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OSIRIS : A RUNGE KUTTA SOLVER OF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

by

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ABSTRACT: The Code OSIRIS (Order and Step Idently Adjusting <u>Runge-Kutta Integrator of Systems</u>) has been developed on the basis of both explicit as well as implicit Runge-Kutta processes of various orders: 4(5), 7(8), 8(9), 10 for explicit processes and 4 and 6 for implicit processes of the Rosenbrock type. This permits an <u>optimization</u> of the <u>integra-</u> <u>tion procedure</u> by choosing the appropriate type of Runge-Kutta methods(explicit or implicit) and by adjusting dynamically the order of the process as well as the step-size. The performance of the Code OSIRIS is demonstrated by some representative examples and is compared with the Code GEAR which is applying multistep methods.

<u>OSIRIS</u> : un code de résolution de système d'équations différentielles ordinaires à haute dynamique.

Le code Osiris (Order and Stepsize Idently Adjusting Runge-Kutta Integrator of System) comporte différents algorithmes de Runge-Kutta tant explicites (d'ordres 4(5), 7(8), 8(9), 10) qu'implicites (ordres 4 et 6 de type Rosenbrock). Ceci permet d'optimiser la procédure d'intégration par un ajustement permanent des méthodes utilisées et du pas d'intégration. Quelques exemples représentatifs permettent de comparer les performances du code OSIRIS à celle du code GEAR utilisant des méthodes à pas liés. TABLE OF CONTENTS

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INTRODUCTION

Considerable progress has been made during the last decades in the field of numerical methods for solving initial value problems of systems of ordinary differential equations. Even recent publications on classical numerical methods as RUNGE-KUTTA and multistep are numerous.

Naturally, several computer codes have been developed on the basis of these methods.

Perhaps, the most performant code in this field is the Code GEAR /HI74/ which is based on multistep methods. This Code, since its first release in 1971, has continually benefited from basic mathematical progress as well as from considerable user experience.

However, we have met problems which could not be solved successfully using the Code GEAR. This has obliged us to look for other codes, particularly those based on RUNGE-KUTTA methods, because they are a natural alternative to multistep methods. Surprisingly, all those codes which we found in current mathematical program libraries, have major deficiencies:

- Some use RUNGE-KUTTA procedures which are clearly superseded;
- others apply up-to-date, but not optimal RUNGE-KUTTA processes.
- Finally, to our great annoyance, none of these codes is powerful enough to solve problems being modestly to extremely stiff which are the kind of systems with which we deal. This situation has motivated the present work which is primarely devoted to RUNGE-KUTTA methods.

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Approximately speaking, this report is divided into three main parts:

The first is devoted to a concise survey of modern RUNGE-KUTTA processes.

The second is concerned with the choice of those processes which have been used in our ODE-solver code. The third is centered on applications of our code. Essentially, the code which we have developed is based on modern explicit as well as implicit RUNGE-KUTTA processes of both low and high order. It permits, therefore, an efficient solution of systems, which are low to extremely stiff, to accuracies lying in the range 10^{-1} to 10^{-7} .

All in all, we have incorporated six RUNGE-KUTTA processes into our code (see TABLE 4.2 in CHAPTER 4); four of them are explicit and two are implicit of the Rosenbrock type. An economical execution is guaranteed by an automatic choice of the locally most efficient RUNGE-KUTTA process and, of course, of an automatic choice of optimal step-size during the integration process.

Concerning the performance of our RUNGE-KUTTA solver in comparison with the Code GEAR the following can be concluded: - The RUNGE-KUTTA code has successfully solved all problems which the Code GEAR failed to do.

- The RUNGE-KUTTA code is competitive with the Code GEAR as far as other problems which we treated are concerned. In ANNEX 1 we present a new algorithm to solve systems of non-linear coupled ordinary differential equations of the type (1.2).

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1.0 FORMULATION OF THE PROBLEM.

