

Runge-Kutta Research in Trondheim

A. Kværnø and S. P. Nørsett and B. Owren*

Abstract

Runge-Kutta research in Trondheim began in 1970 when Syvert P. Nørsett was appointed to the NTH. Although the group has worked on various aspects of Runge-Kutta methods, we have elected, in this paper, to focus on DIRK methods, linear stability, order stars, parallel methods and continuous explicit methods.

1 Introduction

Research activity on Runge-Kutta methods in Trondheim began when Syvert Paul Nørsett accepted a lectureship at NTH in 1970. He has since then been involved in a broad variety of research topics, and has supervised many students at Master and PhD level. From the late eighties there was a notable increase in the number of PhD students who were primarily working on Runge-Kutta methods. These include Ivar Lie, Anne Kværnø, Brynjulf Owren and Harald Simonsen. The activity has increased further in recent years after both Kværnø and Owren were appointed to the NTH. Naturally, with the large number of papers and theses that have been produced in the Trondheim group on Runge-Kutta methods, it is impossible to summarize everything in one short paper. We have therefore elected to emphasize some topics that have been of particular interest to the authors. When discussing these topics, it has been natural to make reference to other authors who have made contributions to the same area, hence the bibliography has become rather voluminous. Still, in such matters there is the danger of leaving out references that have had a considerable influence on the work done by the Trondheim group, and we would like to express our apologies for any such omissions.

*Division of Mathematical Sciences, The Norwegian University of Science and Technology, N-7034 Trondheim, Norway, E-mail: {anne,norsett,bryn}@imf.unit.no

2 Diagonally Implicit Runge-Kutta Methods.

A *Diagonally Implicit Runge-Kutta Method* (DIRK) is characterized by a Butcher tableau given by

$$\begin{array}{c|cccc}
 c_1 & a_{11} & & & \\
 c_2 & a_{21} & a_{22} & & \\
 c_3 & a_{31} & a_{32} & a_{33} & \\
 \vdots & \vdots & \vdots & \vdots & \ddots \\
 c_s & a_{s1} & a_{s2} & a_{s3} & \cdots & a_{ss} \\
 \hline
 & b_1 & b_2 & b_3 & \cdots & b_s
 \end{array} \tag{1}$$

where at least one of the diagonal entries differs from zero. Applied to an ODE

$$y' = f(x, y), \quad y \in \mathbb{R}^m,$$

the method forms the algebraic system

$$Y_i = y_n + h a_{ii} f(x + c_i h, Y_i) + h \sum_{j=1}^{i-1} a_{ij} f(x_n + h c_j, Y_j), \quad i = 1, \dots, s, \tag{2}$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i f(x_n + c_i h, Y_i). \tag{3}$$

The popularity of the DIRK methods springs mainly from two reasons. First, the methods are implicit, so they may preserve the excellent stability properties of implicit Runge-Kutta methods. (Stability properties are further discussed in a later section.) Second, DIRK methods can be more efficiently implemented than fully implicit methods (FIRK). In the latter case, in general a system of ms equations has to be solved simultaneously, usually by some kind of Newton iteration process. To avoid solving a system of ms equations of a FIRK method, the system is usually transformed to either a block diagonal form as in RADAU5 [27] or Jordan form as in STRIDE [8]. However, in the DIRK case, s systems of m equations are solved sequentially in a natural way. In particular, if all a_{ii} are equal, one may hope to use repeatedly the stored LU -factorization of the Newton matrix

$$I - h a_{ii} f_y.$$

The drawback of the DIRK methods is their relatively low order. While FIRK methods can achieve an order of $2s$, the order of A-stable DIRK methods is restricted to $s + 1$, but even this order can not always be achieved. Thus, the practical use of DIRK methods is limited to solving problems for which only low to moderate accuracy is required.

Several names have been used in the literature to denote methods of the form (1). In this paper, we will use the following:

- DIRK (Diagonal Implicit Runge-Kutta) if $a_{ij} = 0$ for all $j > i$ and $a_{ii} \neq 0$ for at least one i .
- SDIRK (Singly DIRK) for DIRKs where $a_{ii} = \gamma$, $i = 1, \dots, s$.

- EDIRK for DIRKs with an explicit first stage, that is $a_{11} = 0$.
- ESDIRK for DIRKs for which $a_{11} = 0$ and $a_{ii} = \gamma$, $i = 2, \dots, s$.

