

# On the History of Runge-Kutta Methods

*To Cor Baayen at the occasion of his retirement*

P.J. van der Houwen

Runge-Kutta methods are widely-used methods for the integration of initial-value problems for ordinary differential equations. They can also be used for the time integration of initial-value problems for time-dependent partial differential equations by applying the so-called Method of Lines. The method of lines transforms the partial differential equation into a system of ordinary differential equations by discretization of the space variables, so that formally any ordinary differential equation solver can be employed for the time integration of the resulting initial-value problem. However, since ordinary differential equations originating from space-discretized partial differential equations have a special structure, not every ordinary differential equation solver is appropriate. For example, the well-known fourth-order Runge-Kutta method is highly inefficient if the partial differential equation is parabolic, but it performs often quite satisfactory if the partial differential equation is hyperbolic. In this contribution, we concentrate on the role played by Runge-Kutta methods in the numerical integration of time-dependent partial differential equations. In particular, we shall describe the research carried out at CWI.

## 1. THE METHOD OF LINES

The method of lines transforms initial-boundary value problems for time-dependent partial differential equations (PDEs) into initial-value problems (IVPs) for systems of ordinary differential equations (ODEs). This is achieved by discretization of the space variables using finite difference, finite element or finite volume approximations. The connection of PDEs with systems of ODEs was already known to Lagrange (see the historical notes in the book of Hairer-Nørsett-Wanner [10, p. 25]). In 1759 Lagrange already observed that his mathematical model for the propagation of sound in terms of a system of second-order ODEs is related to d'Alembert's equation  $u_{tt} = u_{xx}$  for the vibrating string. However, the actual use of

the space-discretized approximation in numerically solving initial-boundary value problems for PDEs seems to start with Rothe in 1930 [32], and is therefore also called Rothe's method (see [10, p. 3]).

In this paper, we shall restrict our considerations to the case where the spatial discretization of the PDE leads to an IVP of the form

$$(1.1) \quad \frac{dy(t)}{dt} = f(t, y(t)), \quad y(t_0) = y_0,$$

where  $t$  is the time variable and  $y_0$  contains the given initial values. Notice that the boundary conditions are lumped into the righthand side function  $f$ .

The IVP (1.1) has a number of specific characteristics that play a crucial role in selecting a suitable integrator. Firstly, the system (1.1) can be extremely large, particularly, if it originates from a problem with 2 or 3 spatial dimensions. Secondly, the system is usually extremely stiff (here, (1.1) is considered to be stiff if the solution components corresponding to eigenvalues of the Jacobian  $\partial f / \partial y$  that are close to the origin are dominating). Thirdly, the required order of accuracy in time is rather modest (usually not exceeding the order of the spatial discretization, that is, at most order three). Hence, we are led to look for low-order, stiff ODEIVP solvers that are storage economic.

One approach is to look for conventional, general purpose ODEIVP methods that meet these requirements. There are two often used integrators, the second-order trapezoidal rule and the first-order backward Euler method, that belong both to the class of Runge-Kutta methods. They were respectively used by Crank and Nicolson [4] and by Laasonen [24] in their papers of 1947 and 1949 for solving heat flow problems. In the PDE literature, these methods also known as the *Crank-Nicolson* and *Laasonen methods*. An integration method that combines the second-order accuracy of the Crank-Nicolson method and the high stability of the Laasonen method is offered by the two-step method based on backward differentiation (known as the *BDF2 method*). BDF methods were proposed in 1952 by Curtiss and Hirschfelder [3] for solving stiff ODEs and became popular by the papers of Gear in 1967-1968, and in particular by his book [7] of 1971. The Crank-Nicolson, Laasonen and BDF2 methods are applicable to a wide class of space-discretized PDEs (not only heat flow problems) and have comparable computational complexity. In order to solve the implicit relations, one usually applies Newton iteration which leads to a large linear system in each iteration. For one-dimensional problems, these linear systems can be solved by *direct* methods that are in general highly efficient because the band structure of the system can be fully exploited. However, in more than one spatial dimension, direct solution methods usually are out of the question and we have to resort to an *iterative* method. If  $L_N$  denotes the number of Newton iterations,  $L_S$  the number of linear system iterations,  $d$  the spatial dimension, and  $\Delta$  the spatial grid size, then the computational complexity of these methods is  $O(L_N L_S \Delta^{-d})$ . Often used linear-system-iteration methods are conjugate gradient type methods that require at least  $O(\Delta^{-1/2})$  iterations. Hence, the total computational work involved for integrating the unit time interval with stepsize  $h$  is at least  $W = O(L_S h^{-1} \Delta^{-d-1/2})$ .

In order to reduce the huge amount of work when integrating higher-dimensional problems, new methods have been developed. The remainder of this paper will be

devoted to such methods. Since it is not feasible to present a complete survey, we shall confine ourselves to Runge-Kutta type methods that are tuned to PDEs in two or more spatial dimensions. We shall discuss explicit RK methods for parabolic and hyperbolic problems (spectrum of the Jacobian  $\partial f / \partial y$  along the negative axis and imaginary axis, respectively), and splitting methods represented as RK methods with fractional stages.

