_2)^3b_{33} - 32r_{32} &= 0, \end{aligned} \right.$$

give us b_{31}, b_{32}, b_{33} and r_{32} .

The coefficients of the fifth order term reduce to $\mathbf{C}_5 = (0, C_{52}, C_{53})^T$ with

$$\begin{aligned} C_{52} &= b_{22}(1-c_2)^2 - 4c_2^2, \\ C_{53} &= \frac{b_0c_2 + b_1c_2b_{22} + b_2c_2b_{22}^2}{24(c_2(2c_2(b_{22}-4) + b_{22} + 2) + 2)}, \end{aligned}$$

where

$$\begin{aligned} b_0(c_2) &= (2-c_2)^2(-194 + 935c_2 - 1393c_2^2 + 757c_2^3 + 279c_2^4 - 192c_2^5), \\ b_1(c_2) &= -12(1-c_2)(2-c_2)^2(-15 + 35c_2 - 17c_2^2 - 23c_2^3 + 12c_2^4), \\ b_2(c_2) &= -24c_2(1-c_2)^3(2-c_2)^3. \end{aligned}$$

To get order 5 we must impose $C_{52} = 0$ which gives $b_{22} = 4c_2^2/(1 - c_2)^2$. The condition $C_{53} = 0$ is then satisfied for the roots of the polynomial

$$p_3(c_2) = -194 + 741c_2 + 68c_2^2 - 135c_2^3.$$

The only root of this polynomial in the interval $[0, 1]$ is $c_2 = 0.2588197469856989$. With this value we get the coefficients

$$\begin{aligned} c_1 &= -0.741180253014301145, & c_2 &= 0.2588197469856989, \\ c_3 &= 1, \\ a_{12} &= 1, & a_{21} &= 0.161238627799772241213, \\ a_{22} &= 0.828412865165948871638, & a_{23} &= 0.0103485070342788871495, \\ a_{31} &= 2.673474934799112431145, & a_{32} &= -1.845062069633163559507, \\ a_{33} &= 0.171587134834051128362, & & \\ b_{21} &= 0.0441913578409199441791, & b_{22} &= 0.4877610622761986795467, \\ b_{23} &= 0.6216160986206665167366, & b_{31} &= 0.8214385374014276549412, \\ b_{32} &= 3.662929452413390864301, & b_{33} &= -4.444462523102436783378, \\ r_{32} &= 4.247572725090730819489. \end{aligned} \tag{21}$$

This method has $[-0.1283, 0]$ as the stability interval.

4.2. Case $\mathbf{c} = (0, c_2, 1)^T$

Imposing the preconsistency condition $\mathbf{A}\mathbf{e} = \mathbf{e}$ and that \mathbf{A} has eigenvalues $1, 0, 0$ (optimal zero stability) we get

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & a_{22} & 1 - a_{22} \\ 0 & a_{22} & 1 - a_{22} \end{pmatrix},$$

that depends only on a_{22} .

The order equations of the second stage are linear in a_{22} , b_{21} , b_{22} , b_{23} and define uniquely these coefficients as a function of $c_2 \neq 0, 1, -1$. The order equations of the third stage are linear in b_{31} , b_{32} , b_{33} , r_{32} and define them as rational functions of c_2 . Then we have a family of fourth order methods given by