The name DIRK was first used by Alexander [1] (but with the meaning we now use for SDIRKs), but an interest in DIRKs is older than this. To our knowledge, they were first mentioned by Butcher in 1964 [10]. We quote from this paper: “On the other hand the semi-explicit process appears to have been previously overlooked even though it is of comparable accuracy and more convenient for the practical use.” But in spite of that, DIRK methods seemed to continue to be overlooked until the beginning of the seventies. Then, from 1971 to 1975 (at least) four different theses were partly devoted to this subject: the theses of Alt [3], Kurdi [37], Nørsett [42] and Crouzeix [14]. The thesis of Syvert P. Nørsett, finished in 1975 actually marked the beginning of the activity on numerical ODEs in Trondheim. In his work, Nørsett realized that the coefficient matrix $A = (a_{ij})_{i,j=1}^s$ of an SDIRK method can be written as

$$A = A_e + \gamma I,$$

where A_e corresponds to the coefficient matrix of an explicit method. Thus, all the order conditions can be written as conditions for an explicit method, corrected by some polynomial of γ . The order conditions up to order three will then look like

$$\begin{aligned} b^T e &= 1, & \text{Order 1,} \\ b^T c_e &= \frac{1}{2} - \gamma, & \text{Order 2,} \\ b^T c_e^2 &= \frac{1}{3} + \gamma^2 - \gamma, & \text{Order 3,} \\ b^T A_e c_e &= \frac{1}{6} + \gamma^2 - \gamma, & \text{Order 3,} \end{aligned}$$

where $c_e = c - \gamma e$, $e = [1, 1, \dots, 1]^T$. By using the terminology of Butcher series and rooted trees, all the order conditions of an SDIRK method can be written as

$$\phi_e(t) = \frac{1}{\gamma(t)} + P_t(\gamma),$$

where $\phi_e(t) = \frac{1}{\gamma(t)}$ is the order condition of an explicit method corresponding to the tree t , while $P_t(\gamma)$ is some polynomial of γ . By using this approach, Nørsett proved that there are only two SDIRK methods of order 3 in 2 stages, and only three methods of order 4 in 3 stages. These are given in Table 1. These methods were simultaneously constructed by Crouzeix [14]. Both the order three methods, but only one of the order four methods are A-stable. Nørsett was also concerned with L-stable methods. In particular, he constructed an embedded pair of order 2(3), and a code was written based on this method. Nørsett first called his code SIRSPN, but later, in a fit of modesty, he changed the name to SIRKUSS.

Of other things worthwhile to mention from this thesis is the conjecture that no SDIRK method of order $p \geq \nu + 1$ exists if ν is even. Nørsett gave some evidence for this conjecture for $\mu = 1, \dots, 10$, but whether it is in general true is, as far as we know, still an open question.

In 1977 Alexander [1] published a paper where some of the results of the four theses mentioned earlier were summarized. He also considered the concept of S- and strong S-stability introduced a few years earlier by Prothero and Robinson [56]. Alexander gave some maximum

| | |
|--------------|---------------------------------|
| γ | γ |
| $1 - \gamma$ | $1 - 2\gamma \quad \gamma$ |
| | $\frac{1}{2} \quad \frac{1}{2}$ |

This method is of order three if γ is a solution of

$$\gamma^2 - \gamma + \frac{1}{6} = 0.$$

| | | | |
|---------------|---------------------------------------|---|---------------------------------------|
| γ | γ | | |
| $\frac{1}{2}$ | $\frac{1}{2} - \gamma$ | γ | |
| $1 - \gamma$ | 2γ | $1 - 4\gamma$ | γ |
| | $\frac{1}{6} \frac{1}{(2\gamma-1)^2}$ | $\frac{2}{3} \frac{6\gamma^2-6\gamma+1}{(2\gamma-1)^2}$ | $\frac{1}{6} \frac{1}{(2\gamma-1)^2}$ |

This method is of order four if γ is a solution of

$$\gamma^3 - \frac{3}{2}\gamma^2 + \frac{1}{2}\gamma - \frac{1}{24} = 0$$

Table 1: SDIRK methods of order 3 and 4 respectively

order results for strongly S-stable SDIRK-methods. Cash [13] extended the work of Alexander by supplying his methods with error estimates. Cash also constructed an embedded method of order 4(3) in 5 stages.

