High Order Explicit Two-Step Runge-Kutta Methods for Parallel Computers

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In this paper we study a class of explicit pseudo two-step Runge-Kutta methods (EPTRK methods) with additional weights v. These methods are especially designed for parallel computers.

We study s-stage methods with local stage order s and local step order $s+2$ and derive a sufficient condition for global convergence order $s+2$ for fixed step sizes. Numerical experiments with 4- and 5-stage methods show the influence of this superconvergence condition.

However, in general it is not possible to employ the new introduced weights to improve the stability of high order methods. We show, for any given s-stage method with extended weights which fulfills the simplifying conditions $B(s)$ and $C(s-1)$, the existence of a reduced method with a simple weight vector which has the same linear stability behaviour and the same order.

Keywords: Runge-Kutta methods, parallelism, two-step methods, superconvergence, linear stability

1. Introduction

For the numerical solution of systems of first-order ordinary differential equations (ODEs)

$$y' = f(t,y), \quad y(t_0) = y_0, \quad y, f \in \mathbb{R}^n, \quad (1)$$

Fei [5], Cong [2] and Cong et al. [3] have recently investigated a class of parallel explicit pseudo two-step Runge-Kutta methods (EPTRK methods). EPTRK methods compute an approximation $y_m \approx y(t_m)$ by the s-stage scheme

$$\begin{aligned} Y_m &= \mathbb{1} \otimes y_m + h_m (A \otimes I) F(t_{m-1}\mathbb{1} \\ &\quad + h_{m-1}c,\, Y_{m-1}), \qquad (2a) \\ y_{m+1} &= y_m + h_m (b^T \otimes I) F(t_m \mathbb{1} + h_m c,\, Y_m) \qquad (2b) \end{aligned}$$

with s (external) stage approximations $Y_m \in \mathbb{R}^{n\times s}$, parameters $A = (a_{ij}) \in \mathbb{R}^{s\times s}$, $c, b \in \mathbb{R}^s$, $\mathbb{1} := (1,\ldots,1)^T$ and step size h_m. F denotes the straightforward extension of f to $\mathbb{R}^{n\times s}$. Here, $\otimes$ denotes the Kronecker tensor product. Notice that the EPTRK method(2) requires only one sequential function evaluation per step on a parallel computer with s processing elements. Numerical experiments with a variable step size implementation on a shared memory computer have shown that EPTRK methods perform well for non stiff ([3]) and for mildly stiff ([10]) problems.

A more general class of two-step RK methods was introduced by Jackiewicz et al. (see [8] and [1] and the references therein). Although Jackiewicz's methods are constructed not with respect to a parallel implementation, it is attractive to borrow the idea of introducing a new weight vector v of s parameters and consider parallel EPTRK methods of the form

$$\begin{aligned} Y_m &= \mathbb{1} \otimes y_m + h_m (A \otimes I) F(t_{m-1}\mathbb{1} \\ &\quad + h_{m-1}c,\, Y_{m-1}), \qquad (3a) \\ y_{m+1} &= y_m + h_m (b^T \otimes I) F(t_m \mathbb{1} + h_m c,\, Y_m) \\ &\quad + h_m (v^T \otimes I) F(t_{m-1}\mathbb{1} + h_{m-1}c,\, Y_{m-1}). \qquad (3b) \end{aligned}$$

The additional effort to compute y_{m+1} in (3b) is small and the parallelization of the method is not affected. The aim of this paper is to study the effects of the new parameters v with respect to order and stability.

2. Superconvergence

Definition 2.1. Let $\triangle_{m,0}$ and $\triangle_m$ denote the residuals of the integration scheme (3) obtained by substituting exact solutions $y(t_m)$ and $Y(t_m) := (y(t_m + c_1 h_m), \ldots, y(t_m + c_s h_m))$ of (1), i.e.

$$\begin{aligned}\triangle_{m,0} &= Y(t_m) - \mathbb{1} \otimes y(t_m) \\ &\quad - h_m(A \otimes I)Y'(t_{m-1}), \qquad (4a)\\ \triangle_m &= y(t_{m+1}) - h_m(b^T \otimes I)Y'(t_m)) \\ &\quad + h_m(v^T \otimes I)Y'(t_{m-1})) \ . \qquad (4b)\end{aligned}$$

An EPTRK method (3) is of *local step order p* if $\triangle_m = \mathcal{O}(h_m^{p+1})$ and of *local stage order q* if $\triangle_{m,0} = \mathcal{O}(h_m^{q+1})$.