$$\begin{aligned} a_{22} &= \frac{c_2^2(-6 - 2c_2 + c_2^2)}{(-1 + c_2)^3(1 + c_2)}, & r_{32} &= \frac{(-1 + c_2)(-17 - 7c_2 - c_2^2 + c_2^3)}{12c_2(1 + c_2)}, \\ b_{21} &= -\frac{c_2}{2(1 + c_2)}, & b_{22} &= \frac{c_2(1 + 4c_2 + 2c_2^2)}{2(-1 + c_2)^2(1 + c_2)}, \\ b_{23} &= \frac{c_2(2 + 4c_2 + c_2^2)}{2(-1 + c_2)^2(1 + c_2)}, & b_{31} &= \frac{-7 + 14c_2 - 12c_2^2 - 2c_2^3 + c_2^4}{12c_2(1 + c_2)}, \\ b_{32} &= -\frac{-7 + 10c_2 + c_2^2 - 36c_2^3 - 13c_2^4 + 2c_2^5 + c_2^6}{12(-1 + c_2)^2c_2(1 + c_2)}, \\ b_{33} &= \frac{17 - 38c_2 - 5c_2^2 + 12c_2^3 - 31c_2^4 + 2c_2^5 + c_2^6}{12(-1 + c_2)^2c_2(1 + c_2)}. \end{aligned}$$

The remaining parameter c_2 can be fixed by considering the error constant and the absolute stability. For this method the norm of the error constant is given by

$$C_5 = \|\mathbf{C}_5\|_2 = \left(\frac{(c_2^2(2+c_2)(1+2c_2))^2}{57600(1+c_2)^2} + \frac{(-31+29c_2+29c_2^2-45c_2^3-11c_2^4+c_2^5+c_2^6)^2}{2073600(1+c_2)^2} \right)^{1/2}. \quad (22)$$

The method can not have order 5 because the above error coefficient C_5 does not vanish for any c_2 . It has a minimum at $c_2 = 0.61968$ and has a value $C_5(0.619682) = 0.0133889$. Unfortunately, the stability interval for this value of c_2 is $[-0.0841, 0]$ which is very small. This interval can be enlarged by reducing c_2 , but in this case the error coefficient is large. For example, for $c_2 = 0.01$ the interval is $[-0.4784, 0]$, but the error coefficient is 0.0422265.

Nevertheless, it is possible to get superconvergence. For this method $\boldsymbol{\nu}^T = (0, a_{22}, 1 - a_{22})$ and hence

$$\boldsymbol{\nu}^T \mathbf{C}_5 = \frac{-31 + 60c_2 + 186c_2^2 - 5c_2^4}{720(-1 + c_2^2)},$$

that has a unique zero at $c_2 = 0.277847$ and for this value the order of convergence (with fixed step) is 6. The stability interval is $[-0.2085, 0]$. The properties of this method, are slightly inferior to those of method (20), which makes the method have a lower performance.

4.3. Case $\mathbf{c} = (c_3 - 1, 0, c_3, 1)^T$

Imposing the preconsistency condition $\mathbf{A}\mathbf{e} = \mathbf{e}$ and that the eigenvalues of matrix \mathbf{A} are 1, 0, 0, 0, we get the relations

$$\begin{aligned} a_{41} &= a_{31} \frac{-a_{32} + (a_{32} + a_{31})a_{33}}{-a_{32} + (a_{31} + a_{32})(a_{31} + a_{32} + a_{33})}, \\ a_{42} &= a_{32} \frac{-a_{32} + (a_{32} + a_{31})a_{33}}{-a_{32} + (a_{31} + a_{32})(a_{31} + a_{32} + a_{33})}, \\ a_{43} &= \frac{a_{32}(a_{32} + (a_{33} - 1)a_{33}) + a_{31}(a_{32} + a_{33}^2)}{-a_{32} + (a_{31} + a_{32})(a_{31} + a_{32} + a_{33})}. \end{aligned}$$

With these conditions we can obtain a family of methods of order 5 with three free parameters c_3, a_{31}, a_{32} . It is even possible to get a method of order 6 but its stability interval is very small, which makes the method not useful in practice. Then the three free parameters are selected to have a reasonable stability interval, small error coefficient and also superconvergence. To this end, we have taken a grid of 100×100 points in the domain $(c_3, a_{32}) \in [0, 1] \times [-24, -14]$ computing at each of them the value of a_{31} that gives superconvergence, removing the points for which the stability interval has a length smaller than 0.15.

