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Functional continuous Runge–Kutta–Nyström methods

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Abstract. Numerical methods for solving retarded functional differential equations of the second order with right-hand side independent of the function derivative are considered. The approach used by E. Nyström for second-order ordinary differential equations with the mentioned property is applied for construction of effective functional continuous methods. Order conditions are formulated, and example methods are constructed. They have fewer stages than Runge–Kutta type methods of the same order. Application of the constructed methods to test problems confirms their declared orders of convergence.

Keywords: delay differential equations, second order equations, Runge–Kutta methods, functional continuous methods.

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1 Introduction

The so-called *standard approach* to solving delay-differential equations (DDEs) is based on the application of continuous extensions of known numerical methods for initial value problems (IVP) in ordinary differential equations (ODEs) [2]. The idea is to construct a method that approximates the IVP solution not only in mesh points but in an arbitrary time point. Continuous extensions for Runge–Kutta methods were developed long ago. Such methods are called Continuous Runge–Kutta methods (CRKs). The same idea was also introduced for Runge–Kutta–Nyström methods for second-order DDEs of special structure about twenty years ago [8,11].

Explicit CRKs can only be applied when delays are greater or equal than the step-size being made. However that cannot be the case for DDEs with vanishing delays, integral-differential or other functional equations with distributed delays. In such problems at least for some steps the situation of *overlapping* occurs, when the demanded delayed values of the solution are yet to be found during the current step, and explicit methods become fully implicit. The most general of such delay problems are retarded functional differential equations (RFDEs), which we consider in this paper.

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Special Runge–Kutta methods for direct application to RFDEs were first developed in the 1970's by Tavernini [13]. But it is only in recent years that these methods have been expanded to a general class of methods called "functional continuous Runge–Kutta methods" for RFDEs [9]. Functional continuous Runge–Kutta methods (FCRKs) among other methods for RFDEs are reviewed in [1], where order conditions and examples of methods are presented.

We introduce the following notations after [9] and [1].

- Let $r \in [0, \infty]$ and $\mathcal{C}$ be the space of continuous functions $[-r, 0] \to \mathbb{R}^d$ equipped with the maximum norm
$$\|\varphi\| = \max_{\theta \in [-r,0]} |\varphi(\theta)|, \qquad \varphi \in \mathcal{C},$$
where $|\cdot|$ is an arbitrary norm on $\mathbb{R}^d$.
- The analogous space of continuously differentiable functions is denoted $\mathcal{C}^1$.
- For a continuous function $u : [a - r, b) \to \mathbb{R}^d$ and $t \in [a, b)$, where $a < b$, let u_t be the function given by
$$u_t(\theta) = u(t + \theta), \qquad \theta \in [-r, 0].$$

In this paper we consider a second order RFDE with right-hand side independent of the derivative of the unknown function
$$\ddot{u}(t) = f(t, u_t), \tag{1.1}$$
where $u_t \in \mathcal{C}^1$, $f : \Omega \to \mathbb{R}^d$ and Ω is an open subset of $\mathbb{R} \times \mathcal{C}^1$.

Such equations describe retarded frictionless motions or damped oscillations, e.g. mechanical or electromagnetic [10], some PDE problems like viscoelasticity with a finite-difference space discretisation, relativistic dynamics, space satellites communication delays etc. [6]

In [10], which is devoted to second order delay equations, existence and uniqueness of solutions for (1.1) through any $(\sigma, \varphi) \in \Omega$ is only shown for linear equations. So we consider the equation (1.1) as a system
$$\begin{cases} \dot{u}(t) = v(t), \\ \dot{v}(t) = f(t, u_t), \end{cases} \tag{1.2}$$
and rewrite the existence and uniqueness conditions for first order equations [5]. It is considered that the function f is continuous and has derivative $f' : \Omega \to \mathcal{L}(\mathcal{C}^1, \mathbb{R}^d)$ with respect to the second argument which is bounded and continuous with respect to the second argument. Thus, for each $(\sigma, \varphi) \in \Omega$ there exists a unique (non-continuable) solution $u = u(\sigma, \varphi) : [\sigma - r, \bar{t}) \to \mathbb{R}^d$ of (1.1) through (σ, φ), where $\bar{t} = \bar{t}(\sigma, \varphi) \in (\sigma, +\infty]$, i.e. u satisfies (1.1) for $t \in [\sigma, \bar{t})$ and $u_\sigma = \varphi$.

In fact, FCRKs can be applied now to solve system (1.2) and thus equation (1.1). However, in case of ODEs, if the right-hand side does not depend on the first derivative, E. Nyström suggested methods that are much more efficient than general Runge–Kutta (RKs) methods applied to the first-order system (see e.g. [4]). The comparison of the number of stages required to provide order p: s stages for RKs and r stages for Runge–Kutta–Nyström methods (RKNs)

p	1	2	3	4	5
s	1	2	3	4	6
r	1	1	2	3	4

suggests trying to construct functional continuous methods for (1.1) analogous to RKNs, which can have the same advantage over FCRKs.

In the next section we recall the necessary information on FCRKs and give the definitions of discrete and uniform convergence orders. After that the general computation scheme of functional continuous Runge–Kutta–Nyström methods (FCRKNs) is given. Then we define local orders, connect them to the convergence orders and write down order conditions. Several example methods up to order 5 are presented after that. Finally numerical tests confirming the convergence order are presented.

2 Functional continuous Runge–Kutta methods

Before introducing FCRKN methods in the next section we first recall some basic definitions and properties of FCRKs for the first order system

$$\dot{u}(t) = f(t, u_t). \tag{2.1}$$

Here all the assumptions made for (1.1) are used with just $\mathcal{C}$ instead of $\mathcal{C}^1$ demanded.

Definition 2.1. Let s be a positive integer. An explicit s-stage functional continuous Runge–Kutta method (FCRK) is a triple ($A(\theta)$, $b(\theta)$, c) where

- $A(\theta)$ is an $\mathbb{R}^{s\times s}$-valued polynomial function such that $A(0) = 0$,
- $b(\theta)$ is an $\mathbb{R}^s$-valued polynomial function such that $b(0) = 0$,
- $c \in \mathbb{R}^s$ with $c_i \geq 0$, $i = 1, \ldots, s$.