Let us consider the general initial value problem $dY_{i}(t)/dt = f_{i}(t, Y_{1}(t), ..., Y_{T}(t))$, (1,1)where i=1.2.3....I . A subclass of (1.1) is the system $dY_{i}(t)/dt = \sum_{j=1}^{S} g_{js}(t) \prod_{j=1}^{I} Y_{j}^{r_{isj}}(t) ,$ (1.2)where g_{is} are either constants or depending on t . r are integers. Eq.(1.2) comprises many applications in natural science in general and in physics in particular. In what follows we shall mention just some of the applications which are somehow relevant in the context of our study. Application 1: A quantitative description of the nuclear fusion processes: $D + T - \rightarrow He - 4 + n$,

b + b > 11e-3 + n , b + b > T + p ,b + He-3 > 11e-4 + p ,

is given by the following equations

$$\frac{dY(t)}{dt} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} b_1 Y_1 Y_2 \\ b_2 Y_1 Y_1 \\ b_3 Y_1 Y_1 \\ b_4 Y_1 Y_3 \end{pmatrix} , \qquad (1.5)$$

where b_i are interaction parameters; Y_1 , Y_2 , Y_3 denote the amount of D, T, He-3, respectively; dY(t)/dt is a one column matrix.

Application 2: Matter which is irradiated by means of a particle beam is changing its composition with time. Such a transformation is described by the following differential equations

$$dY_{i}(t)/dt = \sum_{j=1}^{I} g_{ij}Y_{j}(t)$$
, (1.4)

where Y_i denotes the quantity of the nucleus i . If g_{ij} are constants, then either the particle flux is constant or it is absent (decay). The particle flux depends on time otherwise.

Application 3: Let us consider in abstracto the following chemical reactions

$$\begin{array}{rcl} Y_{1} &> Y_{2} + Y_{3} \\ Y_{1} + Y_{3} &> Y_{4} \\ Y_{4} &> Y_{3} + Y_{5} \\ Y_{2} + Y_{3} &> Y_{0} \end{array},$$

where $Y_{\underline{i}}$ denotes the concentration of the chemical species 1. The equations describing these processes quantitatively read

$$dY(t)/dt = \begin{pmatrix} -1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix} \cdot \begin{pmatrix} b_1 Y_1 \\ b_2 Y_1 Y_3 \\ b_3 Y_4 \\ b_4 Y_2 Y_3 \end{pmatrix}$$
(1.5)

where dY(t)/dt is a one column matrix.

In many applications one has to deal with stiff non-linear ordinary differential equations.

THE NUMERICAL METHODS WHICH WE SHALL DISCUSS IN THIS WORK ARE QUITE GENERALLY APPROPRIATE TO SOLVE THE INITIAL VALUE PROBLEM (1.1).

However, our main numerical effort is focused on the solution of (1.4). We integrate this system for various $g_{i,i}$.

2.0 SOLUTION OF INITIAL VALUE PROBLEMS FOR SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS.

Eq.(1.1) is manifestly complicated. Analytical solutions exist only in rare cases. Usually, to solve it one has to have recourse to numerical methods.

2.1 ANALYTICAL SOLUTIONS.

If (1.1) is non-linear, the analytical solution is only known for some cases, for example, for EULER's equation of motion in a force-free field and for equations resulting from the YANG-MILL theory /RA82/. If (1.1) reduces to a linear system as (1.3), then two cases have to be distinguished: Case 1: g_{ij} are constants. Then, the analytical solution of (1.3) is known. It reads in matrix form

$$Y(t) = P^{T}EC, \qquad (2.1)$$

where $P^{\hat{T}}$ is the transpose of the eigenvector-matrix P,

 $\boldsymbol{\varepsilon} = \begin{pmatrix} e^{-1^{t}} & 0 & \dots & 0 \\ 0 & e^{t} \boldsymbol{\varepsilon}^{t} & \dots & 0 \\ \dots & \dots & \dots & 0 \\ 0 & \dots & \dots & 0 & e^{1^{t}} \end{pmatrix},$

 \prime_{i} (i=1,2,3,...,I) are the eigenvalues of the matrix g_{ij} , and C is a one column matrix containing arbitrary constants which can be determined with the help of (2.1) using the initial values Y(t=t_0). Eq.(2.1) becomes then

$$Y(t) = P^{T}E(P^{T}E(t = t_{o}))^{-1}Y(t = t_{o}) . \qquad (2.2)$$

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Observe that the solution of (2.2) can be obtained without computing explicitely the inverse of a matrix. It can in fact be achieved with the aid of a GAUSSIAN elimination process together with a complete pivoting followed by a back substitution. One should bear in mind that the solution via direct matrix inversion REQUIRES ABOUT THREE TIMES MORE computational effort than via GAUSSIAN elimination. An equivalent representation of the analytical solution (2.1) can be obtained by means of LAPLACE-transformation. This solution method offers for not too large systems (1.3) several advantages because:

- No eigenvalue has to be computed.
- No eigenvector has to be computed.
- Unly the solution of one linear algebraic system is necessary.

