A Class of Explicit Two-Step Runge-Kutta Methods with Enlarged Stability Regions for Parallel Computers

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Abstract. In this paper we study a class of explicit pseudo two-step Runge-Kutta (EPTRK) methods for first-order ODEs for parallel computers. We investigate linear stability and derive methods with enlarged stability regions. In numerical experiments on a shared memory computer we compare a parallel variable step size EPTRK implementation with the efficient sequential Runge-Kutta method `dopri5`.

Key words: Runge-Kutta methods, parallelism, two-step methods, stability
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1 Introduction

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

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

Fei [3], Cong [1] and Cong et al. [2] have recently investigated a class of explicit pseudo two-step Runge-Kutta methods (EPTRK methods). EPTRK methods compute an approximation $u_m \approx y(t_m)$ by the s-stage scheme

$$U_{m+1} = \mathbb{1} \otimes u_m + h_m(A_m \otimes I)F(t_{m-1}\mathbb{1} + h_{m-1}c, U_m), \tag{2a}$$

$$u_{m+1} = u_m + h_m(b^T \otimes I)F(t_m\mathbb{1} + h_m c, U_{m+1}), \tag{2b}$$

with s (external) stage approximations $U_{m+1} \in \mathbb{R}^{n\times s}$, parameters $A_m \in \mathbb{R}^{s\times s}$, $c, b \in \mathbb{R}^s$ and step size h_m. F denotes the straightforward extension of f to $\mathbb{R}^{n\times s}$.

The EPTRK methods are well suited for parallelization with s processors, especially in a shared memory environment. They do not have a sequential bottleneck and need only one effective function evaluation per step. Notice that the parallelism is already in the method. Consequently, using an EPTRK method do not require any additional effort to split the ODE system and this system can be solved by a black-box (library) call yielding coarse grain parallelism.

Numerical tests of a special class of EPTRK methods of high order in [2] have shown the efficiency for problems, where the step size is determined by accuracy only. However, this class suffers from very small stability regions. Therefore, in this paper we construct EPTRK methods of order 3 and 4 with enlarged stability regions.

2 Order Conditions and Convergence

In this section we consider order conditions for EPTRK methods. Assume exact values $U_m = y(t_{m-1}\mathbb{1} + h_{m-1}c)$ and $u_m = y(t_m)$. We perform one EPTRK step with step size h_m and compare the numerical solutions U_{m+1} and u_{m+1} with the exact values $y(t_m\mathbb{1} + h_m c)$ and $y(t_{m+1})$. Let $\alpha := h_m/h_{m-1}$ be the step size ratio. Comparing the Taylor expansions of numerical and analytical solutions yields, analogously with implicit Runge-Kutta Methods, the simplifying conditions

$$C(q): \quad \sum_{j=1}^{s} a_{ij}(c_j - 1)^{\nu-1} = \alpha^{\nu-1}\frac{c_i^\nu}{\nu}, \qquad i = 1,\ldots,s, \quad \nu = 1,\ldots,q \tag{3a}$$

$$B(p): \quad \sum_{i=1}^{s} b_i c_i^{j-1} = \frac{1}{j}, \qquad j = 1,\ldots,p \tag{3b}$$

for stage order q and step order p. From $C(p-1)$ and $B(p)$ follows consistency order p, i.e. $||u_{m+1} - y(t_{m+1})|| = \mathcal{O}(h^{p+1})$, and convergence order p, as stated in the following theorem.

Theorem 1 (Convergence for EPTRK methods). *An EPTRK method with order p and stage order q, i.e. with $B(p)$ and $C(q)$, converges with order $p^* := min(p, q+1)$ if the local errors of starting values U_1 and u_1 for the first EPTRK step are of order p^*.*

Proof. The theorem can be proved by standard techniques. We use $C(q)$ and $B(p)$ to get a recursion for the global error. Using this recursion we can bound the global error. For details see [7]. □

3 Stability of EPTRK Methods

We investigate the stability of the EPTRK methods by means of the linear test equation

$$y' = \lambda y, \quad \mathrm{Re}\lambda \le 0 \tag{4}$$

and constant step size h. The EPTRK solution of (4) fulfills the recursion

$$(U_{m+1}, u_{m+1})^T = M(z)(U_m, u_m)^T, \quad z = h\lambda \ , \tag{5}$$

with the amplification matrix

$$M(z) = \begin{pmatrix} zA & \mathbb{1} \\ z^2 b^T A & 1+z \end{pmatrix} \ . \tag{6}$$