In 1975 Butcher [9] introduced the concept of B-stability, a stability concept for nonlinear equations. Some years later, in 1979, Burrage and Butcher [7] and Crouzeix [15] independently gave an algebraic criterion for B-stability. Methods satisfying this criterion are called algebraically stable. In 1980, Hairer [25] proved that no algebraic stable DIRK method has an order exceeding 4. Now, during a joint stay in Waterloo, Canada 1982-83, Nørsett and Thomsen, from the Technical University of Denmark, started to look for B-stable SDIRK methods. In their paper [44] they gave necessary and sufficient conditions for a three stage method of order (at least) three to be B-stable. In particular, an embedded pair of order 3(2) was constructed. This method was called NTI, and is given by

$$\begin{array}{c|cc}
 \frac{5}{6} & \frac{5}{6} & \\
 \frac{24}{108} & -\frac{61}{108} & \frac{5}{6} \\
 \frac{1}{6} & -\frac{23}{183} & -\frac{33}{61} \quad \frac{5}{6} \\
 \hline
 & \frac{25}{61} & \frac{36}{61} \\
 \hline
 & \frac{26}{61} & \frac{324}{671} \quad \frac{1}{11}
 \end{array} . \tag{4}$$

The order three method is B-stable, the order two method only A-stable. Based on this method, Nørsett and Thomsen wrote the code SIMPLE, which has since then been successfully used for several applications. Some implementation details are described in [30],[45] and [46].

As pointed out in the beginning of this section, SDIRK methods are intended to be used for solving stiff ODEs, and many stability concepts have been taken into account when new methods were constructed. But when Runge-Kutta methods are applied to stiff ODEs, peculiarities like the order reduction phenomenon might occur. This behaviour was for the first time described by Prothero and Robinson [56], who realized that by solving the simple test problem

$$y' = \lambda(y - g(x)) + g'(x)$$

the observed order was lower than expected. Frank et al. [23] made a more general study of order reduction for nonlinear stiff equations, and introduced the concepts of B-consistency

and B-convergence, which can be used to obtain error bounds that are independent of the stiffness of the equation. They also gave results on the relationship between the order of B-consistency and the stage order of a method. From their results, it follows that the order of B-convergence for DIRK methods can in general not exceed 1. This quite pessimistic result seemed to put a curb on the enthusiasm for DIRK methods. In the late eighties, almost no papers about DIRK methods appeared.

Fortunately, this is not the end of the story. In 1988, Hairer et al. [26] studied the singular perturbation problem

$$\begin{aligned} y' &= f(y, z), \\ \varepsilon z' &= g(y, z), \quad 0 < \varepsilon \ll 1, \end{aligned}$$

as a model for stiff equations. From their results one may conclude that the numerical solution behaves more or less as if the semi-explicit differential-algebraic equations (DAE) of index 1,

$$\begin{aligned} y' &= f(y, z), \\ 0 &= g(y, z), \end{aligned} \tag{5}$$

are solved, at least for reasonable values of the stepsize. Runge-Kutta methods applied to (5) have been studied by M. Roche, [57]. Using his order results, one can easily see that methods like NTI (4) do not satisfy the order 2 condition

$$b^T A^{-1} c^2 = 1, \tag{6}$$

and suffer from order reduction in the z -component. It can however be proved that all additional order conditions are automatically fulfilled if $b_i = a_{si}, i = 1, \dots, s$. Such methods are called stiffly accurate. The methods studied by Alexander and Cash [1], [13], and also those proposed by Hairer and Wanner, [27, p. 106-107] are all stiffly accurate. But they are equipped with error estimating methods which are not stiffly accurate. Thus, in practice the order of the error estimate will be lower than expected. This creates a difficulty because strategies like the stepsize selection are usually based on the theoretical order. To overcome this difficulty, Kværnø [38] proposed embedded pairs of ESDIRK methods of the form

$$\begin{array}{c|cccc} 0 & 0 & & & \\ c_2 & a_{21} & \gamma & & \\ \vdots & \vdots & & \ddots & \\ 1 & \hat{b}_1 & \hat{b}_2 & \cdots & \gamma \\ 1 & b_1 & b_2 & \cdots & b_{s-1} \quad \gamma \\ \hline & \hat{b}_1 & \hat{b}_2 & \cdots & \gamma \\ \hline & b_1 & b_2 & \cdots & b_{s-1} \quad \gamma \end{array}$$

Such a pair in 4 stages was first constructed by Alexander and Coyle [2] for solving index 2 DAEs. In [38], pairs of order 3(2), 4(3) and 5(4) are given. The diagonal entry γ has been chosen to make the highest order method L-stable, and the embedded method A-stable. These methods have been successfully implemented in the ODE solver system GODESS, [48].

