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P.J. VAN DER HOUWEN

A NOTE ON TWO-STEP RUNGE-KUTTA METHODS

2e boerhaavestraat 49 amsterdam

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Contents

1. Introduction

Two-step Runge-Kutta methods were first considered by Byrne and Lambert [1]. They give a fourth order exact formula based on six function evaluations of which three coincide with function evaluations of a preceding integration step. For large systems of differential equations, such as the ones originating from partial differential equations, this method may be unattractive because of the high storage requirements and the limited stability range.

In this note we propose a class of two-step Runge-Kutta methods which do not use preceding function evaluations, while the new ones are chosen in such a way that the storage requirements are minimized. In fact, it only uses one array more than the methods described in reference [3].

We have only considered first and second order exact formulae, since our main object was to find integration methods for partial differential equations for which higher order methods are usually not required. A more important aspect in integrating partial differential equations is the stability of the difference scheme. We have considered parabolic and hyperbolic equations. For the parabolic equations we did find a class of first order schemes which allows unrestricted integration steps. Only the rate of increase of the step sizes is limited. Furthermore, a class of second order exact schemes was derived with a stability condition which allows at least about 40% larger step sizes than the stabilized one-step Runge-Kutta methods given in [3]. For hyperbolic equations a first order exact integration formula is given with a stability condition which is effectively identical to the condition associated to the one-step n-point Runge-Kutta method given in [2], section 5 as $n \to \infty$

Finally, the new method is applied to a diffusion problem. A comparison with the results obtained by one-step Runge-Kutta methods which were reported in [5] and [6] confirmed the predicted gain factor of 40%.

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2. General structure of the integration method

Suppose it is required to find the solution of the initial value problem

$$(2.1)\qquad \begin{cases} \dfrac{dU}{dt} = H(t,U), \quad t \geq t_0, \\ U = \tilde{U}_0, \quad t = t_0, \end{cases}$$

where $\tilde{U}_0$ is a given initial vector and H is a given function of t and U which has derivatives with respect to t and U of sufficiently high order. With $\tilde{U}$ the analytical solution of (2.1) will be denoted.

We shall consider the following explicit integration formula:

$$(2.2)\qquad \begin{cases} u_0 = \tilde{U}_0, \\ u_{k+1} = \gamma[u_k + \theta_0 r_k^{(0)} + \ldots + \theta_{n-1} r_k^{(n-1)}] + (1-\gamma)u_{k-1}, \\ r_k^{(0)} = \tau_k H(t_k, u_k), \\ r_k^{(1)} = \tau_k H(t_k + \mu_1 \tau_k, u_k + \lambda_{10} r_k^{(0)}), \\ \qquad \ldots \\ r_k^{(j)} = \tau_k H(t_k + \mu_j \tau_k, u_k + \lambda_{j0} r_k^{(0)} + \ldots + \lambda_{jj-1} r_k^{(j-1)}), \\ \qquad \ldots \\ r_k^{(n-1)} = \tau_k H(t_k + \mu_{n-1} \tau_k, u_k + \lambda_{n-10} r_k^{(0)} + \ldots + \lambda_{n-1n-2} r_k^{(n-1)}), \\ k = 0,1,2,\ldots . \end{cases}$$

In these formula we have

u_k: numerical approximation of the analytical solution $\tilde{U}$ at $t = t_k$,

τ_k: the step length $t_{k+1} - t_k$,

γ, θ_j, μ_j, $\lambda_{j,l}$: real parameters to be determined by consistency and stability conditions.

Note that for $\gamma = 1$ (2.2) reduces to a Runge-Kutta type method.

3. Consistency conditions

In order to simplify the calculations we assume throughout this paper that the following relations are satisfied:

$$(3.1) \qquad \sum_{l=0}^{j-1} \lambda_{jl} = \mu_j, \quad j = 1,2,\ldots,n-1.$$

These relations determine, in fact, the parameters μ_j.