## 2. EXPLICIT RUNGE-KUTTA METHODS

Consider the  $s$ -stage RK method

$$(2.1) \quad \begin{aligned} \mathbf{Y} &= \mathbf{e} \otimes \mathbf{y}_n + h (\mathbf{A} \otimes \mathbf{I}) \mathbf{F}(t_n \mathbf{e} + ch, \mathbf{Y}), \\ \mathbf{y}_{n+1} &= \mathbf{y}_n + h (\mathbf{b}^T \otimes \mathbf{I}) \mathbf{F}(t_n \mathbf{e} + ch, \mathbf{Y}), \end{aligned}$$

where  $h$  is the integration step,  $\mathbf{y}_n$  and  $\mathbf{y}_{n+1}$  represent approximations to the exact solution vector  $\mathbf{y}(t)$  at  $t = t_n$  and  $t = t_{n+1}$ ,  $\otimes$  denotes the Kronecker product, the  $s$ -dimensional vector  $\mathbf{e}$  is the vector with unit entries,  $\mathbf{I}$  is the identity matrix whose dimension equals that of the IVP, and the  $s$ -by- $s$  matrix  $\mathbf{A}$  and the  $s$ -dimensional vectors  $\mathbf{b}$  and  $\mathbf{c} := \mathbf{A}\mathbf{e}$  contain the RK parameters. The  $s$  components  $\mathbf{Y}_i$  of  $\mathbf{Y}$  represent intermediate approximations to the exact solution values  $\mathbf{y}(t_n + c_i h)$  and  $\mathbf{F}(t_n \mathbf{e} + ch, \mathbf{Y})$  contains the derivative values  $(\mathbf{f}(t_n + c_i h, \mathbf{Y}_i))$ . In the following, the dimensions of  $\mathbf{e}$  and  $\mathbf{I}$  may vary, but will always be clear from the context in which they appear.

If  $\mathbf{A}$  is strictly lower triangular, then (2.1) defines an *explicit* RK method (the first method of this type was proposed by Runge [33] about 100 years ago). Explicit RK methods are relatively cheap, provided that the integration step  $h$  can be chosen sufficiently large. For stiff ODEs, the step is restricted by a stability condition of the form

$$(2.2) \quad h < \frac{\beta}{\rho(\mathbf{J}_n)}, \quad \mathbf{J}_n := \frac{\partial \mathbf{f}(t_n, \mathbf{y}_n)}{\partial \mathbf{y}},$$

where  $\rho(\mathbf{J}_n)$  is the spectral radius of  $\mathbf{J}_n$  and  $\beta$  is the so-called stability boundary. In the case of *parabolic* and *hyperbolic* problems, where the Jacobian of the righthand side function respectively has (more or less) negative and imaginary eigenvalues,  $\beta$  denotes the *real* stability boundary  $\beta_{\text{real}}$  or the *imaginary* stability boundary  $\beta_{\text{imag}}$  of the RK method. The real stability boundary is defined by the maximum length of the negative interval  $(-\beta, 0)$  that is contained in the region where the *stability polynomial*  $R_s(z) := 1 + \mathbf{b}^T (\mathbf{I} - z\mathbf{A})^{-1} \mathbf{e}$  assumes values within the unit circle. Similarly, the imaginary stability boundary is defined by the maximum length of the interval  $(0, i\beta)$  where  $R_s$  is bounded by 1.

### 2.1. Conventional RK methods

For conventional RK methods,  $R_s(z)$  is given by the Taylor polynomial of degree  $s$  in  $z$ , that is, the polynomial that coincides with the truncated Taylor expansion of

$\exp(z)$  at  $z = 0$ . Let us first consider the parabolic case. The *real* stability boundary of Taylor polynomials is (approximately) given by (cf. [15, p.236] and [20,21])

$$(2.3) \quad \beta_{\text{real}} \approx 0.368 (s+1) \sqrt[2(s+1)]{19(s+1)} .$$

This approximation is already quite close for  $s \geq 4$ . We conclude from (2.2) and (2.3) that we can take any step we want by choosing  $s$  sufficiently large, but these formulas also show that for large  $s$  the total number of function calls needed for integrating the unit interval with maximum step  $h = \beta_{\text{real}} \rho^{-1}(J_n) \approx 0.368 s \rho^{-1}(J_n)$  is given by  $N_f \approx 2.7\rho(J_n)$ , that is, *independent of  $s$* . Hence, conventional RK methods are as costly as the explicit Euler method (but of course highly accurate as  $s$  increases). Since  $\mathbf{f}$  has  $O(\Delta^{-d})$  components and since for parabolic problems  $\rho(J_n) = O(\Delta^{-2})$ , the computational work can be estimated by  $W = O(\Delta^{-d-2})$ . This differs by a factor of order  $O(h\Delta^{-3/2})$  from the estimate derived for the Crank-Nicolson, Laasonen and BDF2 methods (when applied to higher-dimensional problems). Usually, this factor is quite large (e.g. if  $h = O(\Delta)$ ), so that conventional RK methods are not the way to solve space-discretized PDEs of *parabolic* type. They are "too costly and too accurate".

Next we consider the hyperbolic case. It happens that for the imaginary stability boundary  $\beta_{\text{imag}}$  we do not always obtain nonzero values. If  $z^{-(p+1)}[R_s(z) - \exp(z)] \rightarrow C_{p+1}$  as  $z \rightarrow 0$ , where  $p$  denotes the order of accuracy of the RK method, then it can straightforwardly be shown that  $\beta_{\text{imag}}$  is only nonzero if either  $C_{p+1} i^p < 0$  for  $p$  even or  $C_{p+1} i^{p+1} < 0$  for  $p$  odd. For the Taylor polynomials this implies that the imaginary stability interval is empty for  $p = 1, 2, 5, 6, 9, 10, \dots$ . For the other orders, quite reasonable values are obtained. For example, for  $p = 3, 4, 7, 8$ , we have  $\beta_{\text{imag}} \approx 1.7, 2.8, 1.7, 3.4$ . Taking one of these latter methods and assuming that  $\rho(J_n) = O(\Delta^{-1})$ , the total computational work associated with the unit interval can be estimated by  $W = O(\Delta^{-d-1})$ . This is a factor of order  $O(h\Delta^{-1/2})$  better than the estimate derived for the Crank-Nicolson, Laasonen and BDF2 methods. Hence, unlike the situation for parabolic problems, conventional RK methods seem to be preferable for *hyperbolic* problems.