One open question is whether DIRK methods are suitable for solving DAEs other than (5). One used to believe that because of its low stage order, the order of SDIRK methods could not exceed 2 when applied to fully implicit index 1 DAEs, see e.g. [55]. But in 1988, Kværnø [39] constructed a SDIRK method of order 3. Recently, two more SDIRK methods of order 3 have been presented by Olsson [48]. To our knowledge, no one has so far constructed DIRK methods of order 3 for index 2 DAEs.

The usual thing to do when constructing methods is to maximize order and stability properties. But sometimes it might be more interesting to tailor the methods to the kind of problems solved. Owren and Simonsen have done this, by making low order SDIRK methods for the solution of problems in structural dynamics, [52]. Their methods seem to be worthy competitors to the Newmark methods, which so far have been preferred within this particular field of application.

3 Linear Stability, Order Stars and Parallel Methods

In the first part of this paper we discussed the construction of SDIRK and DIRK methods. One of the properties in that part was the order of a method. Another important feature of a method is stability. A first and important way of getting to know the stability of a method is by the classical scalar test equation of Dahlquist [16]

$$y'(x) = \lambda y(x), \quad y(0) = 1, \quad \lambda \in \mathbb{C}.$$

When we apply a RK method of order p to this test equation we get

$$y_{n+1} = R(z)y_n, \quad \text{with } z = h\lambda,$$

where $R(z)$ is a rational function, an order p approximant to $\exp(z)$. By using the idea of collocation a large class of implicit Runge-Kutta methods can be obtained. Let c_1, \dots, c_s be distinct real numbers. Collocation is then: Find a polynomial u of degree s such that

$$u'(x_n + c_i h) = f(u(x_n + c_i h)), \quad i = 1, \dots, s,$$

and

$$y_{n+1} = u(x_{n+1}).$$

As mentioned earlier collocation gives a subclass of all implicit Runge-Kutta methods, see e.g. the paper of Wright [65]. In order to get an equivalence between these two families of methods we have to modify collocation methods to perturbed collocation. That concept was treated in a paper by Nørsett and Wanner [47]. The polynomial

$$N(t) = \prod_{i=1}^{s-i} (t - c_i),$$

is termed the N -polynomial and plays an important role in connection with stability. That connection was found by Nørsett [42] in his thesis. In that thesis he used the notion C -polynomial. When we apply the collocation method to our test equation we arrive at

$$R(z) = \frac{\sum_{i=0}^s N^{(s-i)}(1)z^i}{\sum_{i=0}^s N^{(s-i)}(0)z^i}.$$

With different choices of the N -polynomial we get different Padé approximants to $\exp(z)$. The linear stability is then linked to the behavior of $R(z)$, termed acceptability of $R(z)$. The way of attacking acceptability before 1978 was by using the maximum modulus theorem in complex analysis. For Padé approximants we use $N(t) = \frac{(-1)^s}{(s+r)!} \frac{\partial^r}{\partial t^r} (t^r(1-t)^s)$ and choose different values of r and s .

Before 1972 we had the following results:

- $r = s$: Diagonal Padé approximant. A -acceptability proven in 1961 by Varga [62] for real z . In 1965 Birkhoff and Varga [5] demonstrated full A -acceptability.
- $r = s - 1$: First subdiagonal Padé approximant. A -acceptability was proven independently by Ehle [18] and Axelson [4].
- $r = s - 2$: Second subdiagonal Padé approximant: A -acceptability proven by Ehle [18].
- $r = s - 3$: Third subdiagonal Padé approximant: Ehle [18] showed then lack of A -acceptability.
- $r = s - 4$ and $r = s - 5$: Nørsett [41] showed that these approximants are not A -acceptable.