Next we introduce for method (2.2) parameters β_j and β_{jl}, of which those used in this paper, are defined by

$$\beta_1 = \theta_0+\theta_1+\ldots+\theta_{n-1} ,$$

$$\beta_2 = \theta_1\mu_1+\ldots+\theta_{n-1}\mu_{n-1} ,$$

$$\beta_3 = \sum_{j=2}^{n-1} \theta_j \sum_{l=1}^{j-1} \lambda_{jl}\mu_l , \quad \beta_{31} = \sum_{j=1}^{n-1} \theta_j\mu_j^2$$

(compare [3], formula (3.6) and (4.1)).
Furthermore, we introduce the parameter

$$(3.3) \qquad q_k = \frac{\tau_{k-1}}{\tau_k} .$$

It will be assumed that both q_k and $1/q_k$ are uniformly bounded with respect to k. In the following analysis we shall omit the index k.

Definition 3.1
Let the integration method (2.2) be written as $L_k(u_{k-1},u_k,u_{k+1}) = 0$. Then the method is said to be of order p at the point $t = t_k$ if

(3.4) $$L_k(U(t_{k-1}), U(t_k), U(t_{k+1})) = O(\tau_k^{p+1}) \text{ as } \tau_k \to 0,$$

where $U(t)$ is a solution of the differential equation which satisfies the condition $U(t_k) = u_k$.

Theorem 3.1

The integration method (2.2) is

(a) of order $p = 1$ if

(3.5) $$\gamma\ \beta_1 - (1-\gamma)q = 1,$$

(b) of order $p = 2$ if, in addition,

(3.6) $$\gamma\ \beta_2 + \frac{1}{2}(1-\gamma)q^2 = \frac{1}{2},$$

(c) of order $p = 3$ if, in addition,

(3.7) $$\gamma\ \beta_3 - \frac{1}{6}(1-\gamma)q^3 = \frac{1}{6},$$

(3.8) $$\gamma\ \beta_{31} - \frac{1}{6}(1-\gamma)q^3 = \frac{1}{3}.$$

Proof

The proof of this theorem can be given by Taylor expansions with respect to τ_k (compare [3], section 3.2). A straightforward calculation yields that the difference scheme (2.2) can written as the differential equation

(3.9) $$\dot{U} = \frac{\gamma\ \beta_1}{1 + (1-\gamma)q} H(t,U) +$$
$$\frac{\gamma\ \beta_2 + \frac{1}{2}(1-\gamma)q^2 - \frac{1}{2}}{1 + (1-\gamma)q} \tau_k\ C_k^{(2)} +$$
$$\frac{\gamma\ \beta_3 - \frac{1}{6}(1-\gamma)q^3 - \frac{1}{6}}{1 + (1-\gamma)q} \tau_k^2\ C_k^{(30)} +$$
$$\frac{\frac{1}{2}\gamma\ \beta_{31} - \frac{1}{6}(1-\gamma)q^3 - \frac{1}{6}}{1 + (1-\gamma)q} \tau_k^2\ C_k^{(31)} + O(\tau_k^3),$$

where the vectors $C_k^{(jl)}$ can be expressed in the partial derivatives of the function $H(t,U)$. From this relation the theorem immediately follows.

4. Stability conditions

Let us define the polynomial

$$(4.1) \qquad P_n(z) = 1 + \beta_1 z + \beta_2 z^2 + \ldots + \beta_n z^n .$$

Theorem 4.1

Suppose that the discrete functions u_k and u_k' satisfy the difference scheme (2.2), i.e.

$$(4.2) \qquad L(u_{k-1}, u_k, u_{k+1}) = 0, \quad L(u'_{k-1}, u'_k, u'_{k+1}) = 0.$$

Then, the function

$$(4.3) \qquad e_k = u_k' - u_k$$

approximately satisfies the difference scheme

$$(4.4) \qquad e_{k+1} = \gamma P_n(\tau_k D_k) e_k + (1-\gamma) e_{k-1},$$

provided that the functions u_k and u_k' are sufficiently close to each other. Here, D_k denotes the Jacobian matrix corresponding to $H(t,U)$ at the point (t_k, u_k).