For the problem (2.1) we look for the solution through (σ, φ). Consider n steps up to t_n ($t_0 = \sigma$, $t_{m+1} = t_m + h_m$, $m = \overline{0, n}$) to be made already. The FCRK method ($A(\theta)$, $b(\theta)$, c) provides the approximation $\eta^n(\theta h_n)$ to the solution $u(t_n + \theta h_n)$ for $\theta \in [0, 1]$

$$\eta^n(\theta h_n) = u^n + h_n \sum_{i=1}^{s} b_i(\theta) K^{n,i}, \quad \theta \in [0,1], \quad u^0 = \varphi(0), \quad u^n = \eta^{n-1}(h_{n-1}), \tag{2.2}$$

where

$$K^{n,i} = f\left(t_n + c_i h_n, Y^{n,i}_{c_i h_n}\right), \qquad i = 1, \ldots, s$$

and $Y^{n,i} : [-\tau, c_i h_n] \to \mathbb{R}^d$ is a stage function given by

$$\begin{aligned} Y^{n,i}(\theta h_n) &= u^n + h_n \sum_{j=1}^{i-1} a_{ij}(\theta) K^{n,j}, && \theta \in [0, c_i], \\ Y^{n,i}(t) &= \eta(t_n + t), && t \in [-\tau, 0], \end{aligned}$$

with $\eta(t)$ being the numerical approximation over all steps

$$\eta(t) = \begin{cases} \eta^m(\theta h_m), & t \in (t_m, t_{m+1}], \quad \theta = \frac{t - t_m}{h_m}, \quad \forall m = 0, 1, \ldots, \\ \varphi(t), & t \leq \sigma. \end{cases}$$

The conditions $A(0) = 0$ and $b(0) = 0$ guarantee $Y^{n,i}_{c_i h} \in \mathcal{C}$ ($i = 1, \ldots, s$) and $\eta^n_h \in \mathcal{C}$ respectively.

Assume that the problem (2.1) is solved in the interval $[\sigma, \sigma + T]$ and N steps are done, so in the mesh points $\sigma = t_0 < t_1 < \cdots < t_N = \sigma + T$ values $\varphi(0) = u^0$, u^1, $\ldots$, u^N are computed and the overall approximation $\eta(t)$ is constructed.

Definition 2.2. A method (2.2) is said to have *discrete* convergence order p if for any solved problem its global discrete error

$$E_d = \max_{0\le m\le N} |u(t_m) - u^m| = O(h^p) \tag{2.3}$$

for sufficiently small h, where $h = \max h_m$, $m = \overline{0, N-1}$.

A method is said to have *uniform* convergence order q if for any solved problem its global uniform error

$$E_u = \max_{t_0\le t\le t_N} |u(t) - \eta(t)| = O(h^q) \tag{2.4}$$

for sufficiently small h.

3 Functional continuous Runge–Kutta–Nyström methods

Now we formulate a functional continuous method for direct application to (1.1).

Definition 3.1. Let s be a positive integer. An explicit s-stage functional continuous Runge–Kutta–Nyström method (FCRKN) is a quadruple ($\bar{A}(\theta)$, $b(\theta)$, $\bar{b}(\theta)$, c) where

- $\bar{A}(\theta)$ is a $\mathbb{R}^{s\times s}$-valued polynomial function such that $\bar{A}(0) = 0$,
- $b(\theta)$ and $\bar{b}(\theta)$ are $\mathbb{R}^s$-valued polynomial functions such that $b(0) = \bar{b}(0) = 0$,
- $c \in \mathbb{R}^s$ with $c_i \ge 0$, $i = 1, \dots, s$.

For the problem (1.1) we look for the solution through (σ, φ). Consider n steps up to t_n ($t_0 = \sigma$, $t_{m+1} = t_m + h_m$, $m = \overline{0, n}$) to be made already. The FCRKN method ($\bar{A}(\theta)$, $b(\theta)$, $\bar{b}(\theta)$, c) provides the approximation $\eta^n(\theta h_n)$ to the solution $u(t_n + \theta h_n)$ and the approximation $\hat{\eta}^n(\theta h_n)$ to its derivative $\dot{u}(t_n + \theta h_n)$ for $\theta \in [0, 1]$

$$\begin{aligned} \eta(\theta h_n) &= u^n + \theta h_n \dot{u}^n + h_n^2 \sum_{i=1}^{s} \bar{b}_i(\theta) K^{n,i}, \quad \theta \in [0,1], \quad u^0 = \varphi(0), \quad u^n = \eta^{n-1}(h_{n-1}),\\ \hat{\eta}(\theta h_n) &= \dot{u}^n + h_n \sum_{i=1}^{s} b_i(\theta) K^{n,i}, \qquad \theta \in [0,1], \quad \dot{u}^0 = \dot{\varphi}(0), \quad \dot{u}^n = \hat{\eta}^{n-1}(h_{n-1}), \end{aligned} \tag{3.1}$$

where

$$K^{n,i} = f\left(t_n + c_i h_n, Y^{n,i}_{c_i h_n}\right), \qquad i = 1, \dots, s \tag{3.2}$$

and $Y^{n,i} : [-\tau, c_i h_n] \to \mathbb{R}^d$ is a stage function given by

$$\begin{aligned} Y^{n,i}(\theta h_n) &= u^n + \theta h_n \dot{u}^n + h_n^2 \sum_{j=1}^{i-1} \bar{a}_{ij}(\theta) K^{n,j}, \qquad \theta \in [0, c_i],\\ Y^{n,i}(t) &= \eta(t_n + t), \qquad t \in [-\tau, 0], \end{aligned} \tag{3.3}$$

with $\eta(t)$ being the numerical approximation over all steps

$$\eta(t) = \begin{cases} \eta^m(\theta h_m), & t \in (t_m, t_{m+1}], \quad \theta = \dfrac{t - t_m}{h_m}, \quad \forall m = 0, 1, \dots,\\ \varphi(t), & t \le \sigma. \end{cases} \tag{3.4}$$

The corresponding approximation to $\dot{u}(t)$ is

$$\hat{\eta}(t) = \begin{cases} \hat{\eta}^m(\theta h_m), & t \in (t_m, t_{m+1}], \quad \theta = \dfrac{t - t_m}{h_m}, \quad \forall m = 0, 1, \ldots, \\ \dot{\varphi}(t), & t \le \sigma. \end{cases} \tag{3.5}$$

The conditions $\bar{A}(0) = 0$, $b(0) = 0$ and $\bar{b}(0) = 0$ guarantee $Y^{n,i}_{c_i h} \in \mathcal{C}$ $(i = 1, \ldots, s)$, $\hat{\eta}^n_h \in \mathcal{C}$ and $\eta^n_h \in \mathcal{C}^1$ respectively.