A Taylor series expansion of $y(t)$ in (4) shows that an EPTRK method is of local stage order q and local step order p if the simplifying conditions $C(q)$ and $B(p)$ defined by

$$\begin{aligned}&\left[c, \sigma\frac{c^2}{2}, \sigma^2\frac{c^3}{3}, \ldots, \sigma^{q-1}\frac{c^q}{q}\right] \\ &\quad = A\left[\mathbb{1}, c-\mathbb{1}, (c-\mathbb{1})^2, \ldots, (c-\mathbb{1})^{q-1}\right], \qquad (\mathrm{C(q)})\\ &\left[1, \frac{\sigma}{2}, \frac{\sigma^2}{3}, \ldots, \frac{\sigma^{p-1}}{p}\right] \\ &\quad = b^T\left[\mathbb{1}, \sigma c, \sigma^2 c^2, \ldots, \sigma^{p-1}c^{p-1}\right] \\ &\qquad + v^T\left[\mathbb{1}, (c-\mathbb{1}), (c-\mathbb{1})^2, \ldots, (c-\mathbb{1})^{p-1}\right] \qquad (\mathrm{B(p)})\end{aligned}$$

are satisfied. Here $\sigma = h_m/h_{m-1}$ denotes the step size ratio.

By standard techniques it can be shown, that a method satisfying $C(s)$ and $B(s+1)$ converges with order $p = s+1$, e.g. [9] for the case $v = 0$. One can find methods which fulfill $C(s+1)$, however the c- vector will include large components and the error constants will be large. On the other hand, it is possible to satisfy $B(l)$ with $l > s+1$. However, this will not increase the order of convergence in general. We will show that, for general c with an additional condition on b and v, the order of convergence is $p = s+2$. For simplicity, we restrict here to the case of a constant step size.

Theorem 2.1. (Superconvergence of EPTRK methods) *Let $C(s)$ and $B(s+2)$ be satisfied. Let further hold the condition*

$$(b^T + v^T)\left(\frac{c^{s+1}}{s+1} - A(c-1)^s\right) = 0. \qquad (5)$$

Then with starting values of order $s+2$ the method will converge with order $p = s+2$.

Proof. Substituting the exact solution into (3) yields

$$\begin{aligned}Y(t_m) &= \mathbb{1}\otimes y(t_m) + h(A\otimes I)F(t_{m-1}\mathbb{1} \\ &\quad + hc, Y(t_{m-1})) + \triangle_{0,m} \\ y(t_{m+1}) &= y(t_m) + h(b^T\otimes I)F(t_m\mathbb{1} + hc, Y(t_m)) \\ &\quad + h(v^T \otimes I)F(t_{m-1}\mathbb{1} + hc, Y(t_{m-1})) + \triangle_m. \qquad (6)\end{aligned}$$

With $C(s)$ and $B(s+2)$ by Taylor expansion follows

$$\begin{aligned}\triangle_{0,m} &= \frac{h^{s+1}}{s!}\left(\frac{c^{s+1}}{s+1} - A(c-1)^s\right) \\ &\quad \otimes y^{(s+1)}(t_m) + \mathcal{O}(h^{s+2}), \\ \triangle_m &= \mathcal{O}(h^{s+3}) \ .\end{aligned}$$

Subtracting (3) from (6) yields a recursion for the global error

$$err_{m+1} = y(t_{m+1}) - y_{m+1}.$$

With the standard convergence result $Y(t_m) - Y_m = \mathcal{O}(h^{s+2})$ for $C(s)$ and $B(s+1)$ we get by the mean value theorem and expanding the Jacobians at $(t_m, y(t_m))$

$$\begin{aligned}err_{m+1} &= (I + \mathcal{O}(h))err_m + \mathcal{O}(h)err_{m-1} \\ &\quad + (b^T + v^T)\left(\frac{c^{s+1}}{s+1} - A(c-1)^s\right)\frac{h^{s+2}}{s!}\times \\ &\quad \times f_y(t_m, y(t_m))y^{(s+1)}(t_m) + \mathcal{O}(h^{s+3}).\end{aligned}$$

With (5) follows

$$\begin{aligned}\|err_{m+1}\| &\le (1 + d_1 h)\|err_m\| + d_2 h\|err_{m-1}\| \\ &\quad + d_3 h^{s+3}, \ d_1, d_2 d_3 > 0.\end{aligned}$$

We can bound $\|err_m\|$ by the solution r_m of

$$r_{m+1} = (1 + d_1 h)r_m + d_2 h r_{m-1} + d_3 h^{s+3}$$

with $r_0 = \|err_0\| = d_4 h^{s+2}$, $r_1 = \|err_1\| = d_5 h^{s+2}$, $d_4, d_5 > 0$, giving finally $err_m = \mathcal{O}(h^{s+2})$.