Ehle [18] gave a conjecture that only for $r \leq s \leq r - 2$ were there A -acceptable approximants. The Ehle conjecture turned out to be a hard problem to solve by using the maximum modulus theorem. It was solved in 1978 in Geneva by Wanner, Hairer and Nørsett [64]. The whole trick was to introduce a new concept, called order stars.

Order Stars

The clue was to study the function,

$$S(z) := \frac{R(z)}{\exp(z)}, \quad z \in \bar{\mathbb{C}}.$$

With this function the relative stability domains, fingers in the paper from 1978 [64] gave rise to the order star.

The **order star of the first kind** of $\{\exp(\cdot), R\}$ is defined as the partition $\{\mathcal{A}_+, \mathcal{A}_0, \mathcal{A}_-\}$ of the closed complex plane, where

$$\begin{aligned} \mathcal{A}_+ &:= \{z \in \bar{\mathbb{C}} : |S(z)| > 1\}; \\ \mathcal{A}_0 &:= \{z \in \bar{\mathbb{C}} : |S(z)| = 1\}; \\ \mathcal{A}_- &:= \{z \in \bar{\mathbb{C}} : |S(z)| < 1\}. \end{aligned}$$

By a simple counting of poles and zeros of $S(z)$ we were in Wanner, Hairer and Nørsett [64] able to prove the Ehle conjecture from 1968. This was for the general Padé approximants. Iserles continued the study of order stars in several papers and the whole theory was put together in a book by Iserles and Nørsett [32]. When working with SDIRK-methods we had to study A -acceptability of **restricted approximants** to $\exp(z)$.

These approximants are obtained by collocation with the N -polynomial

$$N(t) = (-1)^s s! \gamma^n L_s(t/\gamma),$$

with $L_s(t)$ the Laguerre polynomial of degree s . The rational stability function $R(z)$ is

$$R(z) = \frac{P(z)}{(1 - \gamma z)^s},$$

with γ a free parameter and P a certain polynomial of degree at most s . The first detailed study of such approximants appeared in Nørsett [42]. We should mention that Nørsett in his thesis used the word “multiple Padé-approximants”. A more complete study was first possible by the use of order stars, Wanner, Hairer and Nørsett [64]. For DIRK-methods the correct approximants to study was

$$R(z) = \frac{P(z)}{\prod_{i=1}^s (1 - a_{ii} z)}.$$

Such approximants was studied by Keeling [36], Orel [49] and in the thesis by Orel [50].

Parallel Runge- Kutta Methods.

With the increasing interest in numerical algorithms for parallel computers it was natural to consider the possibilities of parallelism in Runge-Kutta methods as well. What the Trondheim group concerns, this work started with a talk, presented in L’Aquila, Italy in 1987 by Nørsett and Simonsen [43]. There the idea was presented of using predictor-corrector techniques in parallel implementations for the first time. Soon after that idea was taken up with interesting results by Van der Houwen and his group in Amsterdam. Lie [40] wrote a report on parallel Runge-Kutta methods. Kalvenes [35] reported some experiments with parallel predictor-corrector methods. Iserles and Nørsett [31] proved a disappointing result suggesting that explicit Runge-Kutta methods have a limited potential in connection with parallel computers. We can give here an interesting remark: Nørsett in his talk in L’Aquila mentioned a forthcoming paper on parallel Runge-Kutta methods by Jackson and Nørsett. The first part of that paper appeared in 1995 [34] and a second part will appear shortly [33].

4 Continuous Explicit Runge-Kutta methods

The material presented here is mostly taken from [21]. Explicit Runge-Kutta formulas were originally designed to approximate the solution of initial value problems on a discrete mesh. The meshpoints are usually determined by a stepsize selection strategy derived from a local error estimator. Such strategies will typically select the largest possible stepsizes under the constraint that some measure of the local error is bounded by a predefined tolerance. But sometimes an approximation to the solution is required at points which do not coincide with the meshpoints. The obvious remedy is to modify the mesh to include these additional points. But apart from the fact that this might severely affect the efficiency of the implementation, it might also happen that the location of the additional points is not known a priori. For instance, after the numerical integration process reaches the point x_n it may become clear

that the solution is required at some x where $x < x_n$. We mention five applications where a continuous extension of the discrete solution obtained by a conventional Runge-Kutta method is required, or at least useful: Monitoring the defect (see [21, Section 3] as a means of error control, global error estimation, and handling discontinuities/singularities. A fourth example arises when the numerical solution is required at a dense set of output points, for instance for the purpose of producing a graphical representation of the solution. Finally, there are *delay differential equations* where one or more *delay arguments* are present in the equations, for instance

$$y'(x) = f(x, y(x), y(x - \tau)), \quad (7)$$

where $\tau > 0$ is a delay that may depend on x , or even on the solution $y(x)$. In many cases this type of system can be solved numerically by a method for standard ODE's, provided an approximation to the delay argument $y(x - \tau)$ can be obtained; for instance by a continuous extension of a Runge-Kutta method.