In addition to (2.3) and (2.4) we measure global discrete

$$\hat{E}_d = \max_{0 \le m \le N} |\dot{u}(t_m) - \dot{u}^m| \tag{3.6}$$

and global uniform

$$\hat{E}_u = \max_{t_0 \le t \le t_N} |\dot{u}(t) - \hat{\eta}(t)| \tag{3.7}$$

errors of the derivative approximation.

Definition 3.2. An FCRKN method (3.1) is said to have *discrete* convergence order p if for any problem being solved both

$$E_d = O(h^p) \quad \text{and} \quad \hat{E}_d = O(h^p),$$

where $h = \max h_m$, $m = \overline{0, N-1}$.

An FCRKN method is said to have *uniform* convergence order q if for any solved problem both

$$E_u = O(h^q) \quad \text{and} \quad \hat{E}_u = O(h^q).$$

4 Order conditions for FCRKNs

In this section first we compare the order conditions of Runge–Kutta methods and FCRKs; and then on the basis of Runge–Kutta–Nyström methods order conditions we present order conditions for FCRKN methods (3.1).

The conception of the method's order is defined from consideration of *local* error, i.e. the error after one step of the method. In [9] the local error is defined (for the first step h_0 from $t_0 = \sigma$) as

$$e(t) = \int_\sigma^t \left(\eta^0(\tau - \sigma) - u(\tau)\right) d\tau, \qquad t \in [\sigma, \sigma + h_0]. \tag{4.1}$$

We add

$$\hat{e}(t) = \int_\sigma^t \left(\hat{\eta}^0(\tau - \sigma) - \dot{u}(\tau)\right) d\tau, \qquad t \in [\sigma, \sigma + h_0] \tag{4.2}$$

for the problem (1.1).

At the second step the local error is measured in respect of the solution of (1.1) that goes through (t_1, φ^1), where $\varphi^1(t) = \varphi(t)$ if $t \le \sigma$ and $\varphi^1(t) = \eta^0(t - \sigma)$ if $t \in (\sigma, \sigma + h_0]$. Notice, that $\hat{\eta}^1$ isn't used for the second step computations.

The presence of deviated argument in RFDEs can cause the appearance of jump discontinuities in $\dot{u}$ or higher derivatives of u in the initial or consequent points, even if the "history" function φ is smooth. But it is known that numerical methods achieve their order of accuracy at a step if the solution is sufficiently smooth within. This means that for a successful application of a method of order p it is important to include the jump discontinuity points of $u^{(s)}$

into the mesh at least for $s = 0, 1, \dots, p-1$ [2]. One of the approaches to find them during the computation cheaply and preserving the explicitness of the methods was suggested in [3]. It can be easily applied for FCRKNs, so we won't discuss it in the present paper. In the following discussion we consider the problem to be smooth enough over each step.

Definition 4.1. It is said, that a FCRKN method (3.1) is of *discrete* (local) order p if for any solved problem with sufficiently small h

$$|e(\sigma + h_0)| = O\left(h_0^{p+1}\right) \quad \text{and} \quad |\hat{e}(\sigma + h_0)| = O\left(h_0^{p+1}\right)$$

and the interval $(\sigma, \sigma + h_0)$ does not contain discontinuity points of $u(t)$.

It is said, that a FCRKN method (3.1) is of *uniform* (local) order q if for any solved problem with sufficiently small h

$$\|e(t)\| = O\left(h_0^{q+1}\right) \quad \text{and} \quad \|\hat{e}(t)\| = O\left(h_0^{q+1}\right)$$

for any $t \in (\sigma, \sigma + h_0)$ and the interval $(\sigma, \sigma + h_0)$ does not contain discontinuity points of $u(t)$.

For ODEs it is easy to show that for smooth enough right-hand sides local order p provides the convergence order p as well. For FCRKs in [9] the theorem is proved that if a method has uniform local order q and discrete local order p then (under certain assumptions on the right-hand side smoothness etc.) its discrete convergence order is $\min\{q+1, p\}$. The similar result can also be stated for FCRKNs, but maybe under slightly different assumptions. We won't give a rigorous proof of such a statement. Anyway all FCRKs properties should preserve when applied to the system (1.2). And FCRKNs can be considered as obtained from some FCRKs (of lower order for general first order RFDEs) by rewriting and simplifying the coefficients when switching from the system (1.2) to the second order equation (1.1).

This effectively means, that it is possible to construct uniform order $p-1$ and discrete order p methods to have the discrete convergence order p. However, some analysis shows that reliable error estimation with means of Runge rule or with an embedded estimator is possible for methods with $q = p$ (see [2] for details). Thus in this paper we will consider methods with uniform order equal to the desired convergence order (which in this case becomes uniform).

Hence the way to construct a method with discrete (uniform) convergence order p is to provide its local discrete order to be p and its local uniform order to be $p-1$ (p as well).

The order conditions are equalities containing method's parameters $\bar{A}(\theta)$, $b(\theta)$, $\bar{b}(\theta)$ and c that provide the equality of Taylor series terms for the solution and it's approximation. We write them down up to order five.

Further it is considered that

- in (1.1) (or (2.1)) f is of class C^l with respect to the second argument for a sufficiently large l: we say that f is of class C^l with respect to the second argument, where l is a positive integer, if f has derivatives $f^{(k)} : \Omega \to \mathcal{L}^k(\mathcal{C}^1, \mathbb{R}^d)$, $k = 1, \dots, l$, with respect to the second argument which are bounded and continuous with respect to the second argument;

- solutions $x = x(\sigma, \varphi)$ of (1.1) (or (2.1)), $(\sigma, \varphi) \in \Omega$ are of piecewise class C^m for a sufficiently large m: we say that x is of piecewise class C^m if there exist $\xi_0, \xi_1, \dots, \xi_I$ called *discontinuity points*, where $t_0 = \xi_0 < \xi_1 < \cdots < \xi_I < t_N$, such that x has continuous derivatives $x^{(k)}$, $k = 1, \dots, m$, on the intervals $[\xi_i, \xi_{i+1}]$, $i = 0, \dots, I-1$, and $[\xi_I, t_N]$.