Searching for a method well balanced between small error constant and large stability interval we have taken $a_{32} = -16.457280303394512$, $a_{31} = -13.020850320747137$ and $c_3 = 0.68$. The resulting method has the error coefficient $\|\mathbf{C}_6\|_2 = 0.0057816$ and a stability interval $[-0.23, 0]$.

The method is determined by the coefficients

$$\begin{aligned}
c_1 &= -0.32, & c_2 &= 0, \\
c_3 &= 0.68, & c_4 &= 1, \\
a_{13} &= 1, & a_{24} &= 1, \\
a_{31} &= -13.020850320747137, & a_{32} &= -16.457280303394512, \\
a_{33} &= 13.863029873184144, & a_{34} &= 16.615100750957505, \\
a_{41} &= 10.8836646940165005, & a_{42} &= 13.7560540352874859, \\
a_{43} &= -10.77668885611984, & a_{44} &= -12.86302987318414, \\
b_{31} &= -0.10475289336554956, & b_{32} &= -13.181978943397285, \\
b_{33} &= -18.04239080932914, & b_{34} &= 2.8004894787301634, \\
b_{41} &= 0.11361995837242606, & b_{42} &= 10.96161489848743367, \\
b_{43} &= 15.122018420408626, & b_{44} &= -1.4681992040025898, \\
r_{43} &= 0.9448969241650209.
\end{aligned} \tag{23}$$

5. Peer methods with three effective stages

There are seven possible families of two-step peer methods with three effective stages: three with four stages ($c_1 = c_2 - 1$, or $c_1 = c_3 - 1$, or $c_1 = c_4 - 1$), three with five stages ($c_1 = c_3 - 1, c_2 = c_4 - 1$, or $c_1 = c_3 - 1, c_2 = c_5 - 1$, or $c_1 = c_4 - 1, c_2 = c_5 - 1$) and one with six stages. With more than six stages, $s_r > s_e$ and the method must be reducible.

In this section we will consider only the case of peer methods with 4 stages and three effective stages with $\mathbf{c} = (c_2 - 1, c_2, c_3, 1)^T$.

By imposing the condition that \mathbf{A} has eigenvalues $1, 0, 0, 0$ and that $a_{11} = a_{13} = a_{14} = 0, a_{12} = 1$, we obtain that the coefficients $a_{41}, a_{42}, a_{43}, a_{44}, a_{24}, a_{34}$ can be expressed in terms of the other 6 coefficients a_{ij} . The remaining 23 parameters can fulfill the order 6 conditions leaving five free parameters $a_{21}, a_{31}, a_{32}, c_2$ and c_3 . It is possible to have order seven, but the absolute stability of the resulting methods is very poor.

Proceeding as in the case of methods with $s = 4$ and two effective stages, we

have obtained a method with

$$\begin{aligned}
c_1 &= -0.8035242525537255, & c_2 &= 0.19647574744627448, \\
c_3 &= 0.72, & c_4 &= 1, \\
a_{21} &= -0.07128783623436709, & a_{22} &= -2.387509763076835, \\
a_{23} &= 0.36944011350403578, & a_{24} &= 3.089357485807169, \\
a_{31} &= -0.62042181681008028, & a_{32} &= -0.6563599502668403, \\
a_{33} &= 0.62955494134947196, & a_{34} &= 1.64722682572745, \\
a_{41} &= 0.098720023563549021, & a_{42} &= -2.0658949190396446, \\
a_{43} &= 0.2092200737487298, & a_{44} &= 2.757954821727366, \\
b_{21} &= -0.01638484510723668, & b_{22} &= -0.600007633856693, \\
b_{23} &= -1.35655864264368, & b_{24} &= 0.22587876143321779, \\
b_{31} &= -0.15949696692096115, & b_{32} &= -1.709290486968977, \\
b_{33} &= 3.486392736696774, & b_{34} &= -6.2893371594343907, \\
b_{41} &= 0.024420393431217120, & b_{42} &= -0.015773121933605, \\
b_{43} &= -2.93561830783985, & b_{44} &= 3.50260698391356795, \\
r_{32} &= 3.9216603283306189245, \\
r_{42} &= -1.77040450882688773, & r_{43} &= 0.713974679388708.
\end{aligned} \tag{24}$$

With this values of the parameters the method has order 6 with error coefficient $C_7 = 0.0006121$ and an absolute stability interval $[-0.15, 0]$ and also superconvergence.