## 2.2. Parabolic RK methods

Our conclusion that for parabolic problems explicit RK methods are "too costly and too accurate" suggests sacrificing accuracy in order to reduce computational costs. By observing that an  $s$ -stage RK method of order  $p$  possesses a stability polynomial  $R_s$  of the form

$$(2.4) \quad R_s^{(p)}(z) := \beta_0 + \beta_1 z + \beta_2 z^2 + \dots + \beta_s z^s, \quad \beta_j = \frac{1}{j!}; \quad j = 0, \dots, p; \quad s > p,$$

where the coefficients  $\beta_j$ ,  $j = p+1, \dots, s$ , are free parameters, it is natural to use these free parameters for obtaining larger stability boundaries. For parabolic problems, where the eigenvalues of the Jacobian often are along the negative axis, we are led to construct polynomials  $R_s^{(p)}(z)$  with increased *real* stability boundary. Having found an appropriate stability polynomial  $R_s^{(p)}$ , it is always possible to

construct an RK method with  $R_s^{(p)}$  as its stability polynomial (see e.g. [15]). Such methods will be called *parabolic RK methods*.

Until now, closed form solutions for the polynomials with maximal real stability boundaries (to be called *optimal polynomials*) are only known for  $p = 1$ . They are given by the shifted Chebyshev polynomials

$$(2.5) \quad C_s^{(1)}(z) := T_s\left(1 + \frac{z}{s^2}\right), \quad \beta_{\text{real}} = 2s^2,$$

where  $T_s(z) := \cos(s \arccos(z))$  denotes the first kind Chebyshev polynomial of degree  $s$ . They have been rediscovered in the literature again and again (even in recent years, see e.g. [2]). As far as I know, they were first mentioned for integrating parabolic equations: in 1958 by Yuan' Chzao-Din in his thesis [41], in 1959 by Franklin in his paper [6] that appeared in the Journal for Mathematical Physics, and in 1960 by Guillou and Lago in the Proceedings [9] of the first conference of AFCAL (the French Association for Computing). These authors were not aware of each others work.

For  $p \geq 2$ , only approximate solutions have been constructed. In the thesis of Metzger [28] in 1967, we find numerical approximations for  $p \leq 4$ ,  $s \leq 5$ , and in a NASA report of Lomax [27] of 1968, a general approach for computing the coefficients was indicated. Lomax conjectured that the optimal polynomials satisfy the so-called *equal ripple* property, that is, the optimal polynomial has  $s-p$  local extrema  $+1$  or  $-1$  (this property was actually proved by Riha [31] in 1972 who also showed the unique existence of the optimal polynomials for all  $p$  and all  $s > p$ ). Using the equal ripple property, an iterative method can be constructed for the numerical computation of the coefficients. However, this equal-ripple-iteration method needs rather accurate initial iterates in order to converge. Presumably for this reason, Lomax did not use the equal-ripple-property approach, and instead, computed least squares approximations for  $p = 2$  and  $s \leq 10$ . Again, Metzger, Lomax and Riha found their results independently.

At CWI we used the least squares approach of Lomax for generating initial iterates to start the equal-ripple-iteration method. In this way, we computed the optimal stability polynomials, together with their real stability boundaries, for  $p \leq 4$  and  $s \leq 10+p$  (tables for the coefficients can be found in [13,14]). These computations indicated that  $\beta_{\text{real}}$  increases quadratically with  $s$  as  $s$  increases. In fact, we found

$$(2.6) \quad \beta_{\text{real}} \approx \gamma_p s^2 \quad \text{as } s \rightarrow \infty, \quad \gamma_2 = 0.814, \quad \gamma_3 = 0.489, \quad \gamma_4 = 0.341.$$

The quadratic behaviour is important. It implies that the total number of function calls needed for integrating the unit interval with maximum step  $h \approx \gamma_p s^2 \rho^{-1} (J_n)$  is now given by  $N_f \approx (\gamma_p s)^{-1} \rho (J_n)$ , which is a factor  $2.7 \gamma_p s$  less than the number of function calls needed for conventional RK methods. Hence, for large values of  $s$ , RK methods generated by (2.5) are much cheaper than conventional RK methods, provided that they are available for large values of  $s$ . Unfortunately, the numerical computation of the optimal polynomials becomes increasingly more difficult as  $s$  increases. This motivated us to look for analytical expressions for nearly optimal polynomials that are valid for arbitrary high values of  $s$ . In 1971, Bakker [1] derived in his Master thesis for  $p = 2$  and  $p = 3$  analytically given polynomials which are

quite close approximations to the optimal stability polynomials, in the sense that the stability boundaries are close to the maximal attainable values. These polynomials, to be called the *Bakker polynomials*, are given by

$$(2.7) \quad B_s^{(2)}(z) = \frac{2s^2 + 1}{3s^2} + \frac{s^2 - 1}{3s^2} T_s\left(1 + \frac{3z}{s^2 - 1}\right), \quad \beta_{\text{real}} \approx \frac{2}{3} (s^2 - 1), \quad s > 2,$$