Also let $c_1^*, \dots, c_{s^*}^*$ such that $c_1^* < \dots < c_{s^*}^*$ and $c_1^*, \dots, c_{s^*}^* = c_1, \dots, c_s$, i.e. $c_1^*, \dots, c_{s^*}^*$ are the distinct c_i's in increasing order.

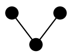
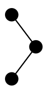
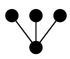
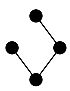
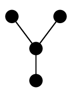
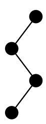
p	T	**Tree**	**RK condition**	**FCRK condition** $\theta \in [0,1]$, $\eta \in [0, c_m^*]$, $\zeta \in [0, c_l^*]$, $m, l = 1, \dots, s^*$
Basic simplifying condition			$\sum_{j=1}^{i-1} a_{ij} = c_i$, $i = 1, \dots, s$	$\sum_{j=1}^{i-1} a_{ij}(\theta) = \theta$ (only here $\theta \in [0, c_i]$), $i = 1, \dots, s$
1	T_1		$\sum_{i=1}^{s} b_i = 1$	$\sum_{i=1}^{s} b_i(\theta) = \theta$
2	T_2		$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}$	$\sum_{i=1}^{s} b_i(\theta) c_i = \frac{\theta^2}{2}$
3	T_{31}		$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}$	$\sum_{i=1}^{s} b_i(\theta) c_i^2 = \frac{\theta^3}{3}$
	T_{32}		$\sum_{\substack{i=\overline{1,s} \\ j=\overline{1,i-1}}} b_i a_{ij} c_j = \frac{1}{6}$	$\sum_{\substack{i=1 \\ c_i = c_m^*}}^{s} b_i(\theta) \left(\sum_{j=1}^{i-1} a_{ij}(\eta) c_j - \frac{\eta^2}{2} \right) = 0$
4	T_{41}		$\sum_{i=1}^{s} b_i c_i^3 = \frac{1}{4}$	$\sum_{i=1}^{s} b_i(\theta) c_i^3 = \frac{\theta^4}{4}$
	T_{42}		$\sum_{\substack{i=\overline{1,s} \\ j=\overline{1,i-1}}} b_i c_i a_{ij} c_j = \frac{1}{8}$	follows from the T_{32} condition
	T_{43}		$\sum_{\substack{i=\overline{1,s} \\ j=\overline{1,i-1}}} b_i a_{ij} c_j^2 = \frac{1}{12}$	$\sum_{\substack{i=1 \\ c_i = c_m^*}}^{s} b_i(\theta) \left(\sum_{j=1}^{i-1} a_{ij}(\eta) c_j^2 - \frac{\eta^3}{3} \right) = 0$
	T_{44}		$\sum_{\substack{i=\overline{1,s} \\ j=\overline{1,i-1} \\ k=\overline{1,j-1}}} b_i a_{ij} a_{jk} c_k = \frac{1}{24}$	$\sum_{\substack{i=1 \\ c_i = c_m^*}}^{s} b_i(\theta) \sum_{\substack{j=1 \\ c_j = c_l^*}}^{i-1} a_{ij}(\eta) \left(\sum_{k=1}^{j-1} a_{jk}(\zeta) c_k - \frac{\zeta^2}{2} \right) = 0$

Table 4.1: RKs and FCRKs order conditions

Deriving the order conditions from direct Taylor series comparison is quite difficult. For ODEs there exists a graphical interpretation of the Taylor series terms (so-called labelled trees theory [4]). Comparison of the FCRKs order conditions from [9] to order conditions of the RKs for ODEs suggests a way to correspond the same trees to FCRKs order conditions. See Table 4.1 for details. The "basic simplifying condition" is necessary to make the methods construction much easier.

The labelled trees theory is also developed for Runge–Kutta–Nyström methods [4] and

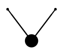
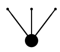
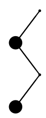
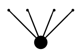
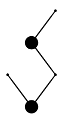
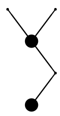
p	NT	**Tree**	**RKN conditions**	
			$\dot{u}$ approximation	u approximation (for the order $p+1$)
Basic simplifying condition			$\sum_{j=1}^{i-1} \bar{a}_{ij} = \frac{c_i^2}{2},\quad i = 1, \dots, s$	
1	NT_1		$\sum_{i=1}^{s} b_i = 1$	$\sum_{i=1}^{s} \bar{b}_i = \frac{1}{2}$
2	NT_2		$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}$	$\sum_{i=1}^{s} \bar{b}_i c_i = \frac{1}{6}$
3	NT_{31}		$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}$	$\sum_{i=1}^{s} \bar{b}_i c_i^2 = \frac{1}{12}$
4	NT_{41}		$\sum_{i=1}^{s} b_i c_i^3 = \frac{1}{4}$	$\sum_{i=1}^{s} \bar{b}_i c_i^3 = \frac{1}{20}$
	NT_{42}		$\sum_{\substack{i=\overline{1,s}\\ j=\overline{1,i-1}}} b_i \bar{a}_{ij} c_j = \frac{1}{24}$	$\sum_{\substack{i=\overline{1,s}\\ j=\overline{1,i-1}}} \bar{b}_i \bar{a}_{ij} c_j = \frac{1}{120}$
5	NT_{51}		$\sum_{i=1}^{s} b_i c_i^4 = \frac{1}{5}$	
	NT_{52}		$\sum_{\substack{i=\overline{1,s}\\ j=\overline{1,i-1}}} b_i c_i \bar{a}_{ij} c_j = \frac{1}{30}$	
	NT_{53}		$\sum_{\substack{i=\overline{1,s}\\ j=\overline{1,i-1}}} b_i \bar{a}_{ij} c_j^2 = \frac{1}{60}$	

Table 4.2: RKNs order conditions

in the Table 4.2 order conditions for them are presented. By analogy to the way the RK order conditions relate to the FCRK order conditions, we write down order conditions for FCRKNs based on the order conditions for RKNs. The FCRKN variant of the basic simplifying condition is

$$\sum_{j=1}^{i-1} \bar{a}_{ij}(\theta) = \frac{\theta^2}{2}, \quad \theta \in [0, c_i], \quad i = 2, \dots, s. \tag{4.3}$$

The meaning of the latter is that $Y^i(\theta h)$ is approximated with order two for any i except 1. At the first stage the approximation is based only on the information known from the previous step (or the history) and is thus of the uniform order of the method itself.