□

	name	conditions	order p	$\|E_{s+1}\|_2$	e_{s+1}
4-stage	gauss4	B(8), C(4)	5	1.051	0.2952
	vgauss4	B(6), C(4)	6	1.051	0
	n4	B(6), C(4)	6	2.334	0
5-stage	cong5	B(7), C(5)	6	2.670	0.0475
	vcong5	B(7), C(5)	7	2.670	0
	n5	B(7), C(5)	7	2.385	0

Table 1. EPTRK methods

3. Numerical Illustration of the Order Results

To discuss the impact of condition (5) for EPTRK methods we construct different sets of coefficients with 4- and 5-stages and apply the resulting methods to three (non stiff) test problems.

Construction of 4-stage Methods

We start with $s = 4$ stages. For any choice of knots c_i a method with $v = 0$ is uniquely determined by $B(4)$ and $C(4)$. The remaining 4 degrees of freedom can be used to satisfy $B(8)$ with c-vector taken as Gaussian collocation points, as done for method gauss4 in Table 1. Here, $E_{s+1} := A(c-1)^s - c^{s+1}/(s+1)$ denotes the local stage error and $e_{s+1} := (b^T + v^T)E_{s+1}$ denotes the residual of condition (5) in Theorem 2.1. Since e_{s+1} does not vanish, the global convergence order is only 5.

Global order 6 can be achieved by satisfying $C(s)$, $B(s+2)$ and (5) for given c by computing v or for $v = 0$ by a special choice of c. To attain global order 6 with the same points c_i we choose v as a solution of $e_{s+1} = 0$. But $B(6)$ depends on v and has to be satisfied, too. With the help of Maple V we calculated a solution

$$\begin{aligned} v = [&0.0, -0.006632901980013884, \\ &-0.319483842974888, \\ &0.06964740132900621]. \end{aligned}$$

for this method vgauss4, see Table 1.

Although it is natural to guarantee condition (5) for arbitrarily chosen knots c_i by introducing a suitable v vector, it is not necessary. By choosing special points c one can find EPTRK methods with $v = 0$ which satisfy (5), $B(s+2)$ as we did for the method n4 with

$$\begin{aligned} c = [&0.1493506562434243, \\ &0.6535456428480576,\ 1.123, \\ &1.6391116441727]\ . \end{aligned}$$

Construction of 5-stage Methods

The method cong5 was proposed in [3]. Due to small error coefficients, this method performs well for non stiff problems. Since $e_{s+1} \neq 0$ the global order is $p = 6$ only, see Table 1. The method cong5 has the knots

$$\begin{aligned} c = [&0.08858795951270395, \\ &0.4094668644407347, \\ &0.7876594617608471,\ 1, \\ &1.409466864440735]\ . \end{aligned} \qquad (6)$$

With the choice $v = [0, 0, 0, 0, -0.018424462471253 09]$ and the c-vector (6) the method vcong5 fulfills (5), $B(s+2)$ and has global order $p = 7$.

The method n5 has been constructed with $v = 0$ and

$$\begin{aligned} c = [&0.1365941578442505, 0.625, \\ &1.230436842527931, 1.5, \\ &1.6911642569218]\ . \end{aligned}$$

These values guarantee (5) and $B(s+2)$ and give a small leading stage error coefficient $\|E_{s+1}\|$.

Test Problems

We consider the following test problems:

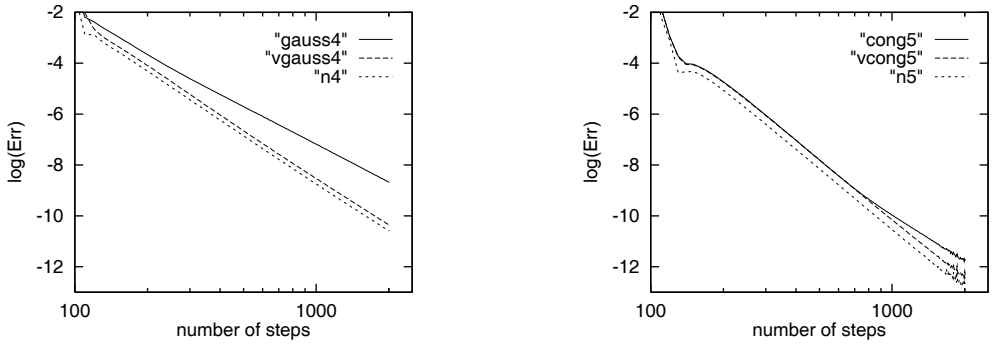

Fig. 1. Results for problem NOFE(8)