$$(2.8) \quad B_s^{(3)}(z) = 1 + \frac{3\beta^2 - 2(40k^2 - 1)\beta}{576k^4} - \frac{3\beta^2 - 2(36k^2 - 1)\beta}{512k^4} T_{2k}\left(1 + \frac{2z}{\beta}\right) \\ + \frac{3\beta^2 - 2(4k^2 - 1)\beta}{4608k^4} T_s\left(1 + \frac{2z}{\beta}\right), \quad k := \frac{s}{6}, \quad s = 6, 12, 18, \dots,$$

$$\beta_{\text{real}} \approx \beta := \frac{2}{9} s^2 - 1 + \frac{1}{9} \sqrt{\frac{8s^4 - 60s^2 + 297}{5}} \\ \approx \frac{2}{9} s^2 \left(1 + \sqrt{\frac{2}{5}}\right) \approx 0.363 s^2 \text{ as } s \rightarrow \infty,$$

where again  $T_s$  denotes the first kind Chebyshev polynomial of degree  $s$  (in addition, Bakker actually proved the quadratic behaviour of the real stability boundaries of the optimal polynomials and obtained lower and upper bounds for  $\gamma_p$  up to  $p = 15$ ). A comparison of (2.6) with (2.7) and (2.8) reveals that the Bakker polynomials respectively possess 80% and 75% of the maximal attainable, asymptotic stability boundary. Later on in 1982, we found for  $p = 2$  an even better approximation given by (cf. [17])

$$(2.9) \quad A_s^{(2)}(z) = \frac{2}{2 - z} - \frac{z}{2 - z} T_s\left(\cos(\pi/s) + z \frac{1 - \cos(\pi/s)}{2}\right), \\ \beta_{\text{real}} = \frac{2}{[\tan(\pi/2s)]^2} \approx 8 \frac{s^2}{\pi^2} \approx 0.810 s^2 \text{ as } s \rightarrow \infty.$$

These polynomials are not the optimal ones, but yield 99.5 % of the maximal attainable, asymptotic stability boundary!

The parabolic RK methods generated by the analytically given polynomials (2.5), (2.7) and (2.9) enable us to select an integration step  $h$  on the basis of accuracy considerations and to adapt the number of stages according to the stability condition  $s \approx (\gamma_p^{-1} h \rho(J_n))^{1/2}$ . Hence, effectively, we have an *unconditionally stable* method. As we remarked earlier, given the stability polynomial, many RK methods possessing this stability polynomial are possible. One of the most simple implementations of first-order or second-order RK methods with stability polynomial (2.4) reads

$$\begin{aligned}
& \mathbf{Y}_i = \mathbf{y}_n + a_i h \mathbf{f}(t_n + c_{i-1}h, \mathbf{Y}_{i-1}), \quad a_i := \frac{\beta_{s-i+2}}{\beta_{s-i+1}}, \quad i = 1, \dots, s, \\
(2.10) \quad & \mathbf{y}_{n+1} = \mathbf{y}_n + h \mathbf{f}(t_n + h, \mathbf{Y}_s),
\end{aligned}$$

where  $a_1$  is assumed to vanish. This implementation is of the form (2.1) with  $\mathbf{b} = \mathbf{e}_s$  and a matrix  $A$  with zero entries except for the lower off-diagonal entries. We shall call (2.10) the *diagonal* implementation. Unfortunately, when we actually applied the diagonal implementation with  $s \approx (\gamma_p^{-1} h \rho(J_n))^{1/2}$ , it turned out that the numerical solution lost accuracy for larger values of  $s$ . On a computer with 14 digits arithmetic,  $s$  should not be greater than 12. This is caused by the development of *internal* instabilities within a single step. Just as the step values  $\mathbf{y}_n$  are required to be stable by imposing the (external) stability condition  $h < \beta_{\text{real}} / \rho(J_n)$ , we also have to require that the internal values  $\mathbf{Y}_i$  are stable. In the implementation (2.10), the internal perturbations satisfy the recursion  $\Delta \mathbf{Y}_i = a_i h J_n \Delta \mathbf{Y}_{i-1} = R_{i-1}(h J_n) \Delta \mathbf{Y}_1$ , where the so-called *internal stability polynomials*  $R_i(z)$  are of degree  $i$  in  $z$ . This leads to the *internal* stability conditions  $h < \alpha_i / \rho(J_n)$ ,  $i = 1, \dots, s$ , where  $\alpha_i$  denotes the stability boundary associated with  $R_i$ . For large values of  $s$ , these conditions are much more restrictive than the external stability condition  $h < \beta_{\text{real}} / \rho(J_n)$ . As a consequence, the main advantage of the polynomials (2.5), (2.7) and (2.9), viz. that they are available for arbitrarily large values of  $s$ , cannot be exploited.

Fortunately, it is possible to avoid, or at least to suppress the internal instabilities, just by choosing another implementation than (2.10). The first attempt to internal stabilization of RK methods with many stages is due to Gentsch and Schlüter [8] in 1978, who 'rediscovered' the shifted Chebyshev polynomials (2.5) and exploited the fact that these polynomials possess  $s$  real zeroes  $z_i$  on the negative axis. Although their approach was restricted to linear IVPs, it can directly be extended to nonlinear problems to obtain an RK method of the form

$$\begin{aligned}
& \mathbf{Y}_1 = \mathbf{y}_n, \quad \mathbf{Y}_{i+1} = \mathbf{Y}_i - \frac{1}{z_i} h \mathbf{f}(t_n + c_i h, \mathbf{Y}_i), \quad i = 1, \dots, s-1, \\
(2.11) \quad & \mathbf{y}_{n+1} = \mathbf{Y}_s - \frac{1}{z_s} h \mathbf{f}(t_n + c_s h, \mathbf{Y}_s).
\end{aligned}$$

This implementation may be interpreted as an RK method that is factorized in a sequence of Euler steps and will be called the *factorized* implementation. If the zeroes  $z_i$  are ordered such that  $z_i < z_{i+1}$  or  $z_i > z_{i+1}$ , then the performance the factorized implementation is hardly better than that of the diagonal implementation as  $s$  increases. However, Gentsch and Schlüter reported satisfactory results for extremely large values of  $s$  (up to 997) if special orderings of the  $z_i$  are used. A disadvantage in actual applications is that a suitable ordering depends on  $s$ .