The corresponding NT-tree is given in brackets for every condition. Note, that each tree corresponds to two conditions: one including $b_i(\theta)$ summations and the other with $\bar{b}_i(\theta)$ sums. They have common inner $\bar{a}$ and c factors and different right-hand sides.

First order

A FCRKN is of uniform order one iff

$$\sum_{i=1}^{s} b_i(\theta) = \theta, \quad \theta \in [0,1]. \quad (NT_1) \tag{4.4}$$

Discrete order one is provided by the RKN condition for NT_1.

Second order

A FCRKN method of uniform order one of uniform order two iff

$$\sum_{i=1}^{s} \bar{b}_i(\theta) = \frac{\theta^2}{2}, \quad \theta \in [0,1], \quad (NT_1) \tag{4.5}$$

$$\sum_{i=1}^{s} b_i(\theta) c_i = \frac{\theta^2}{2}, \quad \theta \in [0,1], \quad (NT_2) \tag{4.6}$$

and of discrete order two iff corresponding RKN conditions are satisfied.

Third order

A FCRKN method satisfying (4.3) and of uniform order two is of uniform order three iff

$$\sum_{i=1}^{s} \bar{b}_i(\theta) c_i = \frac{\theta^3}{6}, \quad \theta \in [0,1], \quad (NT_2) \tag{4.7}$$

$$\sum_{i=1}^{s} b_i(\theta) c_i^2 = \frac{\theta^3}{3}, \quad \theta \in [0,1]. \quad (NT_3) \tag{4.8}$$

A FCRKN method satisfying (4.3) and (4.5) and of discrete order two is of discrete order three iff the corresponding RKN conditions are satisfied.

Fourth order

A FCRKN method satisfying (4.3) and of uniform order three is of uniform order four iff

$$\sum_{i=1}^{s} \bar{b}_i(\theta) c_i^2 = \frac{\theta^4}{12}, \quad \theta \in [0,1], \quad (NT_3) \tag{4.9}$$

$$\sum_{i=1}^{s} b_i(\theta) c_i^3 = \frac{\theta^4}{4}, \quad \theta \in [0,1], \quad (NT_{41}) \tag{4.10}$$

and

$$\sum_{\substack{i=1 \\ c_i = c_m^*}}^{s} b_i(\theta) \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j - \frac{\eta^3}{6} \right) = 0, \quad \theta \in [0,1], \quad \eta \in [0, c_m^*] \quad (NT_{42}) \tag{4.11}$$

for $m = 1, \dots, s^*$.

A FCRKN method satisfying (4.3), (4.5) and (4.7) and of discrete order three is of discrete order four iff

$$\begin{aligned} \sum_{i=1}^{s} \bar{b}_i c_i^2 &= \frac{1}{12}, \quad (NT_3) \\ \sum_{i=1}^{s} b_i c_i^3 &= \frac{1}{4}, \quad (NT_{41}) \\ \sum_{\substack{i=1\\c_i=c_m^*}}^{s} b_i \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j - \frac{\eta^3}{6} \right) &= 0, \quad \eta \in [0, c_m^*] \quad (NT_{42}) \end{aligned} \tag{4.12}$$

for $m = 1, \ldots, s^*$.

Fifth order

A FCRKN method satisfying (4.3) and of uniform order four is of uniform order five iff

$$\sum_{i=1}^{s} \bar{b}_i(\theta) c_i^3 = \frac{\theta^5}{20}, \quad \theta \in [0,1], \quad (NT_{41}) \tag{4.13}$$

$$\sum_{\substack{i=1\\c_i=c_m^*}}^{s} \bar{b}_i(\theta) \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j - \frac{\eta^3}{6} \right) = 0, \quad \theta \in [0,1], \quad \eta \in [0, c_m^*] \quad (NT_{42}) \tag{4.14}$$

for $m = 1, \ldots, s^*$,

$$\sum_{i=1}^{s} b_i(\theta) c_i^4 = \frac{\theta^5}{5}, \quad \theta \in [0,1], \quad (NT_{51}) \tag{4.15}$$

and

$$\sum_{\substack{i=1\\c_i=c_m^*}}^{s} b_i(\theta) \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j^2 - \frac{\eta^4}{12} \right) = 0, \quad \theta \in [0,1], \quad \eta \in [0, c_m^*] \quad (NT_{53}) \tag{4.16}$$

for $m = 1, \ldots, s^*$. Note that the NT_{52} condition is automatically satisfied by the NT_{42} condition in case of functional continuous methods (as it was for T_{42} for FCRKs).

A FCRKN method satisfying (4.3), (4.5), (4.7) and (4.9) and of discrete order four is of discrete order five iff

$$\begin{aligned} \sum_{i=1}^{s} \bar{b}_i c_i^3 &= \frac{1}{20}, \quad (NT_{41}) \\ \sum_{\substack{i=1\\c_i=c_m^*}}^{s} \bar{b}_i \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j - \frac{\eta^3}{6} \right) &= 0, \quad \eta \in [0, c_m^*] \quad (NT_{42}) \end{aligned}$$

for $m = 1, \ldots, s^*$,

$$\begin{aligned} \sum_{i=1}^{s} b_i c_i^4 &= \frac{1}{5}, \quad (NT_{51}) \\ \sum_{\substack{i=1\\c_i=c_m^*}}^{s} b_i \left(\sum_{j=1}^{i-1} \bar{a}_{ij}(\eta) c_j^2 - \frac{\eta^4}{12} \right) &= 0, \quad \eta \in [0, c_m^*] \quad (NT_{53}) \end{aligned}$$

for $m = 1, \ldots, s^*$.

5 FCRKN examples

We'll use the same approach of satisfying the order conditions as in [9], namely using in the final computations (3.1) only those stages, which themselves provide an approximation accurate enough.

In FCRKs (2.2) Y^i are computed with use of K_j values, which are multiplied by h. So the error of Y^i Taylor expansion starts from h^{r+1} term, where r is the lowest order of Y^j used in K_j. It means, that stages of order q can only be constructed with use of stages of order at least $q-1$ to provide their stage order. As a result, an FCRK of order p contains a method of order $p-1$ within.