Proof.

The operator L', defined by

$$(4.5) \qquad L'(v_{k-1}, v_k, v_{k+1}) = v_{k+1} - \gamma P_n(t_k D_k) v_k - (1-\gamma) v_{k-1},$$

is, in fact, the first derivative of the non-linear operation L at the point (u_{k-1}, u_k, u_{k+1}). This may be verified by a straightforward calculation

(compare [3], section 3.3). From this it follows that for functions u_k and u_k', which are sufficiently close to each other, we may write

$$L(u_{k-1}+e_{k-1}, u_k+e_k, u_{k+1}+e_{k+1}) \tilde{=} L(u_{k-1}, u_k, u_{k+1}) +$$

$$+ L'(e_{k-1}, e_k, e_{k+1}) .$$

From (4.2), (4.3) and (4.5) relation (4.4) follows.

Definition 4.1
The solutions of the equation

$$(4.6) \qquad a^2 - \gamma P_n(\tau_k \delta)a - (1-\gamma) = 0,$$

where δ is an eigenvalue of the matrix D_k, are said to be the amplification factors of the integration method corresponding to δ at the point $t = t_k$. Next we derive similar relations for the difference of two solutions U and U' of equation (2.1) and its amplification factor.

Theorem 4.1'
Let U and U' be two solutions of equation (2.1) and define

$$(4.3') \qquad E = U' - U.$$

For integral curves which are sufficiently close to each other, the function E approximately satisfies the relation

$$(4.4') \qquad E_{k+1} = (e^{\tau_k D_k} - (1-\gamma)e^{-\tau_{k-1} D_k})E_k + (1-\gamma)E_{k-1},$$

where E_k denotes the function E at $t = t_k$ and γ is an arbitrary parameter.

Proof
We have for $U' \tilde{=} U$

$$\dot{E} = \dot{U}'-\dot{U} = H(t,U') - H(t,U) \tilde{=} D(U'-U) = DE.$$

By integrating this equation we obtain

$$E(t) = \exp(tD)\, E(t_0)$$

from which (4.4') immediately follows.

Definition 4.1
The solutions of the equation

$$(4.6') \qquad A^2 - (e^{\tau_k \delta} - (1-\gamma)e^{-\tau_{k-1}\delta})\, A - (1-\gamma) = 0$$

are said to be the amplification factors of equation (4.4') corresponding to the eigenvalue δ at the point $t = t_k$.

Ideally, the polynomial $P_n(z)$ associated to the numerical integration methods, should be such that equations (4.6) and (4.6') are identical, i.e.

$$(4.7) \qquad \gamma\, P_n(\tau_k \delta) = e^{\tau_k \delta} - (1-\gamma)e^{-\tau_{k-1}\delta}$$

for all eigenvalues δ of D_k, since then perturbations introduced into the numerical scheme and the differential equation are propagated in the same manner. As an additional condition, one should require that the numerical local amplification factors a are within or on the unit circle for all δ with a non-positive real part.
To be more specific, let S be the domain in the complex z-plane which is bounded by the curve

$$(4.8) \qquad P_n(z) = e^{-i\phi} + \frac{2i}{\gamma} \sin\phi,\ 0 \leq \phi \leq 2\pi,\ 0 \leq \gamma \leq 2.$$

Then the points $\tau_k \delta$ for which $\mathrm{Re}\,\delta \leq 0$ should belong to the region S.
The reason is that in numerical calculations with two-step methods

parasitic solutions are introduced which do not correspond to solutions of the analytical initial value problem

First, we consider condition (4.7). When the values of $\tau_k\delta$ and $\tau_{k-1}\delta$ are relatively small, the right hand side may be approximated by a finite number of terms of the series

$$\gamma\left[1 + \frac{1-(\gamma-1)q}{\gamma}\tau_k\delta + \frac{1}{2}\frac{1+(\gamma-1)q^2}{\gamma}\tau_k^2\delta^2 + \ldots\right] .$$