Having established the need for a continuous approximation to the solution, there are several ways to proceed. The first interpolants for explicit Runge-Kutta methods were based on interpolation over two or more meshpoints using Hermite or Hermite-Birkhoff interpolation. However, with this approach the desirable one-step nature possessed by the Runge-Kutta method is lost if more than two meshpoints are included in the continuous approximation. Thus, in this paper we will restrict our attention to one-step piecewise polynomial continuous extensions of the form

$$u_i(x_i + \theta h_i) = y_{i-1} + h_i \sum_{r=1}^s b_r(\theta) k_r, \quad i = 1, 2, \dots, \quad \theta \in [0, 1], \quad (8)$$

where k_r , $r = 1 \dots, s$ are the stages of the RK method, h_i is the stepsize, and $b_r(\theta)$, $r = 1 \dots, s$ are polynomials. It is natural to define the *uniform order* of the continuous extension as the greatest integer q for which

$$\max_{\theta \in [0, 1]} \| u_i(x_{i-1} + \theta h_i) - y(x_{i-1} + \theta h_i) \| = O(h_i^{q+1}), \quad \text{where } u_i(x_{i-1}) = y_i(x_{i-1}) \quad i = 1, 2, \dots \quad (9)$$

We will assume that the continuous extension evaluated at the endpoint, $\theta = 1$, reduces to the discrete formula, i.e. $b_r(1) = b_r$, thus it follows that $q \leq p$ where p is the order of the discrete formula. Another consequence is that the piecewise polynomial approximation is globally continuous. It has been argued (see, for example, [17]) that for the purpose of treating dense output, it is sufficient that $q = p - 1$. To see this, recall that the global error at the meshpoints is of order p while the continuous formula contributes an error term of order $q + 1$. However, there are other applications where it is necessary to have $q = p$ so that the local error in the continuous extension is asymptotically negligible compared with the global error at the meshpoints (see, for example, [20, 19]).

Surveying the literature of the past decade, we find that a large variety of techniques have been applied for the construction of continuous explicit Runge-Kutta formulas. These techniques fall naturally into two classes: those which are based exclusively on solving the continuous version of the order conditions [53, 54, 63] and those which apply classical interpolation theory, possibly combined with solving order conditions, see, [21] and the references therein.

The first significant contributions to the theory of one-step or local interpolants were made

by Horn [29] and Shampine [60, 59]. We shall not discuss the details of this approach here, since the Trondheim group has not been involved in developing or using it.

When Nørsett and Thomsen visited in Waterloo 1982-83, they initiated a collaboration with Enright and Jackson that resulted in two papers. One of these was [22], where a general approach for finding interpolants for Runge-Kutta methods was developed. Given a RK formula of order p and some C^1 interpolant of uniform order $q_0 < p$ this technique provides a general algorithm for the construction of a C^1 interpolant of order $q = p$ or $q = p - 1$. The algorithm is based on a “boot-strapping” procedure such that, starting with the interpolant of uniform order q_0 each step produces a new interpolant of one order higher. Notice that it is always possible to obtain $q_0 \geq \min\{3, p\}$ simply by computing the cubic Hermite interpolant from the function and derivative values at the end points. We describe here one such step. Assume that an interpolant of uniform order $q \geq q_0$ is available through a polynomial $u_q(x)$ of degree q . Assume also that $q < p$. Choose points $\theta_j \in (0, 1), j = 1, \dots, q - 2$ and compute the polynomial $u_{q+1}(x)$ of degree $q + 1$ such that

$$\begin{aligned} u_{q+1}(x_{i-1}) &= y_{i-1}, & u_{q+1}(x_i) &= y_i, \\ u'_{q+1}(x_{i-1}) &= k_1, & u'_{q+1}(x_i) &= k_{s+1} := f(x_i, y_i), \\ u'_{q+1}(x_{i-1} + \theta_j h_i) &= k_{s+j+1} := f(x_{i-1} + \theta_j h_i, u_q(x_{i-1} + \theta_j h_i)). \end{aligned} \quad (10)$$