The main difference is now that we multiply stage functions (3.2) by h^2 and thus stages of two orders lower than the desired can be used. So, to minimise the number of stages we separate methods with even order from those with odd order. Still for order p of η' we need stages of order $p-1$.

5.1 Odd order methods

For order 1 there is nothing to improve, since explicit Euler method with one stage satisfies all the definitions and in (3.3) the second option $Y^i(t) = \varphi(t)$ is always used due to the method's explicitness ($c_1 = 0$). Continuous extensions are provided by $b_1 = \theta$ and $\bar{b}_1 = \theta^2/2$.

An order 3 RKN method for ODEs can be constructed with 2 stages, but to get a uniform order 3 FCRKN we need at least 3 stages (just to provide the order 3 continuous extension). So a uniform order 3 method (FCRKN33) is

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{\theta^2}{2} & & \\ 1 & \frac{\theta^2}{2} & & \\ \hline \bar{b} & \frac{1}{6}\theta^4 - \frac{1}{2}\theta^3 + \frac{1}{2}\theta^2 & \frac{2}{3}\theta^3 - \frac{1}{3}\theta^4 & \frac{1}{6}\theta^4 - \frac{1}{6}\theta^3 \\ \hline b & \frac{2}{3}\theta^3 - \frac{3}{2}\theta^2 + \theta & 2\theta^2 - \frac{4}{3}\theta^3 & \frac{2}{3}\theta^3 - \frac{1}{2}\theta^2 \end{array} \tag{5.1}$$

However a discrete order 3 and uniform order 2 method can be constructed with only two stages

$$\begin{array}{c|cc} 0 & & \\ \frac{2}{3} & \frac{\theta^2}{2} & \\ \hline \bar{b} & \frac{1}{2}\theta^2 - \frac{1}{4}\theta^3 & \frac{1}{4}\theta^3 \\ \hline b & \theta - \frac{3}{4}\theta^2 & \frac{3}{4}\theta^2 \end{array} \tag{5.2}$$

An order 5 method (FCRKN57) is based on (5.1):

$$
\begin{array}{c|ccccccc}
0 & & & & & & & \\
\frac{1}{2} & \frac{\theta^2}{2} & & & & & & \\
1 & \frac{\theta^2}{2} & & & & & & \\
\frac{1}{4} & \frac{1}{6}\theta^4 - \frac{1}{2}\theta^3 + \frac{1}{2}\theta^2 & \frac{2}{3}\theta^3 - \frac{1}{3}\theta^4 & \frac{1}{6}\theta^4 - \frac{1}{6}\theta^3 & & & & \\
\frac{1}{2} & \frac{1}{6}\theta^4 - \frac{1}{2}\theta^3 + \frac{1}{2}\theta^2 & \frac{2}{3}\theta^3 - \frac{1}{3}\theta^4 & \frac{1}{6}\theta^4 - \frac{1}{6}\theta^3 & & & & \\
\frac{3}{4} & \frac{1}{6}\theta^4 - \frac{1}{2}\theta^3 + \frac{1}{2}\theta^2 & \frac{2}{3}\theta^3 - \frac{1}{3}\theta^4 & \frac{1}{6}\theta^4 - \frac{1}{6}\theta^3 & & & & \\
1 & \frac{1}{6}\theta^4 - \frac{1}{2}\theta^3 + \frac{1}{2}\theta^2 & \frac{2}{3}\theta^3 - \frac{1}{3}\theta^4 & \frac{1}{6}\theta^4 - \frac{1}{6}\theta^3 & & & & \\
\hline
\bar{b} & \bar{b}_1(\theta) & 0 & 0 & \bar{b}_4(\theta) & \bar{b}_5(\theta) & \bar{b}_6(\theta) & \bar{b}_7(\theta) \\
\hline
b & b_1(\theta) & 0 & 0 & b_4(\theta) & b_5(\theta) & b_6(\theta) & b_7(\theta)
\end{array}
\tag{5.3}
$$

where

$$
\begin{aligned}
\bar{b}_1(\theta) &= \frac{16}{45}\theta^6 - \frac{4}{3}\theta^5 + \frac{35}{18}\theta^4 - \frac{25}{18}\theta^3 + \frac{1}{2}\theta^2, & b_1(\theta) &= \frac{32}{15}\theta^5 - \frac{20}{3}\theta^4 + \frac{70}{9}\theta^3 - \frac{25}{6}\theta^2 + \theta, \\
\bar{b}_4(\theta) &= -\frac{64}{45}\theta^6 + \frac{24}{5}\theta^5 - \frac{52}{9}\theta^4 + \frac{8}{3}\theta^3, & b_4(\theta) &= -\frac{128}{15}\theta^5 + 24\theta^4 - \frac{208}{9}\theta^3 + 8\theta^2, \\
\bar{b}_5(\theta) &= \frac{32}{15}\theta^6 - \frac{32}{5}\theta^5 + \frac{19}{3}\theta^4 - 2\theta^3, & b_5(\theta) &= \frac{64}{5}\theta^5 - 32\theta^4 + \frac{76}{3}\theta^3 - 6\theta^2, \\
\bar{b}_6(\theta) &= -\frac{64}{45}\theta^6 + \frac{56}{15}\theta^5 - \frac{28}{9}\theta^4 + \frac{8}{9}\theta^3, & b_6(\theta) &= -\frac{128}{15}\theta^5 + \frac{56}{3}\theta^4 - \frac{112}{9}\theta^3 + \frac{8}{3}\theta^2, \\
\bar{b}_7(\theta) &= \frac{16}{45}\theta^6 - \frac{4}{5}\theta^5 + \frac{11}{18}\theta^4 - \frac{1}{6}\theta^3, & b_7(\theta) &= \frac{32}{15}\theta^5 - 4\theta^4 + \frac{22}{9}\theta^3 - \frac{1}{2}\theta^2.
\end{aligned}
$$

5.2 Even order methods

An order 2 method (FCRKN22) is

$$
\begin{array}{c|cc}
0 & & \\
1 & \frac{\theta^2}{2} & \\
\hline
\bar{b} & \frac{1}{2}\theta^2 - \frac{1}{6}\theta^3 & \frac{1}{6}\theta^3 \\
\hline
b & \theta - \frac{1}{2}\theta^2 & \frac{1}{2}\theta^2
\end{array}
\tag{5.4}
$$