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 $(U_m, u_m) \to 0$ for $m \to \infty$. We compute $\varrho(M(z))$ by computing the zeros of the stability polynomial $\varrho(x, z) := \det(xI - M(z))$. From (6), it can be seen that EPTRK methods are always zero-stable. In $z = 0$ the matrix $M(z)$ has the single eigenvalue $x = 1$ and the s-fold eigenvalue zero. Furthermore, by calculating the derivative by the implicit function theorem, we can see that the absolute value of the maximal eigenvalue x is less than 1 in a whole region locally left to the origin and hence an EPTRK method is stable there. To construct methods with large stability regions we calculate the coefficients of the stability polynomial in the following theorem.

Theorem 2. *A consistent s stage EPTRK method has the stability polynomial*

$$\varrho(x, z) = \sum_{k=0}^{s} x^{s-k} \left[(p_k - \sum_{i=0}^{k-1} p_{k-i-1} b^T A^i \mathbb{1}) x - p_k \right] z^k \tag{7}$$

with parameters p_k defined by

$$\det(\lambda I - A) = \sum_{i=0}^{s} p_i \lambda^{s-i}, \quad p_0 = 1 \ . \tag{8}$$

Proof. Starting with the definition

$$\varrho(x, z) = \det(xI - M(z)) = \det \begin{pmatrix} xI - zA & -\mathbb{1} \\ -z^2 b^T A & x - 1 - z \end{pmatrix}$$

we get

$$\begin{aligned} \varrho(x, z) &= \det \left\{ \begin{pmatrix} xI - zA & -\mathbb{1} \\ -z^2 b^T A & x - 1 - z \end{pmatrix} \begin{pmatrix} (xI - zA)^{-1} & (xI - zA)^{-1} \mathbb{1} \\ 0 & 1 \end{pmatrix} \right\} \\ &\quad \times \frac{1}{\det(xI - zA)^{-1}} \\ &= \left[x - 1 - z - z^2 b^T A (xI - zA)^{-1} \mathbb{1} \right] \det(xI - zA) \ . \end{aligned}$$

Using (8) and a Neumann series for the inverse matrix yields

$$\varrho(x,z) = \sum_{i=0}^{s} p_i z^i x^{s-1} \left[(x-1-z) - z^2 b^T A \sum_{i=0}^{\infty} z^i \left(\frac{1}{x}\right)^{i+1} A^i 1\!\!1 \right] . \tag{9}$$

The polynomial $\varrho(x,z)$ has degree s in z and degree $s+1$ in x and therefore almost all terms in (9) vanish. This proves the theorem. □

Since for many applications with (nearly) real eigenvalues only stability is crucial along the real axis we optimize the boundary $r_{\max}$ of the real stability interval defined as $r_{\max} = \sup\{x : (-x,0) \subset S^*\}$. We determine analytically optimal values $r_{\max}$ for one-stage EPTRK methods and for two-stage EPTRK methods of order $p=2$ in Theorem 3. For EPTRK methods with more than 2 stages we have found stability polynomials with large values $r_{\max}$ by a numerical search.

Theorem 3. *The optimal value for r_{max} of a consistent s-stage EPTRK method of order p is given by*

(i) $r_{max} = 4$, *if* $s = p = 1$, *and*
(ii) $r_{max} = 2$, *if* $s = p = 2$.

Proof. We prove only (ii). The result (i) can be obtained similarly. According to Theorem 2, we have

$$\varrho(x,z) = x^3 + (-1 + p_1 z - z)x^2 + (-p_1 z + p_2 z^2 - p_1 z^2 - b^T A 1\!\!1 z^2)x - p_2 z^2.$$

Order $p = 2$ implies $b^T A 1\!\!1 = b^T c = 1/2$. Assume $r_{\max} \geq 2$. Then all zeros w_1, w_2 and w_3 of

$$\varrho(x,-2) = x^3 + (-2p_1 + 1)x^2 + (4p_2 - 2 - 2p_1)x - 4p_2 \tag{10}$$

lie in the unit circle. Define

$$\begin{aligned} g &= w_1 + w_2 + w_3 + w_1 w_2 + w_1 w_3 + w_2 w_3 - w_1 w_2 w_3 \\ &= w_1 + (1 + w_1)[w_2 + w_3] + (1 - w_1) w_2 w_3 \end{aligned}$$