It is always possible to find points θ_j such that $u_{q+1}(x)$ is uniquely determined, but since this is a Hermite-Birkhoff interpolation problem, the points must be chosen with some care to ensure that a solution of (10) exists. Now, again assuming that f is sufficiently smooth, it can be shown that the new polynomial $u_{q+1}(x)$ approximates the solution with uniform order $q + 1$. This procedure can be applied repeatedly until $q = p - 1$ or $q = p$ depending on which is desired. We remark that this approach is general, and does not require information obtained from the order conditions. But naturally, to minimize the cost of the interpolant, it is recommended to use as much information as possible from the stages of the underlying discrete method.

It can be easily verified that all the interpolants above can be written in the form (8). In the Trondheim group, it was discussed how one could classify all continuous methods which satisfy (9). The solution to this problem was found when the Trieste group, particularly represented by Zennaro, got involved. At that time, Zennaro had already published several papers on the subject of continuous RK-methods, see for instance [66, 67, 68]. The material we present here on this topic is mainly due to Owren and Zennaro [53, 54], the material is synthesized in the PhD thesis of Owren [51]. But also Verner [63] was working on these topics simultaneously. Standard theory (see, for example, [11]) shows that a RK method is of order p iff the method satisfies the order conditions up to order p ; that is, $\Phi(t) = 1/\gamma(t)$ for all rooted trees t with order $r(t) \leq p$. Here $\gamma(t)$ is the *density* of the rooted tree while $\Phi(t)$ depends on the coefficients that define the RK method. For all t , $\Phi(t)$ depends linearly on the weights b_r of the method, hence $\Phi(t) = \sum_r b_r \phi_r(t)$ where $\phi_r(t)$ depends only on the coupling coefficients a_{ij} . Now, observe that for a fixed θ a continuous method of the type (8) reduces to a conventional RK method with weights $b_r(\theta)$ using step size θh_i . It then follows from the discrete theory that the continuous method (8) satisfies (9) if and only if for every $\theta \in [0, 1]$

$$\sum_{r=1}^s b_r(\theta) \phi_r(t) = \frac{\theta^{r(t)}}{\gamma(t)}, \quad \text{for all } t : r(t) \leq q. \quad (11)$$

By assigning a unique index to each tree we may define the matrix $\Phi := ((\phi_{ij}))$ where $\phi_{ij} := \phi_j(t_i)$. The matrix Φ is $N_q \times s$, where N_q is the number of trees in (11). Defining the two vectors of polynomials $b(\theta) = (b_1(\theta), \dots, b_s(\theta))^T$ and $p(\theta) = (p_i(\theta))$ with $p_i(\theta) = \theta^{r(t_i)}/\gamma(t_i)$ we can write (11) simply as

$$\Phi b(\theta) = p(\theta).$$

Notice that the right hand side is independent of the coefficients of the method. Observe that if Φ has full rank then all the polynomial weights must be of degree $\leq q$ and satisfy $b_r(0) = 0$. It is customary (see, for example, [53, 63]) to assume that $b_r(\theta) = \sum_{k=1}^q b_{rk} \theta^k$. Thus, by defining the $s \times q$ matrix $B := ((b_{rk}))$ and the $N_q \times q$ matrix $P := ((p_{jk}))$ where $p_{ik} := 1/\gamma(t_i)$ if $k = r(t_i)$ and $p_{ik} = 0$ otherwise, we arrive at the matrix equation

$$\Phi B = P. \tag{12}$$

This equation characterizes all continuous Runge-Kutta methods of order q . The least number of stages required to obtain an explicit method of uniform order q is known for $q \leq 6$ and is given in the accompanying table along with the corresponding numbers for conventional (discrete) RK methods. These numbers are denoted $\text{EN}(q)$ and $\text{CEN}(q)$, respectively. For a general theory of such order barriers, see [53]. The result for $\text{CEN}(6)$ in the table below was obtained by Santo [58].