An order 4 method (FCRKN45) is

$$
\begin{array}{c|ccccc}
0 & & & & & \\
1 & \frac{\theta^2}{2} & & & & \\
\frac{1}{3} & \frac{1}{2}\theta^2-\frac{1}{6}\theta^3 & \frac{1}{6}\theta^3 & & & \\
\frac{2}{3} & \frac{1}{2}\theta^2-\frac{1}{6}\theta^3 & \frac{1}{6}\theta^3 & & & \\
1 & \frac{1}{2}\theta^2-\frac{1}{6}\theta^3 & \frac{1}{6}\theta^3 & & & \\
\hline
\bar{b} & \bar{b}_1(\theta) & 0 & \bar{b}_3(\theta) & \bar{b}_4(\theta) & \bar{b}_5(\theta) \\
\hline
b & b_1(\theta) & 0 & b_3(\theta) & b_4(\theta) & b_5(\theta)
\end{array} \tag{5.5}
$$

where

$$
\begin{aligned}
\bar{b}_1(\theta) &= -\frac{9}{40}\theta^5+\frac{3}{4}\theta^4-\frac{11}{12}\theta^3+\frac{1}{2}\theta^2, & b_1(\theta) &= -\frac{9}{8}\theta^4+3\theta^3-\frac{11}{4}\theta^2+\theta,\\
\bar{b}_3(\theta) &= \frac{27}{40}\theta^5-\frac{15}{8}\theta^4+\frac{3}{2}\theta^3, & b_3(\theta) &= \frac{27}{8}\theta^4-\frac{15}{2}\theta^3+\frac{9}{2}\theta^2,\\
\bar{b}_4(\theta) &= -\frac{27}{40}\theta^5+\frac{3}{2}\theta^4-\frac{3}{4}\theta^3, & b_4(\theta) &= -\frac{27}{8}\theta^4+6\theta^3-\frac{9}{4}\theta^2,\\
\bar{b}_5(\theta) &= \frac{9}{40}\theta^5-\frac{3}{8}\theta^4+\frac{1}{6}\theta^3, & b_5(\theta) &= \frac{9}{8}\theta^4-\frac{3}{2}\theta^3-\frac{1}{2}\theta^2.
\end{aligned}
$$

For all the methods constructed, order conditions of the form (4.11), (4.14) and (4.16) are satisfied by assuring that each term in the outer sum vanishes by setting $b_i(\theta) \equiv 0$ or $\bar{b}_i(\theta) \equiv 0$ if the term in brackets does not vanish. For instance $b_2(\theta) \equiv 0$ for order 4 method (5.5) or $b_2(\theta) \equiv 0$ and $b_3(\theta) \equiv 0$ for order 5 method (5.3). The same approach was used in [9] for FCRKs. The calculation of stages sufficient for certain orders is made using this approach. Methods constructed differently, if they exist, possibly have fewer stages, but we are unaware of any such method.

Thanks to the special structure of the FCRKNs the total number of stages r sufficient to get uniform order p is thus much less than s of FCRKs

p	1	2	3	4	5	6	7	8	9	10
s	1	2	4	7	11	16	22	29	37	46
r	1	2	3	5	7	10	13	17	21	26

The advantage is even more noticeable than in case of basic RKs and RKNs.

6 Test problems

We choose state-dependent delay problems with overlapping (so that $\bar{A}(\theta)$ part of methods is used to find the delayed values).

The first is a modification of the problem 1.2.6 from [12]

$$
\begin{aligned}
&\ddot{u}(t) = u\left(\frac{t}{(1+2t)^2}\right)^{(1+2t)^2}, \qquad t \geq 0,\\
&u(0) = 1, \qquad \dot{u}(0) = -1,
\end{aligned} \tag{6.1}
$$

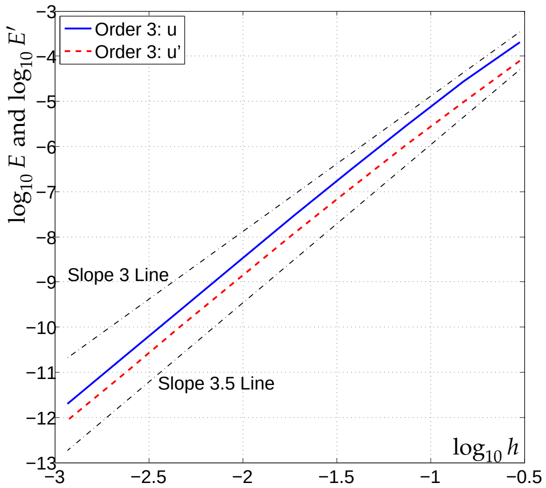


Figure 6.1: Global error of FCRKN33 applied to test problem (6.1) over time interval $[0, 3]$.

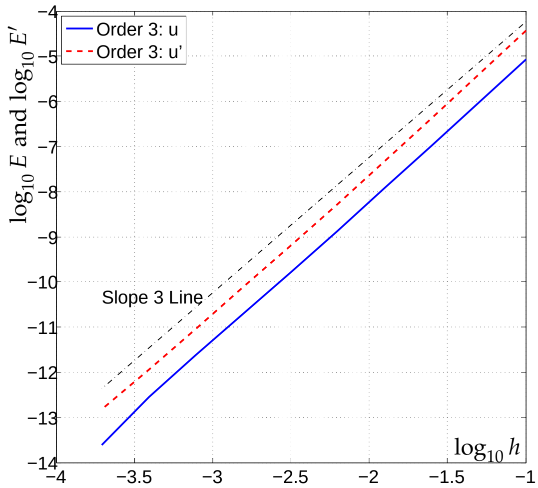


Figure 6.2: Global error of FCRKN33 applied to test problem (6.2) over time interval $[0, 0.5]$.