6. Numerical experiments

To show the performance of the peer methods above developed we present some numerical experiments to compare them with other previously developed peer methods and to check the correctness of the order results. In order to do that, we consider two non-linear problems of low dimension used by many authors as non-stiff test problems:

1. The Euler's equations that describe the motion of a free rigid body

$$\begin{aligned}
y'_1 &= (\alpha - \beta)y_2y_3, \\
y'_2 &= (1 - \alpha)y_1y_3, \\
y'_3 &= (\beta - 1)y_1y_2, \\
y(0) &= (0, 1, 1)^T,
\end{aligned} \quad t \in [0, 10], \tag{25}$$

where

$$\alpha = 1 + 1/\sqrt{1.51}, \quad \beta = 1 - 0.51/\sqrt{1.51}.$$

The solution of this problem is

$$y(t) = \left(\sqrt{1.51} \operatorname{sn}(t, 0.51), \operatorname{cn}(t, 0.51), \operatorname{dn}(t, 0.51) \right)^T,$$

where sn, cn, dn are the Jacobi elliptic functions with elliptic modulus 0.51.

2. The Duffing's equation

$$\begin{aligned} y'' + (w^2 + k^2)y &= 2k^2y^3, \quad t \in [0, 20], \\ y(0) &= 0, \quad y'(0) = w, \end{aligned}$$

with $k = 0.035$ and $w = 1$. This problem has the solution

$$y(t) = \operatorname{sn}\left(wt, (k/w)^2\right).$$

We have selected in our experiments the following peer methods (we use the notation ijk to indicate: i total number of stages, j effective stages and order k and $ijks$ to indicate that the method has superconvergence order $(k + 1)$):

New324 The peer method with three stages, two effective stages and order 4 with $c_1 = c_2 - 1$, given in (19). This method has an stability interval larger than the other selected peer methods.

New324s The peer method with three stages, two effective stages and order 4 with $c_1 = c_2 - 1$, given in (20). This method has superconvergence of order 5.

New325 The peer method with three stages, two effective stages and order 5 with $c_1 = c_2 - 1$, given in (21).

New425s The peer method with four stages, two effective stages and order 5 with $c_1 = c_3 - 1, c_2 = c_4 - 1 = 0$, given in (23). It has also superconvergence of order 6.

New436s The peer method with four stages, three effective stages and order 6 with $c_1 = c_2 - 1, c_4 - 1 = 0$, given in (24). It has also superconvergence of order 7.

Calvo335 The peer method with three stages, three effective stages and order 5 proposed in [3].

Klinge425 The peer method with four stages, two effective stages and order 5 with $c_1 = c_3 - 1, c_2 = c_4 - 1 = 0$, proposed in [12].

In Table 1 we give the main properties of the methods used in the experiments

In the above problems we have used a fixed stepsize, taking $h = T/2^i$, for $i = 3, 4, \dots$

To start the integration, the stages corresponding to the first step were defined as the exact solution, that is, $Y_{0,k} = (y(t_0 + c_1h)^T, \dots, y(t_0 + c_s h)^T)^T$.