By Vieta's Theorem and (10) we have $g = -3$. Let w_1 be a real zero. Assume $|w_1| < 1$. Then we get

$$g > w_1 + (1 + w_1)(-2) + (1 - w_1)(-1) = -3 \ ,$$

in contradiction to $g = -3$. Therefore, $|w_1| = 1$. A simple calculation shows now that $\varrho(x,-2)$ has the zeros $-1, -1$ and 1. A study of the unique polynomial with these zeros shows $r_{\max} = 2$. □

By using Theorem 2 we can determine stability polynomials of EPTRK methods with more than 2 stages and large stability regions. In Sect. 4 we will construct appropriate methods corresponding to these polynomials. The properties for these EPTRK methods are given in Tab. 1. Here, *emb. order* denotes the order of an embedded method used for step size selection and *#procs* the number of processors for parallelization. Note, that the parameters $b^T A^i \mathbb{1}$, $i = 0, \dots, p-1$ are already determined by $C(p-1)$ and $B(p)$, but we can choose p_k, $k = 1, \dots, s$ and $b^T A^i \mathbb{1}$, $i = p \dots, s$ arbitrarily to optimize the stability regions. Figure 1 shows these stability regions. For comparison we have also drawn the stability region of the 5-stage 5-order collocation EPTRK method `cong5` [2] and the stability region S^*_{dopri} of the well known explicit Runge-Kutta method `dopri5` [4] and the smaller scaled stability region $S^{\text{scal}}_{\text{dopri}} := \{z/6 : z \in S^*_{\text{dopri}}\}$ which takes into account the six effective sequential functions evaluations per step. Numerical experiments [2] show that `cong5` performs well for non-stiff problems. But for mildly stiff problems `dopri5` is superior due to better stability properties. The new methods `p33, p43` and `p44` of this paper have a larger stability region than `dopri5` (scaled). Therefore we can expect that these methods are more efficient than `dopri5` if stability is important and the function evaluations are not too cheap.

Table 1. EPTRK methods

name	stages	conditions	order	emb. order	#proc
`p33`	3	$C(2)$, $B(3)$	3	2	3
`p43`	4	$C(3)$, $B(3)$	3	4	4
`p44`	4	$C(4)$, $B(4)$	4	3	4
`cong5`	5	$C(5)$, $C(5)$	5	3	5

4 Constructing the Methods from the Polynomials

The 5-stage 5-order method `cong5` [2] fulfills $C(5)$. Here, for constructing the s-stage EPTRK methods `p33`, `p43` and `p44` with better stability properties, we require $C(s-1)$ only. First consider fixed step sizes. We start by choosing vector c of distinct nodes and a stability polynomial calculated in Sect. 3. We have $C(s-1)$ and the polynomial, i.e.

$$AV = P, \qquad V_{ij} = (c_i - 1)^{j-1}, \quad P_{ij} = c_i^j / i, \quad P, V \in \mathbb{R}^{s \times s-1}, \qquad \text{(11a)}$$

$$\det(\lambda I - A) = \sum_{i=0}^{s} p_i \lambda^{s-i}, \quad p_0 = 1 \qquad \text{(11b)}$$