When reading the paper of Gentsch and Schlüter, we suddenly realized, that the problem of internal stabilization was already solved a long time ago by numerical analysts working in *elliptic* PDEs! The spatial discretization of elliptic PDEs leads

to the problem of solving linear systems  $Ay = \mathbf{b}$ , where  $A$  is known to have a negative spectrum in the negative interval  $(-\rho(A), 0)$  with  $\rho(A)$  large positive. A well-known iterative method for solving such problems is due to Richardson, who proposed in his paper [30] of 1910 the recursion  $y_i = y_{i-1} + \alpha_i(Ay_{i-1} - \mathbf{b})$ , where the parameters  $\alpha_i$  are chosen such that after  $s$  iterations, the polynomial  $P_s$  occurring in the error formula  $y_s - y = P_s(A)(y_0 - y)$  has a small norm in the eigenvalue interval  $(a, b)$  of  $A$ . Various approaches to achieve this have been proposed. Richardson suggested choosing  $P_s$  such that it has uniformly distributed zeros in  $(a, b)$ , Stiefel proposed to minimize an integral measure of  $P_s$  (cf. [36]), but most numerical analysts prefer to minimize the maximum norm of  $P_s$ . The latter approach leads to shifted Chebyshev polynomials that are very similar to (2.5). This process is now known as Richardson's method of *first* degree. However, application of this method for large values of  $s$  suffers the same internal instability as the method (2.11). Just as Gentsch and Schlüter, one has tried to improve the stability by special choices of the ordering of the parameters  $\alpha_i$  (see e.g. the experiments of Young [40] in 1954), but a real break-through was due to Stiefel [36] in 1958. He observed that Chebyshev polynomials satisfy a *stable* three-terms recursion, so that using a three-terms recursion for the iterates  $y_i$ , rather than the two-terms recursion of Richardson, would avoid the instability problem. This two-step iteration method is known as Richardson's method of *second* degree or, in the more recent literature, the *Chebyshev semi-iterative* method. Realizing that the stability polynomials (2.5), (2.7) and (2.9) are also expressions in terms of shifted Chebyshev polynomials, brought us to construct internally stable implementations of the corresponding parabolic RK methods (cf. [15,16]). For the second-order consistent polynomials  $A_s^{(2)}$  and  $B_s^{(2)}$ , it was pointed out by Sommeijer (see [15]), that it is even possible to make the  $Y_i$  not only stable, but also second-order accurate approximations to the exact solution at the intermediate points  $t_n + c_i h$ ,  $i = 1, \dots, s$ .

The internally stable Runge-Kutta method generated by the Bakker polynomials  $B_s^{(2)}$  performs slightly better than the method generated by  $A_s^{(2)}$  (its smaller stability boundary is compensated by its smaller error constants). It is a highly efficient integrator for general heat flow problems, particularly for 2D and 3D problems. We called it the *Runge-Kutta-Chebyshev method*, but it could equally well have been called the *Runge-Kutta-Bakker method*. A detailed study of its convergence is presented in [37] and an extensive performance evaluation can be found in [12]. The Runge-Kutta-Chebyshev method has been implemented by Sommeijer as the code RKC and is available through netlib [34].

Another code that is based on stabilized RK methods is the code DUMKA developed by Lebedev and his coworkers of the Institute for Numerical Mathematics of the Russian Academy of Science. They approximate the optimal stability polynomials by so-called Zolotarev polynomials. Like Gentsch and Schlüter, internal stability is achieved by a special ordering of the stages rather than using recurrence relations. More details can be found in the references [25, 26].

Finally, we compare the total computational work of conventional and parabolic RK methods needed for integrating the unit interval with a given step  $h$ . Assuming that  $s$  is defined by  $s \approx (\gamma_p^{-1} h \rho(J_n))^{1/2}$ , we find for the stabilized RK methods  $W = h^{-1} s O(\Delta^{-d}) \approx h^{-1} (\gamma_p^{-1} h \rho(J_n))^{1/2} O(\Delta^{-d}) \approx O(h^{-1/2} \Delta^{-d-1})$ . Comparing this estimate with that derived for conventional RK methods, we see that the computational complexity of the stabilized RK methods differ by a factor of order



$O(h^{1/2}\Delta^{-1})$ . With respect to the Crank-Nicolson, Laasonen and BDF2 methods using conjugate gradient type iteration methods, the stabilized RK methods are at least competitive.

### 2.3. Hyperbolic RK methods

Instead of maximizing the *real* stability boundary of stability polynomials of the form (2.4), we may also maximize the *imaginary* stability boundary, to obtain a *hyperbolic RK method* that should be suitable for integrating hyperbolic problems that have Jacobians with imaginary eigenvalues.