For each integration we have computed at each step the Euclidean norm of the global error, and we have obtained the maximum of these values, GE. We

Table 1: Properties of the methods

Method	Order	Stab	Error coef.	s_e	Super conv.
Calvo335	5	2.02	0.003642	3	No
Klinge425	5	0.38	0.044127	2	No
New324	4	0.82	0.019172	2	No
New324s	4	0.31	0.032019	2	Yes
New325	5	0.13	0.014686	2	No
New425	5	0.23	0.005781	2	Yes
New436	6	0.15	0.000612	3	Yes

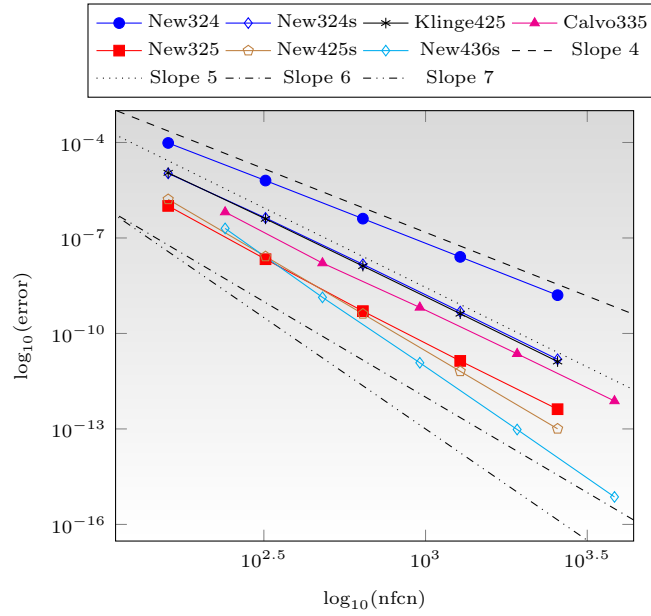


Figure 1: Efficiency plot for Euler's equations

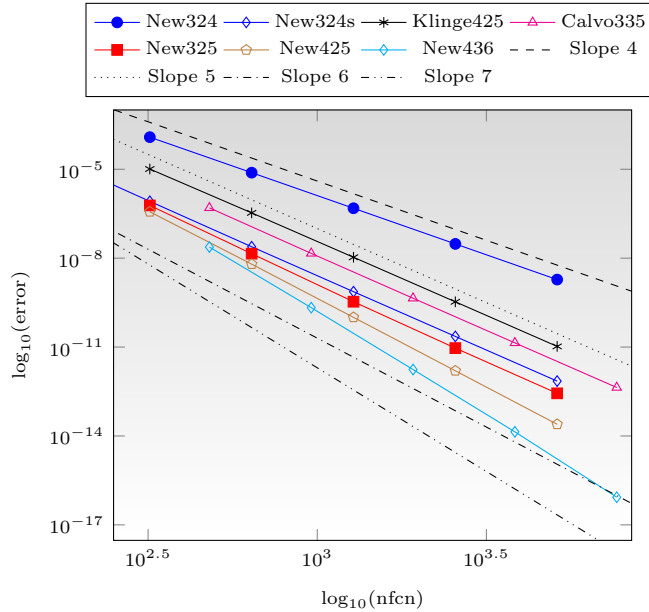


Figure 2: Duffing's equation: efficiency plot

have also computed the number of function evaluations $nfcn$ required for the corresponding integration.

In Figures 1 and 2 we display the efficiency plots, $\log_{10}(GE)$ versus $\log_{10}(nfcn)$, corresponding to the problems 1 and 2.

From Figures 1 and 2, we can see that all the methods exhibit the order deduced from the theory. Moreover, in general, the higher the order, the more efficient the method. It is also seen that the new methods are more efficient than the existing methods with the same order. It is worth to note that the methods New436s, New425s and New324s show numerical orders 5, 6 and 7 respectively, due to the superconvergence property.

Secondly, we want to compare the performance of the proposed methods with some existing state of the art methods such as the classical sixth-order Adams-Bashforth-Moulton implemented in PECE mode and the well-known fifth-order Runge-Kutta scheme of Dormand and Prince [6]. In this case, we have considered two problems with high dimension.