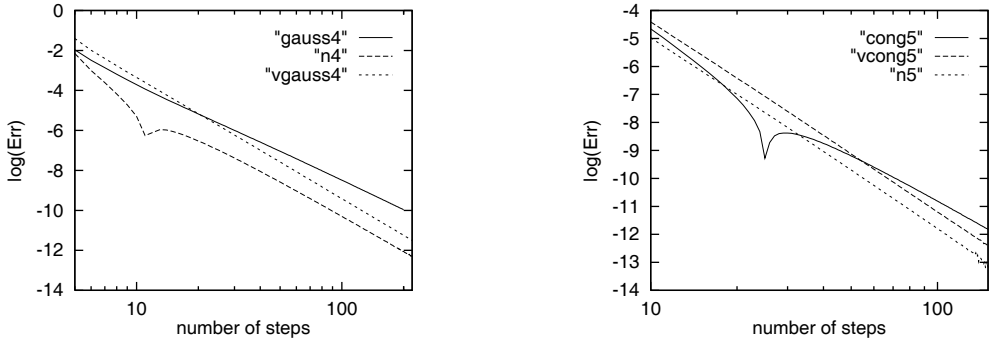

Fig. 2. Results for problem PROTH (9)

- NOFE – a nonlinear problem proposed by Fehlberg [4].

$$y_1' = 2ty_1 \log(\max(y_2, 0.001)) \quad (8a)$$
$$y_2' = -2ty_2 \log(\max(y_1, 0.001)) \quad (8b)$$
$$t \in [0, 5] \quad (8c)$$

  with initial values taken from the exact solution $y_1(t) = \exp(\sin(t^2))$, $y_2(t) = \exp(\cos(t^2))$.

- PROTH – a (non stiff) Prothero-Robinson problem, see [7].

$$y' = \lambda(y - \sin(t)) + \cos(t), \quad t \in [0, 10], \quad \lambda = 0.1, \quad (9)$$

  with exact solution $y(t) = \sin(t)$.

- ORBIT – a two-body orbit problem, see [6].

$$y_1' = y_3, \quad y_2' = y_4 \quad (10a)$$
$$y_3' = -\frac{y_1}{r^3}, \quad y_4' = -\frac{y_2}{r^3}, \quad t \in [0, 10], \quad (10b)$$

  $r = \sqrt{y_1^2 + y_2^2}$, with exact solution $y(t) = [\cos(t), \sin(t), -\sin(t), \cos(t)]$.

We implemented the EPTRK methods of Table 1 in FORTRAN using double precision and applied them to the test problems. (The code for the method cong5 can be obtained from our web site http://www.mathematik.uni-halle.de/institute/numerik/software.)

In the figures below we have plotted the number of steps versus the error *ERR* in the endpoint of the integration, defined by

$$ERR = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - y_i(t_{end})}{1 + |y_i(t_{end})|}\right)^2}.$$

Notice, from $ERR \approx Ch^p$ follows $\log(ERR) \approx \log(C) - p \cdot \log(h^{-1})$ and therefore the order of an EPTRK method can be estimated by the slope of the lines in the figures.

The order 6 of the 4-stage methods n4 and vgauss4 compared with the order 5 of the method gauss4 leads to a better accuracy for all step sizes. Due to smaller error constants in the step formula (3b) (not shown in Table 1) the method n4 with $v = 0$ performs slightly better as vgauss4 in particular in example PROTH, Fig. 2.