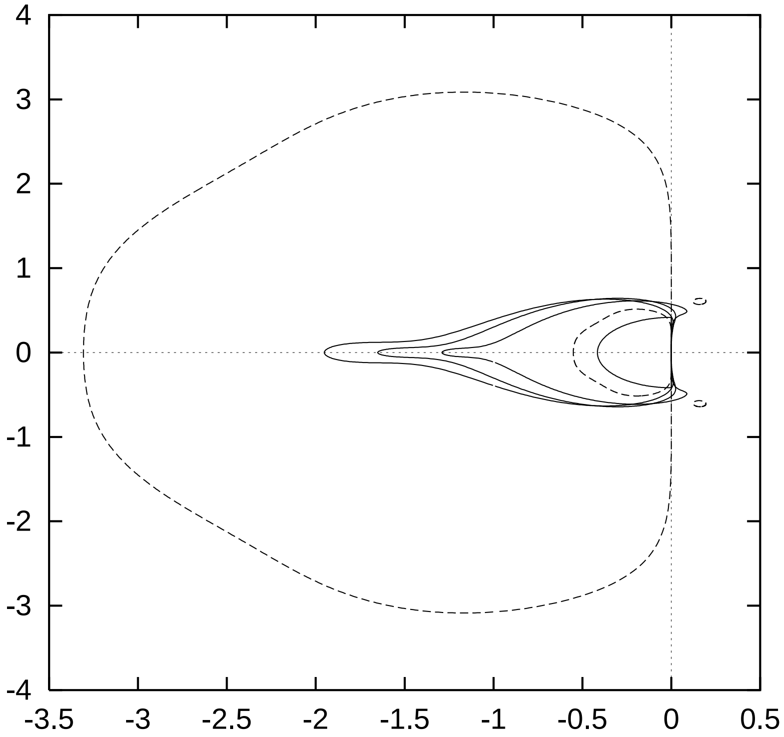

Fig. 1. Stability regions for the EPTRK methods drawn with solid lines and for `dopri5` with dashed lines. Regions from biggest to smallest: `dopri5, p43, p33, p44,` $\texttt{dopri5}^{\mathrm{scal}}$`, cong5`

holds. We calculate A from (11): the solution of (11a) has s free parameters which can be determined by substituting this solution into (11b). Now, A is known and we get the weights b directly from the polynomial coefficients $b^T A^i \mathbb{1}$, $i = 0, \ldots, s-1$.

For variable step sizes $C(s-1)$ becomes

$$A(\alpha)V = PD(\alpha), \quad \text{with} \quad D(\alpha) = \mathrm{diag}(1, \alpha, \ldots, \alpha^{s-2}), \tag{12}$$

and with (11a) we have

$$(A(\alpha) - A)V = P(D(\alpha) - I) \ . \tag{13}$$

We calculate a row minimal 2-norm solution $A(\alpha) - A$ of this underdetermined system (13) in order to preserve the stability properties for $A(1) = A$.

5 Numerical Experiments

Implementation

We have implemented the EPTRK methods in FORTRAN 77. The code for the collocation method `cong5` is available at URL `http://www.mathematik.uni-halle.de/institute/numerik/software` .

The numerical tests below were performed on a shared memory HP/Convex-Exemplar X-Class computer. Parallelism is expressed by means of the compiler-directives for loop-parallelization. For step size selection we computed an approximation of the local error

$$err = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{u_{m+1,i}-\tilde{u}_{m+1,i}}{\mathrm{ATOL}+\mathrm{RTOL}|u_{m+1,i}|}\right)^2},$$

and the new step size

$$h_{m+1} = \begin{cases} h_m & \text{for} \quad \alpha \in [0.9, 1.1] \\ \alpha h_m & \text{else} \end{cases}, \quad \text{with}$$
$$\alpha = \min\left\{3, \max\left\{0.3, 0.8\cdot \mathrm{err}^{-1/p^*}\right\}\right\}.$$

We compare the computing time in seconds with the error *ERR* in the endpoint of the integration interval,

$$ERR = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{u_i - u_{\mathrm{ref},i}}{1+|u_{\mathrm{ref},i}|}\right)^2} \ .$$

The reference solutions u_{ref} were obtained by `dop853` with ATOL=RTOL=10^{-14}. The version of `dopri5` was 03/14/93.

Test problems

As a first test example we take the seven body problem **Plei** in two spatial dimensions from Hairer et al. [4]. This problem models the gravity forces between seven stars leading to a second order ODE system of dimension 14, respectively a first order $y' = f(y)$ system with 28 equations. To illustrate how the speedup depends on the dimension of the problem we enlarge this system by a factor d and we get

$$Y' = F(Y), \quad Y(0) = Y_0, \quad \text{with} \tag{14}$$
$$Y = (\mathbb{1}\otimes y), \quad F(Y) = (\mathbb{1}\otimes f(y)), \quad Y_0 = \mathbb{1}\otimes y_0, \quad \text{and} \quad \mathbb{1}\in\mathbb{R}^d \ . \tag{15}$$

We discuss the speedup for different values $d = 1,\ldots,1000$.