From theorem 3.1 it follows that for a p-th order consistent scheme the first p+1 terms of this series coincide with the polynomial $\gamma P_n(\tau_k\delta)$. Hence condition (4.7) is approximately satisfied for sufficiently small values of $\tau_k\delta$ and $\tau_{k-1}\delta$.
When these values are not small we have to choose $P_n(z)$ in a very special way. Ideally, the coefficients β_j should depend on the local values of $\tau_k\delta$ and $\tau_{k-1}\delta$. In general, this problem is too difficult to solve, since the eigenvalues δ are not easily found.

In this paper we shall concentrate on the cases where it is known that the eigenvalues δ are either negative or purely imaginary. Such situations are frequently met in the numerical solution of partial differential equations where the space variables are discretized.

5. Integration formulae with n = p = 1

The most simple integration formulae are those for which n = p = 1. From (3.5) and (4.8) it follows that the local stability region S is bounded by the curve

$$(5.1) \qquad z = \gamma\,\frac{-1+\cos\phi + i(\frac{2}{\gamma}-1)\sin\phi}{1+(1-\gamma)q} \quad , \quad 0 \leq \phi \leq \pi \quad .$$

In figure (5.1) the stability region S is indicated by the shaded region.

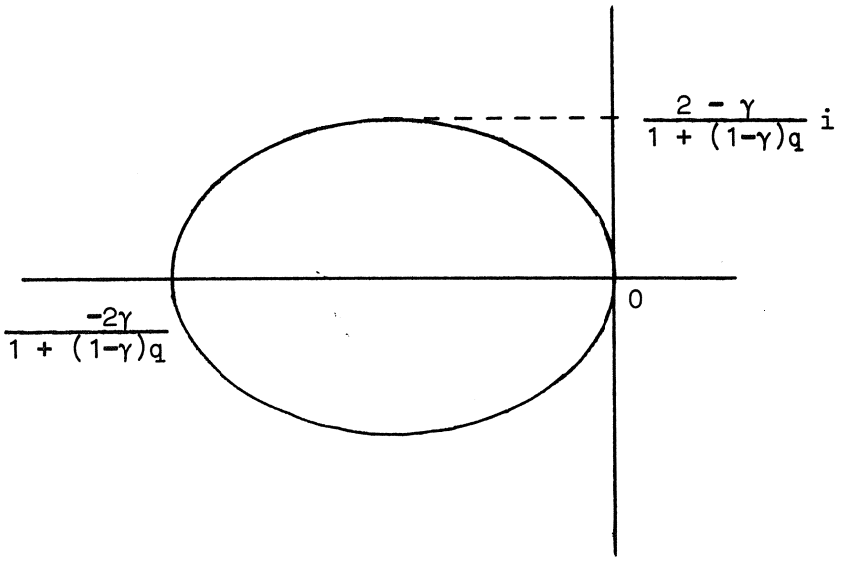

fig. 5.1 Stability region for $n = p = 1$ and $0 < \gamma < 2$.

From this figure it follows that for negative eigenvalues we have stability when

$$(5.2)\qquad \begin{cases} \gamma \leq 2, \\ \dfrac{2\gamma}{1+(1-\gamma)q} \geq \tau_k \sigma(D_k) \ , \end{cases}$$

or, equivalently,

$$(5.2')\qquad \begin{cases} \gamma \leq 2 \\ \tau_k \leq (\gamma-1)\tau_{k-1} + \dfrac{2\gamma}{\sigma(D_k)} \ . \end{cases}$$

Hence, the maximal step allowed by stability equals

$$(5.3)\qquad \tau_{stab} = \tau_{k-1} + \frac{4}{\sigma(D_k)} \ .$$

In these formulas $\sigma(D_k)$ denotes the spectral radius of the Jacobian matrix D_k.