3 The reaction-diffusion equation (Brusselator with diffusion) ([9], page 248)

$$\begin{cases} \frac{\partial u}{\partial t} = 1 + u^2v - 4.4u + \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ \frac{\partial v}{\partial t} = 3.4u - u^2v + \alpha \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \end{cases}$$

for $0 \leq x \leq 1, 0 \leq y \leq 1, t \geq 0, \alpha = 2 \cdot 10^{-3}$ together with the initial conditions

$$u(x, y, 0) = 0.5 + y, \quad v(x, y, 0) = 1 + 5x,$$

and the Neumann boundary conditions

$$\frac{\partial u}{\partial \mathbf{n}} = 0, \quad \frac{\partial v}{\partial \mathbf{n}} = 0,$$

where \mathbf{n} is the normal vector to the boundary of the square $[0, 1] \times [0, 1]$. The method of lines using centered finite differences with

$$x_i = (i - 1)/(N - 1), \quad y_j = (j - 1)/(N - 1), \quad i, j = 1, \dots, N,$$

and defining

$$U_{ij}(t) = u(x_i, y_j, t), \quad V_{ij}(t) = v(x_i, y_j, t),$$

yields the system of ODEs for $i, j = 1, \dots, N$,

$$\begin{aligned} U'_{ij} &= 1 + U_{ij}^2 V_{ij} - 4.4U_{ij} + \alpha(N - 1)^2 (U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} - 4U_{ij}) \\ V'_{ij} &= 3.4U_{ij} - U_{ij}^2 V_{ij} + \alpha(N - 1)^2 (V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{ij}) \end{aligned} \quad (26)$$

of dimension $2N^2$.

Because of the boundary conditions we have

$$U_{0j} = U_{2j}, \quad U_{N+1j} = U_{N-1j}, \quad U_{i0} = U_{i2}, \quad U_{iN+1} = U_{iN-1},$$

and similarly for V_{ij} . We choose $N = 21$, giving a dimension of 882 and as the integration interval $t \in [0, 10]$.

We have solved it with the 4-stage peer methods deduced in the previous section, the DOPRI5 and the sixth-order Adams-Bashforth-Moulton (ABM6) to show the behaviour of this class of methods in high dimension problems.

- 4 As another problem with large dimension, we consider the ROPE problem ([9], page 247)

$$\begin{aligned} \sum_{k=1}^n a_{lk} \ddot{\theta}_k &= - \sum_{k=1}^n b_{lk} \dot{\theta}_k^2 - n \left(n + \frac{1}{2} - l \right) \sin(\theta_l) \\ &\quad - n^2 \sin(\theta_l) F_x(t) + \begin{cases} n^2 \cos(\theta_l) F_y(t) & \text{if } l \leq 3n/4, \\ 0 & \text{if } l > 3n/4, \end{cases} \end{aligned}$$

for $l = 1, 2, \dots, n$, and

$$a_{lk} = g_{lk} \cos(\theta_l - \theta_k), \quad b_{lk} = g_{lk} \sin(\theta_l - \theta_k), \quad g_{lk} = n + \frac{1}{2} - \max\{l, k\},$$

with the horizontal force $F_y(t) = 1/(\cosh(4t - 2.5))^4$ and the vertical force $F_x(t) = 0.4$. The initial conditions are $\theta_l(0) = \dot{\theta}_l(0) = 0$, the integration interval is $[0, 3.723]$ and choosing $n = 40$ we obtain a system of ODEs of dimension 80.