A well known test problem is the **Brusselator**, see [5] and [6], a two-dimensional diffusion-reaction equation

$$\begin{aligned} u_t =& B + u^2 v - (A+1)u + \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \quad , \\ v_t =& A - u^2 v + \alpha \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \end{aligned}$$

with $A = 3$, $B = 1$ and initial values

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

and Neumann boundary conditions

$$\frac{\partial u}{\partial n} = 0 \ , \quad \frac{\partial v}{\partial n} = 0 \quad \text{auf} \quad \partial \Omega, \quad \Omega = [0,1] \times [0,1], \quad t \in [0,1] \ .$$

Semidiscretization by the method of lines with second order central differences in x and y on a 100×100 uniform grid leads to a first order system of 20000 ordinary differential equations. For small values α this system is non-stiff. We consider $\alpha = 2 \cdot 10^{-4}$ and $\alpha = 5 \cdot 10^{-3}$.

The second test problem is the two dimensional diffusion-convection equation **Difkon** from [8]:

$$\begin{aligned} &u_t = \alpha \Delta u + \beta(-y u_x + x u_y) + g(t, x, y), \quad \text{with} \\ &\alpha = 10^{-3}, \quad \beta = 1, \quad \Omega = [0,1]^2, \quad t \in [0,1] \ , \end{aligned}$$

with function g and initial values and Dirichlet boundary conditions chosen according to the exact solution $u(t, x, y) = \sin(\pi x) \sin(\pi y) \left(1 + 4xy \exp(-2\alpha\pi^2 t)\right)$. We use second order differencing on a 69×69 grid to get a semidiscrete system of ODEs. Due to the convection term the Jacobian of this system is unsymmetric and has non-real eigenvalues. We obtain a variation of this problem with even larger imaginary parts if we set $\beta = 10$.

Results and Discussion

Figure 2 shows the speedups for the s-stage EPTRK methods on s processors over the same method on one processor. Although the function evaluations are not very expensive we get speedups between 3 and 4 with five processors (`cong5`). Of course, increasing the dimension of an ODE systems yields better speedups as demonstrated with example Plei. Figure 2 depends strongly on the parallel computer.

For the celestial mechanic example Plei (see Fig. 3) the the collocation EPTRK method `cong5` in sequential mode and `dopri5` show nearly the same efficiency. Thus

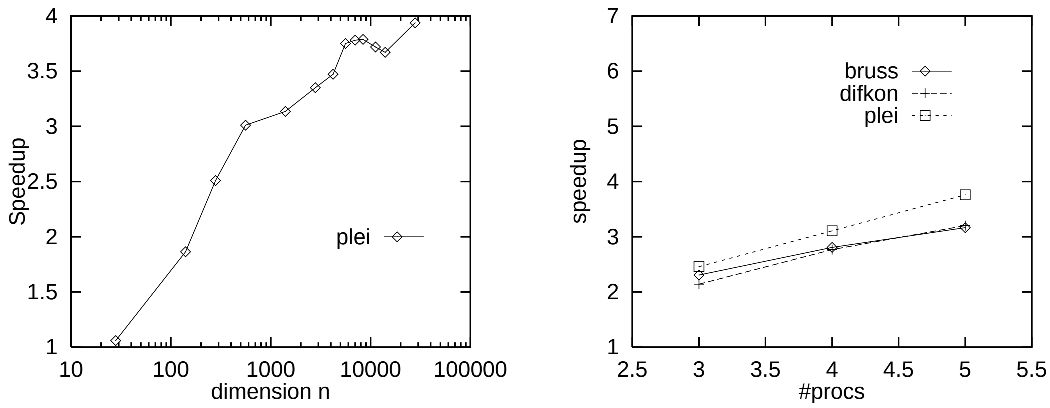

Fig. 2. The speedup for `cong5` for different dimensions of the ODE system Plei (left figure) and for EPTRK methods with $s = \#\text{procs}$

we get a speedup of about 4 of `cong5` over `dopri5` with 5 processors. For low tolerances the parallel `p44` is also competitive with `dopri5`. For the non-stiff Brusselator (see Fig. 4, left), for crude tolerances `p33` and for more stringent tolerances `cong5` are most efficient. For the mildly stiff Brusselator with increased α (right figure) the stability enlarged EPTRK methods `p33` and `p43` become the most efficient ones, except for very high accuracy. Consider problem Difkon (see Fig. 5) with $\beta = 1$ (left). The best method for low tolerances is `p33` and for high tolerances `dopri5`. If we set $\beta = 10$ (right figure) the imaginary parts of the eigenvalues of the Jacobian become larger and the stability of the method near the imaginary axis becomes crucial. Accordingly `p44` and `p33` perform well.