When the eigenvalues δ are purely imaginary we have to choose

$$(5.4)\qquad \begin{cases} \gamma = 0 \\ \tau_k \leq \frac{1}{2}\,\tau_{k-1}\left[\sqrt{1 + \frac{8}{\sigma(D_k)\tau_{k-1}}} - 1\right] . \end{cases}$$

Note that for $\gamma = 1$ the integration methods reduce to Euler's method. From (5.2') it follows that Euler's method for the negative eigenvalue case is stable when

$$\tau_k \leq \frac{2}{\sigma(D_k)} ,$$

while no stability is obtained for the imaginary eigenvalue case.

Furthermore, it may be remarked that γ has to be chosen such that

$$(5.5)\qquad \gamma \neq 1 + \frac{1}{q}.$$

Otherwise, the error constant becomes infinite (compare (3.9)).

Finally, we give the complete integration formula for $n = p = 1$:

$$(5.6)\qquad \begin{cases} u_0 = \tilde{U}_0 , \\ u_{k+1} = \gamma u_k + [(1 + (1-\gamma)q]\tau_k H(t_k,u_k) + (1-\gamma)u_{k-1}, \quad k = 0,1,2,\ldots . \end{cases}$$

6. First order consistent integration formulae for equations with negative eigenvalues

In this section we consider formulae with $p = 1$, $n > 1$ which apply to differential equations of which the Jacobian D has negative eigenvalues. From equation (4.6) we conclude that the stability conditions in the case of negative eigenvalues reduce to

$$(6.1)\qquad \begin{cases} \gamma \leq 2 \ , \\ -1 \leq P_n(\tau_k \delta) \leq 1. \end{cases}$$

The stability interval defined by (6.1) is maximized by the polynomial

$$(6.2)\qquad P_n(z) \equiv T_n\left(1 + \frac{\beta_1 z}{n^2}\right)$$

(compare [2], section 4.1).
The polynomial (6.2) remains between -1 and +1 in the interval

$$\frac{-2n^2}{\beta_1} \leq z \leq 0, \quad \beta_1 > 0 \ ,$$

hence the stability conditions (6.1) become

$$(6.1')\qquad \begin{cases} \gamma \leq 2 \\ \beta_1 \tau_k \sigma(D_k) \leq 2n^2, \end{cases}$$

By substituting the consistency condition (3.5) we find

$$(6.2')\qquad \begin{cases} \gamma \leq 2, \\ \tau_k \leq (\gamma-1)\tau_{k-1} + \dfrac{2n^2\gamma}{\sigma(D_k)} \ . \end{cases}$$

The maximal step for which the integration process remains stable is given by

$$(6.3)\qquad \tau_{stab} = \tau_{k-1} + \frac{4n^2}{\sigma(D_k)} \ .$$

As in the preceding section, where n = 1, we have a bound for the rate of increase of the step sizes. When $\gamma = 1$ an absolute bound for τ_k is obtained.

An explicit formulation of integration formula (2.2) is given by (cf. [3], p.7)

$$
(6.4)\qquad \left\{
\begin{aligned}
& u_0 = \tilde{U}_0, \\
& u_{k+1} = \gamma[u_k + \beta_1 r_k^{(n-1)}] + (1-\gamma)u_{k-1}, \\
& r_k^{(0)} = \tau_k H(t_k, u_k), \\
& r_k^{(1)} = \tau_k H(t_k + \frac{\beta_n}{\beta_{n-1}}\tau_k,\ u_k + \frac{\beta_n}{\beta_{n-1}} r_k^{(0)}), \\
& \qquad \cdots \\
& r_k^{(j)} = \tau_k H(t_k + \frac{\beta_{n-j+1}}{\beta_{n-j}}\tau_k,\ u_k + \frac{\beta_{n-j+1}}{\beta_{n-j}} r_k^{(j-1)}), \\
& \qquad \cdots \\
& r_k^{(n-1)} = \tau_k H(t_k + \frac{\beta_2}{\beta_1}\tau_k,\ u_k + \frac{\beta_2}{\beta_1} r_k^{(n-2)}),
\end{aligned}
\right.
$$

where

$$
(6.5)\qquad \left\{
\begin{aligned}
& \beta_1 = \frac{1 + (1-\gamma)q}{\gamma}, \\
& \beta_j = \beta_1^j c_j,\ j = 2,3,\ldots,n,
\end{aligned}
\right.
$$

c_j being the coefficient of z^j of the polynomial $T_n(1 + \frac{z}{n^2})$.