For  $p = 1$ , the optimal polynomials are given by

$$(2.12) \quad I_s^{(1)}(z) = (-i)^s \left[ i T_{s-1}\left(\frac{iz}{s-1}\right) - \left(1 + \frac{z^2}{(s-1)^2}\right) U_{s-2}\left(\frac{iz}{s-1}\right) \right], \quad \beta_{\text{imag}} = s - 1,$$

where  $s \geq 2$  and  $U_s(z) := \sin((s+1) \arccos(z)) / \sin(\arccos(z))$  denotes the second kind Chebyshev polynomial of degree  $s$ . For *odd* values of  $s$ , these polynomials were given in 1972 in [13] (a proof can be found in [14]). At the time, it was not realized that (2.12) is also valid for *even* values of  $s$ , because in [13] the polynomials  $I_s^{(1)}$  were represented in the form

$$(2.13) \quad I_s^{(1)}(z) = T_k\left(1 + \frac{z^2}{2k^2}\right) + \frac{z}{k} \left(1 + \frac{z^2}{4k^2}\right) U_{k-1}\left(1 + \frac{z^2}{2k^2}\right), \quad \beta_{\text{imag}} = s - 1,$$

with  $s = 2k+1$ ,  $k \geq 1$ , which cannot directly be extended to even values of  $s$ . It turns out that the odd-degree polynomials are identical to the optimal polynomials corresponding to  $p = 2$ , i.e.  $I_s^{(2)}(z) = I_s^{(1)}(z)$  for  $s$  odd.

In 1984 Kinnmark and Gray [22] derived the representation (2.12) which is valid for all values of  $s$ . This result was also obtained, independently, by Sonneveld and van Leer [35] in 1985.

Kinnmark and Gray [23] have also derived approximations to the optimal polynomials  $I_s^{(3)}$  for  $s$  odd and to  $I_s^{(4)}$  for  $s$  even. These *Kinnmark-Gray polynomials* are given by

$$(2.14) \quad K_s^{(3)}(z) = \frac{1}{\beta^2 + 1} \left[ 1 + z + i^{s-1} \beta^2 T_{s-1}\left(\frac{iz}{\beta}\right) + \frac{1}{2} i^{s+2} \beta \left\{ (s-2) T_s\left(\frac{iz}{\beta}\right) - s T_{s-2}\left(\frac{iz}{\beta}\right) \right\} \right],$$

$$\beta_{\text{imag}} = \beta := \sqrt{(s-1)^2 - 1}, \quad \text{odd } s \geq 3$$

and

$$(2.15) \quad K_s^{(4)}(z) = \sqrt{\frac{1}{\beta^2 + 1}} \left[ i^{s+1} \beta T_{s-1}\left(\frac{iz}{\beta}\right) + \frac{1}{2} i^s \left\{ (s-2) T_s\left(\frac{iz}{\beta}\right) - s T_{s-2}\left(\frac{iz}{\beta}\right) \right\} \right],$$

$$\beta_{\text{imag}} = \beta := \sqrt{(s-1)^2 - 1}, \quad \text{even } s \geq 4.$$

Earlier, in 1983, Vichnevetsky [38] had already proved that  $\beta_{\text{imag}} \leq s - 1$  for all  $p$  and  $s$ . Hence, this result of Vichnevetsky indicates that the Kinnmark-Gray polynomials are extremely close approximations to the optimal ones. However, it also indicates that, unlike the situation for parabolic problems, *hyperbolic* RK methods are hardly more effective than conventional RK methods with nonempty imaginary stability intervals.

### 3. SPLITTING METHODS

Just as RK methods, splitting methods compute in each step two or more intermediate stages. However, unlike RK methods, these stages are not expressed in the full righthand side of the PDE, but in *fractions* of the righthand side. Almost all splitting methods proposed in the literature can be represented in RK format. This approach was followed in [19] to develop a unified treatment of splitting methods and allows a straightforward derivation of the order conditions and stability functions.

Let the righthand side function in (1.1) is reduced to autonomous form and split according to

$$(3.1) \quad \mathbf{f}(\mathbf{y}(t)) = \sum_{i=1}^{\sigma} \mathbf{f}_i(\mathbf{y}(t)),$$

and consider the RK type method

$$(3.2) \quad \begin{aligned} \mathbf{Y} &= \mathbf{e} \otimes \mathbf{y}_n + h \sum_{k=1}^{\sigma} (\mathbf{A}^{(k)} \otimes \mathbf{I}) \mathbf{F}_k(\mathbf{Y}), \\ \mathbf{y}_{n+1} &= (\mathbf{e}_s^T \otimes \mathbf{I}) \mathbf{Y}, \end{aligned}$$

where  $\mathbf{F}_k(\mathbf{Y})$  contains the derivative values  $(\mathbf{f}_k(\mathbf{Y}_j))$ . If  $\sigma = 1$ , then (3.2) reduces to the RK method (2.1) with  $\mathbf{b}^T = \mathbf{e}_s^T \mathbf{A}$ . The method  $\{(3.1), (3.2)\}$  will be called a  $\sigma$ -terms RKS method with  $s$  fractional stages. RKS methods consist of two components, the righthand side splitting (3.1) and the splitting scheme (3.2).

Restricting our discussion to first-order and second-order methods and using the compact notation in terms of the matrices  $\mathbf{A}^{(k)}$ , we have first-order accuracy if

$$(3.3) \quad \mathbf{e}_s^T \mathbf{A}^{(j)} \mathbf{e} = 1, \quad j = 1, \dots, \sigma,$$

and second-order accuracy if, in addition,

$$(3.4) \quad \mathbf{e}_s^T \mathbf{A}^{(j)} \mathbf{A}^{(k)} \mathbf{e} = \frac{1}{2}, \quad j, k = 1, \dots, \sigma.$$

In actual computations, the time-dependent parts originating from time-dependent boundary conditions, cannot be dealt with by simply writing (1.1) in autonomous form and need a more careful treatment. In this overview, we shall not elaborate on this aspect of splitting methods (see e.g. [5]).