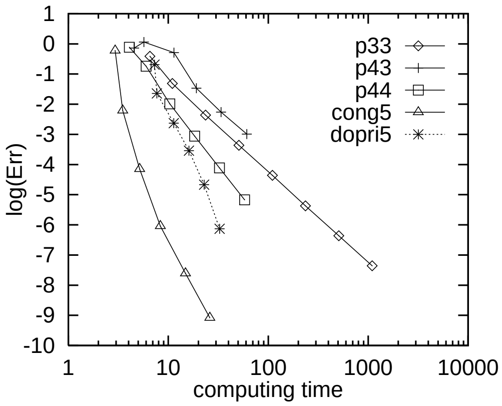

Fig. 3. Test problem Plei with dimension $n = 7000$

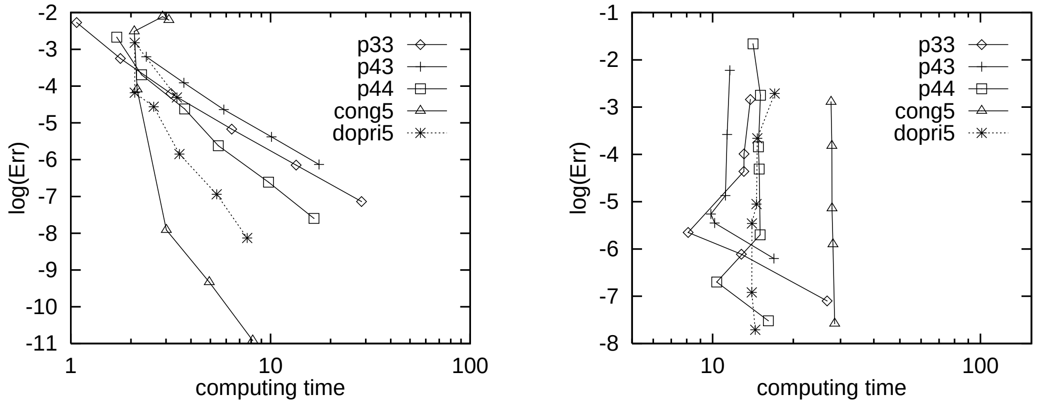

Fig. 4. Test problem Brusselator, left $\alpha = 4 \cdot 10^{-4}$, right $\alpha = 5 \cdot 10^{-3}$

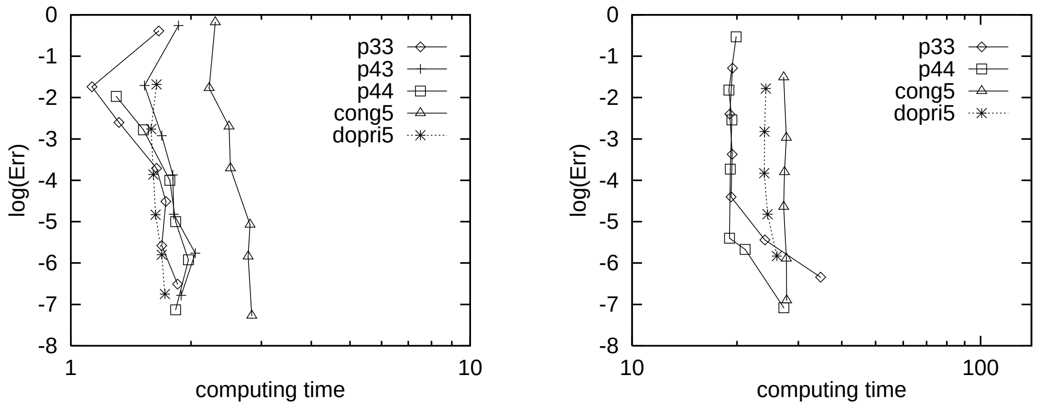

Fig. 5. Test problem Difkon, left $\beta = 1$, right $\beta = 10$

6 Conclusions

The class of explicit two-step Runge-Kutta (EPTRK) methods is an interesting subject for solving ODE systems of large dimension and/or with expensive f-evaluations in a parallel environment. For problems where accuracy is more important than stability the high order collocation method `cong5` [2] performs better than the sequential Runge-Kutta method `dopri5`. On the other hand, for mildly stiff problems and not too stringent tolerances, where stability is important, EPTRK methods `p33, p43` and `p43` with stability regions are a good choice.

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