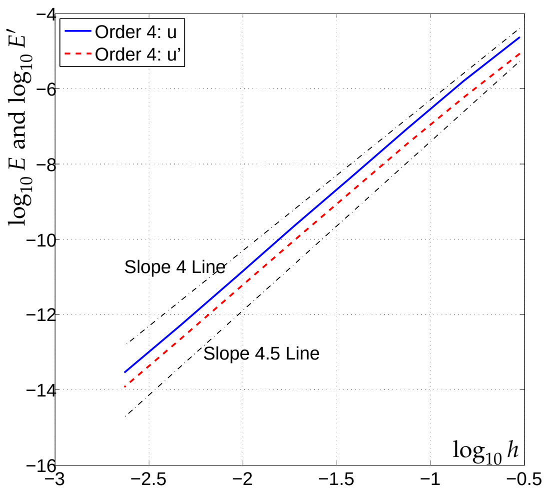


Figure 6.3: Global error of FCRKN45 applied to test problem (6.1) over time interval $[0, 3]$.

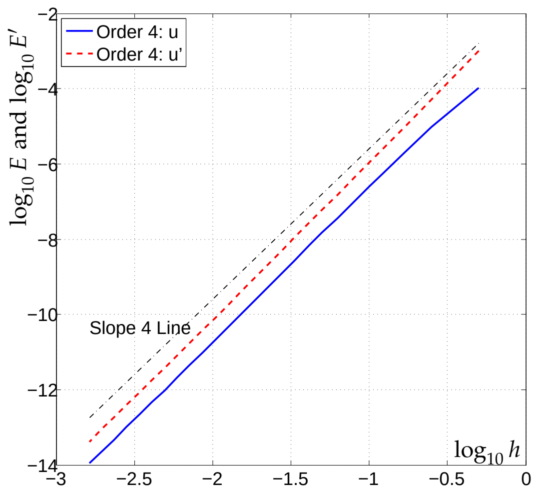


Figure 6.4: Global error of FCRKN45 applied to test problem (6.2) over time interval $[0, 0.5]$.

with the analytical solution

$$u(t) = e^{-t}, \qquad \dot{u}(t) = -e^{-t}, \qquad t \geq 0.$$

The problem is interesting, since it is an *initial value* DDE. The overlapping here occurs at one or more steps in the beginning of the interval.

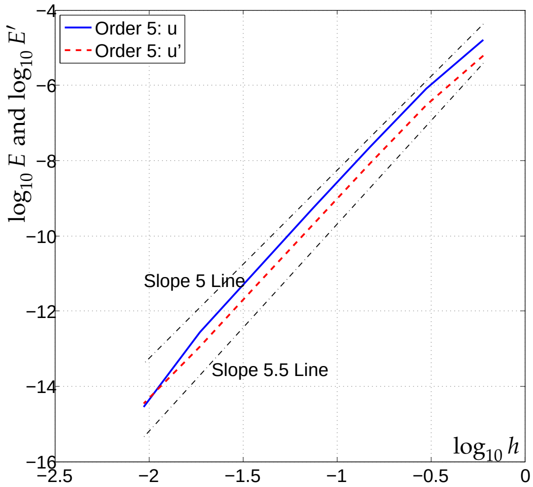


Figure 6.5: Global error of FCRKN57 applied to test problem (6.1) over time interval $[0, 3]$.

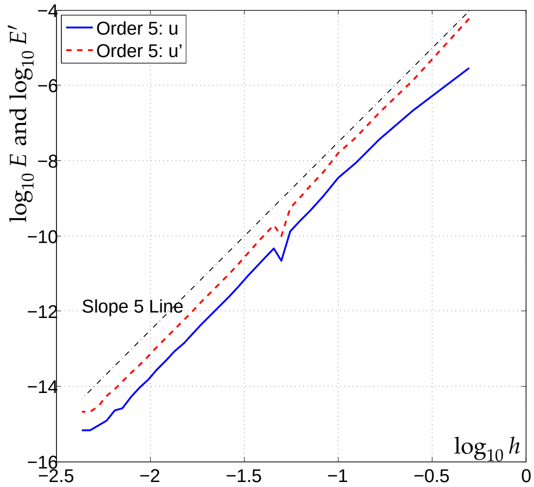


Figure 6.6: Global error of FCRKN57 applied to test problem (6.2) over time interval $[0, 0.5]$.

The second

$$\begin{aligned} \ddot{u}(t) &= u(\alpha(t))\, u(t)\, e^{\alpha(t)}, \qquad t \geq 0, \\ \alpha(t) &= t - \frac{\sin^2(100\pi t)}{100}, \\ u(t) &= e^{-t}, \qquad t \leq 0, \\ \dot{u}(0) &= -1 \end{aligned} \tag{6.2}$$

is a problem with vanishing delay and the overlapping here periodically occurs in the whole time interval. It has the same analytical solution as the previous problem

$$u(t) = e^{-t}, \qquad \dot{u}(t) = -e^{-t}, \qquad t \geq 0.$$

For both problems we run FCRKN methods of orders three (5.1), four (5.5) and five (5.3) multiple times with different constant time steps and measure the global uniform errors of the solution (2.4) and of its derivative (3.7) by computing the absolute value of the difference in 1000 equidistant points per step.

The error to step-size ratio is presented on the plots in double logarithmic scale. Reference lines with fixed slopes are given for comparison.

Results for the problem (6.1) show the global order of all methods to be some value *higher* than the theoretical expectation (at least for small enough steps). In [7] there were presented some similar results for the original problem 1.2.6 from [12], to which (6.1) is quite similar. However the methods described in [7] had different orders in case of overlapping (lower order) and without it (higher order) and the observed convergence order over an interval with both types of steps was in between the two.

In our case the situation is different though. Indeed, for few tested problems without overlapping FCRKN33 and FCRKN57 show global orders 4 and 6 respectively, but FCRKN45 remains of order 4. At the same time the test for local orders do not show increases values for any methods in absence of overlapping (we will not present figures here).

Another interesting fact is, that considering the problem (6.1) with different initial conditions $u(0) = \dot{u}(0) = 1$ and the solution $u(t) = \dot{u}(t) = e^t$ leads to much lower difference between the shown and theoretical global orders.

A possible explanation of the observed order increase can be that errors cancel for some problems and do not for other, and its relation to overlapping if any is not clear. More careful study and various tests should be done.

For the problem (6.2) the order of all the methods is confirmed.

Conclusion

Exploiting specific structure of retarded functional differential equations (such as right-hand side being independent of the function derivative in second order equations) one can construct functional continuous methods, which have fewer stages than Runge–Kutta type methods applicable to the most general problems. Usage of such methods provides the same accuracy with fewer computations, which makes the solution process faster.

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