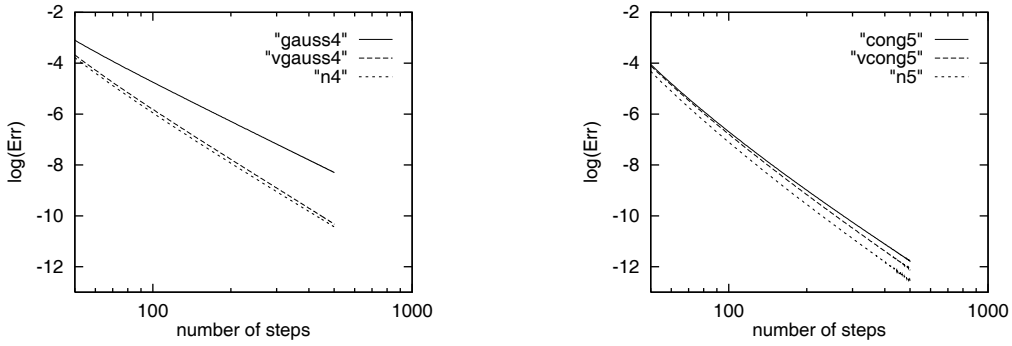

Fig. 3. Results for problem ORBIT (10)

The fact that cong5 is of order 6 only can be seen for sufficient small step sizes, i.e. the slope of the lines in the figures is smaller than the slopes of the (nearly parallel) lines of vcong5 and n5. The best overall performance gives the method n5 with $v = 0$ and small error constants.

4. Stability

The stability of EPTRK methods with $v = 0$ has been investigated in [10]. The adaption of the concepts there to the case $v \neq 0$ is straightforward. Here, we start with a short review of the notations:

We apply the EPTRK methods to the linear test equation $y' = \lambda y, \quad \mathrm{Re}\lambda \leq 0$ with constant step size h. Then the solution fulfills the recursion

$$(Y_m, y_{m+1})^T = M(z)(Y_{m-1}, y_m)^T, \quad z = h\lambda \ , \tag{11}$$

with the amplification matrix

$$M(z) = \begin{pmatrix} zA & \mathbb{1} \\ z^2 b^T A + z v^T & 1 + z b^T \mathbb{1} \end{pmatrix} \ . \tag{12}$$

We define the stability region S^* of an EPTRK method by

$$S^* := \{z : \varrho(M(z)) \leq 1\}$$

and have $\varrho(M(z)) < 1$ if z is an inner point of S^* and hence $(Y_m, y_{m+1}) \to 0$ for $m \to \infty$. We obtain $\varrho(M(z))$ by computing the zeros of the stability polynomial $\varrho(x, z) := \det(xI - M(z))$.

But surprisingly, the new parameters v do not give us any new degree of freedom in the corresponding stability polynomial. We have the following theorem:

Theorem 4.1. *For every method (3) with $C(s-1)$ and $B(s)$ there exists a corresponding method with $v^T = 0$, satisfying $C(s-1)$, $B(s)$ and having the same stability polynomial.*

Proof. The rather lengthy proof requires a careful study of the stability polynomial. It is given in [11].

□

A consequence of Theorem 4.1 is that it is not possible to improve the stability of EPTRK methods with a choice $v \neq 0$ for high order methods. However, a nontrivial choice of the v-vector may be useful to conserve the stability for variable step sizes.

5. Conclusion

We have proposed a superconvergence condition (5) in Theorem 2.1, which allows the construction of s-stage EPTRK methods with stage order s and convergence order $s + 2$. To satisfy this condition with a given set of knots c_i we have introduced new parameters v into the integration scheme(3). Numerical tests with fixed step size and 4- and 5-stage methods have illustrated the convergence result. Though it has been possible to find special knots c_i which guarantee condition (5) for constant step size with $v = 0$, for variable step sizes we are forced to choose $v \neq 0$. Equation (5) becomes

$$b_m^T \left[\frac{c^{s+1}}{s+1} \sigma_m^{s+1} - \sigma_m A(\sigma_m)(c-1)^s \right] + v_m^T \left[\frac{c^{s+1}}{s+1} - \frac{1}{\sigma_{m-1}} A(\sigma_{m-1})(c-1)^s \right] = 0 \tag{13}$$

with step size ratios $\sigma_m := h_m/h_{m-1}$ and σ_m-dependent RK matrix $A = A(\sigma_m)$ and condition (5) cannot longer be satisfied with $v = 0$. Since with $v \neq 0$ the error behavior is smoother, we hope to obtain a more reliable error estimation and step size control in this case. This generalization to variable step sizes will be a topic of further work.

In Theorem 4.1 we have shown that it is not possible to enlarge the stability regions of the EPTRK methods with $B(s)$ and $C(s-1)$ with the new parameters v of the integration scheme. However, the construction in [10] of a EPTRK method based on a given stability polynomial can be simplified with $v \neq 0$.

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Received: May 15, 1999
Accepted in revised form: January 21, 2000

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