The linear stability of RKS methods can be analysed by means of the test equation

$$(3.5) \quad \mathbf{y}'(t) = \sum_{k=1}^{\sigma} \mathbf{J}_k \mathbf{y}(t),$$

where  $\mathbf{J}_k$  is the Jacobian matrix  $\partial \mathbf{f}_k(\mathbf{y}_n) / \partial \mathbf{y}$ . It will be assumed that  $\mathbf{J}_k$  has its eigenvalues in the left halfplane. Defining  $\mathbf{Z}_k = h\mathbf{J}_k$ ,  $k = 1, \dots, \sigma$ , we deduce

$$\mathbf{Y} = \mathbf{e} \otimes \mathbf{y}_n + \sum_{k=1}^{\sigma} (\mathbf{A}^{(k)} \otimes \mathbf{Z}_k) \mathbf{Y} = (\mathbf{I} - \mathbf{S})^{-1} (\mathbf{e} \otimes \mathbf{y}_n),$$

$$\mathbf{S} := \sum_{k=1}^{\sigma} (\mathbf{A}^{(k)} \otimes \mathbf{Z}_k).$$

Hence,

$$\begin{aligned} \mathbf{y}_{n+1} &= (\mathbf{e}_s^T \otimes \mathbf{I}) \mathbf{Y} = (\mathbf{e}_s^T \otimes \mathbf{I}) (\mathbf{I} - \mathbf{S})^{-1} (\mathbf{e} \otimes \mathbf{y}_n) \\ &= (\mathbf{e}_s^T \otimes \mathbf{I}) (\mathbf{I} - \mathbf{S})^{-1} (\mathbf{e} \otimes \mathbf{I}) \mathbf{y}_n. \end{aligned}$$

Thus, the *stability function* is given by

$$(3.6) \quad \mathbf{R} = (\mathbf{e}_s^T \otimes \mathbf{I}) \left( (\mathbf{I} \otimes \mathbf{I}) - \sum_{k=1}^{\sigma} (\mathbf{A}^{(k)} \otimes \mathbf{Z}_k) \right)^{-1} (\mathbf{e} \otimes \mathbf{I}).$$

### 3.2. Splitting methods as RKS methods

This survey paper is concluded with an example of a family of splitting methods that can be represented as an RKS method. For a more detailed analysis of RKS methods we refer to [18].

Consider the two-terms, three-stage splitting scheme defined by

$$(3.7) \quad \mathbf{A}^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 1/2 & 0 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix}, \quad \mathbf{A}^{(2)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

This scheme is second-order accurate whatever we choose for  $\mathbf{f}_1$  and  $\mathbf{f}_2$ . Presumably, the first splitting method proposed in the literature generated by the splitting scheme (3.7) is the Peaceman-Rachford method [29] of 1955. If (3.7) is applied to a space-discretized, two-dimensional PDE in which the righthand side  $\mathbf{f}$  can be split into an

x-dependent part  $f_1$  and a y-dependent part  $f_2$ , then the so-called ADI (Alternating Direction Implicit) method of Peaceman and Rachford is obtained. Other well-known splitting methods generated by (3.7) are the Hopscotch methods proposed by Gourlay in 1970. These methods are obtained by dividing the grid points on which the PDE is discretized in two groups  $G_1$  and  $G_2$ , and by defining  $f_1$  and  $f_2$  such that they vanish on  $G_1$  and  $G_2$ , respectively. On rectangular grids, often used examples are the Line Hopscotch and the Odd-Even Hopscotch methods which arise if  $G_1$  and  $G_2$  contain grid points lying on alternating lines and diagonals, respectively.

#### ACKNOWLEDGEMENT

The author is grateful to Dr. B.P. Sommeijer for his interest in this survey paper and for his many comments to improve the presentation of the available material.

#### REFERENCES

- [1] Bakker, M. (1971): Analytic aspects of a minimax problem (Dutch), Report TN 62, Mathematisch Centrum, Amsterdam.
- [2] Burrage, K. (1985): Order and stability properties of explicit multivalued methods, *Appl. Numer. Math.* 1, 363-379.
- [3] Curtiss, C.F. & Hirschfelder, J.O. (1952): Integration of stiff equations, *Proc. Nat. Acad. Sci. U.S.* 38, 235-43.
- [4] Crank, J. & Nicolson, P. (1947): A practical method for numerical integration of solutions of partial differential equations of heat-conduction type, *Proc. Cambridge Philos. Soc.* 43, 50-67.
- [5] Fairweather, G. & Mitchell, A.R. (1967): A new computational procedure for A.D.I. methods, *SIAM J. Numer. Anal.* 4, 163-170.
- [6] Franklin, J.N. (1959): Numerical stability in digital and analogue computation for diffusion problems, *J. Math. Phys.* 37, 305-315.
- [7] Gear, C.W. (1971): Numerical initial value problems in ordinary differential equations, Prentice Hall, Englewood Cliffs N.J..
- [8] Gentzsch, W. & Schlüter, A. (1978): On one-step methods with cyclic stepsize changes for solving parabolic differential equations (German), *Z. Angew. Math. Mech.* 58, T415-T416.
- [9] Guillou, A. & Lago, B. (1960): Stability regions of one-step and multistep formulas for differential equations; Investigation of formulas with large stability boundaries (French), 1<sup>e</sup> Congrès de l'Association Française de Calcul, AFCAL, Grenoble, Sept. 1960, 43-56.
- [10] Hairer, E., Nørsett, S.P. & Wanner, G. (1987/91): Solving ordinary differential equations I. Nonstiff problems, Springer-Verlag, Berlin.
- [11] Henrici, P. (1962): Discrete variable methods in ordinary differential equations, Wiley, New York.
- [12] Hofmann, S. (1992): First and second-order Runge-Kutta-Chebyshev methods for the numerical integration of parabolic differential equations and stiff ordinary differential equations (in German), Master's thesis, University of Wuppertal, Germany.
- [13] Houwen, P.J. van der (1972): Explicit Runge-Kutta methods with increased stability boundaries, *Numer. Math.* 20, 149-164.