It is shown in [54] that for $q = 3, 4, 5$ the value of $\text{CEN}(q)$ can be effectively reduced by one using a FSAL (first-same-as-last) stage. Studying the table, one sees that for $2 \leq p \leq 5$ the formula $\text{CEN}(p) = 2p - 2$ holds. Carnicer [12] has shown that for general p one has the lower bound $\text{CEN}(p) \geq 2p - 2$ under the condition that either $c_i \neq 0$, $i = 2, \dots, s$ or $a_{i,i-1} \neq 0$, $i = 2, \dots, p$.

| Order q | EN(q) | CEN(q) |
|---------|-------|--------|
| 1 | 1 | 1 |
| 2 | 2 | 2 |
| 3 | 3 | 4 |
| 4 | 4 | 6 |
| 5 | 6 | 8 |
| 6 | 7 | 11 |

Sometimes it may also be useful to consider the matrix obtained by attaching the rows of Φ to the rows of P , i.e. we consider the $N_q \times (s + q)$ matrix $\Psi = [\Phi, P]$. Observe that a solution to (12) exists if and only if $\text{rank}(\Psi) = \text{rank}(\Phi)$. Moreover, given a RK method of order p with a corresponding matrix Φ of elementary weights, it is easy to verify that at least $\text{rank}(\Psi) - \text{rank}(\Phi)$ additional stages are required to construct a continuous extension of uniform order p .

As for higher order discrete Runge-Kutta methods, the analysis of continuous methods becomes exceedingly more difficult as the order increases. It also seems that the discrepancy between the number of stages needed for discrete and continuous methods increases rapidly. To our knowledge, the cheapest known continuous method of order 8 has 20 stages. Verner [63] has investigated high-order continuous extensions by considering the continuous order conditions. Starting with a RK pair of some order $(p, p - 1)$ he constructs continuous extensions of order p or $p - 1$ simply by adding new stages successively until a solution to (12) can be found. This procedure, like the one in [22], is general in the sense that it will always lead to a continuous extension of the desired uniform order. However, it is not guaranteed that the total number of stages needed to obtain uniform order p equals $\text{CEN}(p)$ as defined above. We mention that some authors argue that the order of the interpolant is not necessarily its most

important property. For example, [6] and [24] investigate the use of low order interpolants that guarantee to reproduce monotonicity or convexity in the discrete data.

A third way to obtain continuous explicit RK methods of arbitrary order is by means of extrapolation with an explicit basis method. Simonsen [61], in another PhD thesis from the Trondheim group, shows that extrapolation based on the Euler method with harmonic step sequence yields an extrapolation table similar to the discrete one where all the entries are polynomial approximations with uniform order equal to the (discrete) order of the corresponding entries in the discrete extrapolation table. A similar result holds for the smoothed midpoint rule, but in that case there is the restriction on the step sequence, n_k , that it cannot grow more slowly than $n_k = 4k + 2$.

Finally, we address the question of global smoothness of continuous extensions. This question is particularly easy to answer for the case where classical interpolation techniques are used. In that case it is clear that the global polynomial approximation is C^1 if Hermite interpolation conditions are imposed at the end points. In the approach with continuous order conditions, it can be shown [54], that the uniform approximation is C^1 if and only if the matrix Φ of (12) has full rank and that one of the stages is the so called FSAL evaluation, i.e. $f_{i,j} = f(x_i, y_i)$ for some j . We remark that this stage cannot be involved in the discrete approximation, since, if so, the method would be implicit. Higham [28] considers continuous extensions with a higher degree of smoothness. He gives a procedure for constructing piecewise polynomial approximations such that the k th derivative is continuous at the meshpoints for arbitrary non-negative k . In this case, since the degree of the polynomial exceeds the uniform order when $k > 1$, it follows that some higher derivatives of the local error will become unbounded as the stepsize tends to zero.

In this paper, we have discussed some of the research on Runge-Kutta methods that has been conducted by the Trondheim group over the past 25 years. It is clear that many of the ideas behind this work have been conceived through interaction with other research groups throughout the world. The people who work in this area have kindly accepted invitations to visit Trondheim and enriched us with ideas and inspiration. Likewise, they have always generously hosted people from our group, academic staff as well as students. It is our sincere hope that this cordial atmosphere will continue to be the trademark of Runge-Kutta researchers also in the future, thus we may hope there will be another 100 years of fruitful Runge-Kutta research.

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