7. Second order consistent integration formulae for equations with negative eigenvalues

When we choose in scheme (6.4) the parameter γ such that (see (3.6))

$$
(7.1)\qquad \gamma = \frac{1}{2}\,\frac{1 - q^2}{\beta_2 - \frac{1}{2}q^2}
$$

then the scheme becomes second order exact.

Substitution of expression (6.5) for β_2 into (7.1) yields the following equation for γ

$$(7.2) \qquad 2c_2(1 + (1-\gamma)q)^2 = \gamma(1 - (1-\gamma)q^2).$$

Thus, we have to determine values for γ and τ_k which satisfy (7.2) and which are in the stability domain defined by (6.2').
Here, we shall consider the case $q = 1$. It is easily seen that (6.2') and (7.2) together, reduce to

$$(7.3) \qquad \tau_k \leq \frac{2n^2\sqrt{2c_2}}{\sigma(D_k)} .$$

Table 7.1 Stability parameters $\beta(n) = \tau\sigma(D)$ of some second order exact integration formulae.

n	$\beta(n)$, $\gamma = 1$	$\beta(n)$, γ according to (7.2)
2	2	4
3	6.264	9.796
4	12.048	17.888
	...	...
∞	$.82\ n^2$	$1.16\ n^2$

The results for $\gamma = 1$ given in table 7.1 are taken from [4], table 4.1.

As can be seen we may expect an increase of efficiency varying from 100% for $n = 2$ to 40% for $n \to \infty$ over the corresponding one-step Runge-Kutta methods.

8. Numerical results

We have applied the second order consistent version of (2.3) with $n = 4$ to the initial boundary value problem (cf. [5])

$$(8.1)\qquad \begin{cases} U_t = U_{xx} + e^{-t}(x^{10}+90x^{8}-x), \ 0 \le t \le .3 \\ U(0,t) = U(1,t) = 1, \ U(x,0) = 1+x-x^{10}. \end{cases}$$

We have done experiments with a three-point and a five-point representation for U_{xx} (cf. [6]). In table 8.1 results obtained for $n = 4$ are given for a number of values of the mesh size Δx.

Table 8.1 Numerical results obtained for problem (8.1)

Δx	3-point formula			5-point formula		
	K	C	ε_r	K	C	ε_r
1/5	3	.6	$7.0\ 10^{-2}$	4	1.6	$2.0\ 10^{-2}$
1/6	4	1.0	$4.7\ 10^{-2}$	5	2.4	$9.7\ 10^{-3}$
1/7	5	1.4	$3.5\ 10^{-2}$	6	3.4	$4.7\ 10^{-3}$
1/8	6	1.9	$2.7\ 10^{-2}$	8	5.1	$2.5\ 10^{-3}$
1/9	7	2.5	$2.1\ 10^{-2}$	9	6.5	$1.3\ 10^{-3}$
1/10	9	3.6	$1.7\ 10^{-2}$	11	8.8	$7.9\ 10^{-4}$

In this table K denotes the number of integration steps, C a measure for the computational labour ($C = \frac{Kcn}{100\Delta x}$ where $c = 1$ for the 3-point formula and $c = 2$ for the 5-point formula), and ε_r the relative accuracy defined by

$$(8.2)\qquad \varepsilon_r = \max_k \frac{||\tilde{U}_k - u_k||_2}{||\tilde{U}_k||_2},$$

where $\tilde{U}$ is the analytical solution $1 \ e^{-t}(x^w-x)$ and $||\ ||_2$ the Euclidean norm.

A comparison with the results given in [5] shows the superiority of the two-step Runge-Kutta method over the one-step Runge-Kutta method.

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