- [14] Houwen, P.J. van der (1977): Construction of integration formulas for initial-value problems, North-Holland, Amsterdam.
- [15] Houwen, P.J. van der (1981): On the time integration of parabolic differential equations, in: G.A. Watson (ed.): Numerical analysis, Lecture Notes in Mathematics 912, Springer, New-York, 157-168.
- [16] Houwen, P.J. van der & Sommeijer, B.P. (1980): On the internal stability of explicit m-stage Runge-Kutta methods for large values of m, Z. Angew. Math. Mech. 60, 479-485.
- [17] Houwen, P.J. van der & Sommeijer, B.P. (1982): A special class of multistep Runge-Kutta methods with extended real stability interval, IMA J. Numer. Anal. 2, 183-209.
- [18] Houwen, P.J. van der & Sommeijer, B.P. (1994): Runge-Kutta splitting methods, in preparation.
- [19] Houwen, P.J. van der & Verwer, J.G. (1979): One-step splitting methods for semi-discrete parabolic equations, Computing 22, 291-309.
- [20] Jeltsch, R. & Nevanlinna, O. (1981): Stability and accuracy of time discretizations for initial value problems, Report HTKK-MAT-A187, Helsinki University of Technology.
- [21] Jeltsch, R. & Nevanlinna, O. (1981): Stability of explicit time discretizations for solving initial value problems, Numer. Math. 37, 61-91.
- [22] Kinnmark, I.P.E. & Gray, W.G. (1984): One-step integration methods with maximum stability regions, Math. Comput. Simulation 16, 87-92.
- [23] Kinnmark, I.P.E. & Gray, W.G. (1984): One-step integration methods of third-fourth order accuracy with large hyperbolic stability limits, Math. Comput. Simulation 16, 181-184.
- [24] Laasonen, P. (1949): On a method for solving the heat flow equation (German), Acta Math. 81, 309-323.
- [25] Lebedev, V.L. (1987): Explicit difference schemes with time-variable steps for solving stiff systems of equations (in Russian), Preprint No. 177, Dept. of Numerical Mathematics, USSR Acad. Sc., Moscow.
- [26] Lebedev, V.L. (1994): How to solve stiff systems of equations by explicit difference schemes, In: Numerical Methods and Applications (ed. G.I. Marchuk), CRC Press, Boca Raton, Ann Arbor, London-Tokyo, 45-80.
- [27] Lomax, H. (1968): On the construction of highly stable, explicit numerical methods for integrating coupled ODEs with parasitic eigenvalues, NASA Technical Note NASAIN D/4547.
- [28] Metzger, C.L. (1967): Runge-Kutta methods whose number of stages exceeds their order (French), These (Troisieme cycle), Université de Grenoble.
- [29] Peaceman, D.W. & Rachford, H.H. Jnr. (1955): The numerical solution of parabolic and elliptic differential equations, J. Soc. Indust. App. Math. 3, 28-41.
- [30] Richardson, L.F. (1910): The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam, Philos. Trans. Roy. Soc. London, Ser. A 210, 307-357 and Proc. Roy. Soc. London, Ser. A 83, 335-336.
- [31] Riha, W. (1972): Optimal stability polynomials, Computing 9, 37-43.

- [32] Rothe, E. (1930): Two-dimensional parabolic boundary value problems as limiting case of one-dimensional boundary value problems (German), *Math. Annalen*, 102, 650-670.
- [33] Runge, C. (1895): On the numerical solution of differential equations (German), *Math. Ann.* 46, 167-178.
- [34] Sommeijer, B.P. (1991): RKC, a nearly-stiff ODE solver, available through netlib (mail: netlib@ornl.gov, send rkc.f from ode).
- [35] Sonneveld, P & Leer, B. van (1985): A minimax problem along the imaginary axis, *Nieuw Archief voor Wiskunde* (4) 3, 19-22.
- [36] Stiefel, E.L. (1958): Kernel polynomials in linear algebra and their numerical applications, *Nat. Bur. Stand. Appl. Math. Series* 49, 1-22.
- [37] Verwer, J.G., Hundsdorfer, W.H. & Sommeijer, B.P. (1990): Convergence properties of the Runge-Kutta-Chebyshev method, *Numer. Math.* 57, 157-178.
- [38] Vichnevetsky, R. (1983): New stability theorems concerning one-step numerical methods for ordinary differential equations, *Math. Comput. Simulation* 25, 199-205.
- [39] Yanenko, N.N. (1971): *The method of fractional steps*, Springer-Verlag, Berlin.
- [40] Young, D.M. (1954): On Richardson's method for solving linear systems with positive definite matrices, *J. Math. Phys.* 32, 243-255.
- [41] Yuan' Chzao-Din (1958): Some difference schemes for the solution of the first boundary value problem for linear differential equations with partial derivatives (Russian), Thesis, Moskow State University.