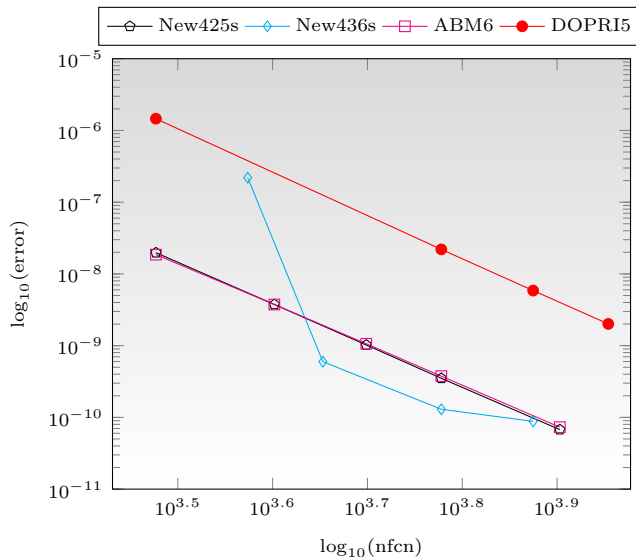


Figure 3: Efficiency plot for the Brusselator equation

In problems 3 and 4 we have used different values for the number of integration steps (fixed stepsize). To obtain the exact solution, we have taken the DOPRI853 with stringent tolerances to compute the global error at the end point of the integration interval.

In Figures 3 and 4 we display the efficiency plots, $\log_{10}(GE)$ versus $\log_{10}(nfcn)$, corresponding to the two problems considered.

In the non-stiff Brusselator equation, the most efficient method when the step is small corresponds to the New436s. Also, the efficiency of the peer New425s is the same as the ABM6.

For the ROPE problem, the efficiency of New425s is very similar to ABM6 and the peer scheme New436s appears to be better when the step size is small.

This numerical experiments indicate that both methods are quite competitive when are compared against the DOPRI5 method.

7. Conclusions

In general an two-step explicit s -stage peer method requires the computation of s vector fields $f(t_{n,j}, Y_{n,j})$, ($j = 1, 2, \dots, s$) per step but under some relation between the nodes it is possible to construct s -stage methods that require $s_e < s$ effective computations at each step. In this paper a new technique to construct explicit s -stage peer methods with $s_e \leq s/2$ effective stages of the previous step is presented.

We have derived new peer methods with three stages and two effective stages that attain order 4 and 5. With four stages we have developed methods with

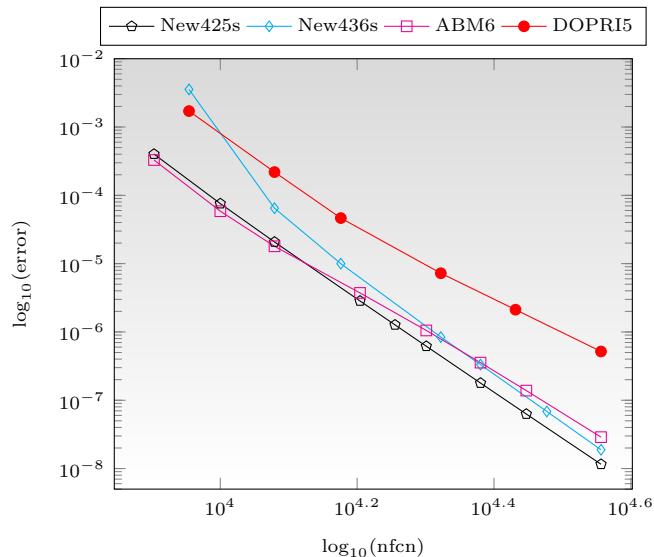


Figure 4: Efficiency plot for the ROPE equation

and 2 and 3 effective stages that attain order 5 and 6 respectively. By choosing the available parameters to get the highest order of accuracy with smallest error constant and maximum real stability interval. Since optimal methods with each of these requirements is achieved for different values of the available parameters a compromise between these objectives is considered.

The results of some numerical experiments are presented to show that with a fixed step size the new methods have orders of accuracy that are those predicted by the theory and can be more efficient than some standard explicit formulas used in the solution of non-stiff IVPs. At the moment an extension of the present formulas to a variable step size environment is under study as well as local error estimators with the purpose to use these formulas in codes that may adjust the size step along the integration to have an efficient computation.

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