Here, we will only sketch this method to exhibit its underlying principles.

The transformation \pounds of (1.3) into the image space yields

$$\mathcal{L}(dY_{i}(t)/dt - g_{ij}Y_{j}(t)) = sZ_{i} - Y_{i}(t=t_{o}) - g_{ij}Z_{j} = 0 \quad (2.3)$$

The determination of the unknowns Z_{i} by solving (2.3) and the transformation of Z_{i} back to the original space, i.e.,

$$\mathcal{L}_{i} = Y_{i}(t) , \qquad (2.4)$$

yield directly the solution functions $Y_i(t)$. Finally, we wish to emphasize that an analytical solution, despite its mathematical beauty is not necessarely THE NOST

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APPROPRIATE METHOD FOR PRACTICAL COMPUTATION. This is especially true, if the input data are only known within a certain accuracy and, therefore, the solution do not need to be computed exactly either. Integration using numerical methods might in such a case be more economical than the use of the analytical representation of the functions, because the former permits a flexible adaptation to the accuracy requirements and avoids thus wasteful computational effort.

Case 2: g_{ij} are not constants. Then, for some specific functions $g_{ij}(t)$, analytical solutions of (1.3) are known. In general, however, the solution of (1.3) and of course of (1.1) can only be obtained using numerical methods. To solve such a system several numerical methods are at our disposal. ALL OF THEM ARE ESSENTIALLY EXTRAPOLATORY IN A SENSE THAT THEY START FROM A POINT AND DEVELOP THE SOLUTION FOR A NEIGHBOURING POINT.

We are now going to enumerate the common numerical methods and to outline their essential features.

2.2 NUMERICAL METHODS.

2.2.1 Categories and characteristics.

For obvious reasons, a great deal of attention has in literature been given to this subject and comprehensive books have been published on it /GE71/, /HA76/, /LA73/. It is of course not our aim to repeat here details on these methods, but to exhibit their fundamental features and to select among the various methods those which seem to be

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most appropriate and performant to sove problems with which we have to deal. Five categories of numerical methods are of particular interest: the Taylor series method, the RUNGE-KUTTA methods, the multistep methods, the hybrid method and the OBRECHKOFF method.

• The Taylor series method.

This is conceptually the most attractive numerical method. Essentially, one uses there all information of a function (value plus derivatives) at a point to determine the function at another point. The LIE-series method /GR6o/ can be regarded as a more elegant form of it. The Taylor series method permits in principle an automatic choice of both the order of approximation as well as the step size. It has the obvious demerit of requiring derivatives of functions.

• The RUNGE-KUTTA methods.

These methods can be considered as approximations to the Taylor series method. However, it uses only the knowledge of the value of the function at a point (none or only one derivative) to determine another function value in its vicinity. This simplification is gained at the price of the determination of the socalled RUNGE-KUTTA schemes for each order of approximation separately. That involves tedious and laborious calculations, especially for RUNGE-KUTTA processes of high order.

• The multistep methods.

Essentially, these methods use the knowledge of the functions at several points (multistep) to determine the value of the function at a further point. Also for these methods one has

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to determine coefficients prior to computation.

• The hybrid method.

This method is a combination of the RUNGE-KUTTA and the multistep formalism.

The OBRECHKOFF method.

This method is a combination of the Taylor series and the multistep formalism.

Each of these methods has its merits and drawbacks. They are complementary. For most purposes one of the methods mentioned above should prove sufficient. As for our applications, we need first of all methods which do not require derivatives of functions involved. Therefore, only two basically different methods remain for our aim: The RUNGE-KUTTA and the multistep methods.

2.2.2 The multistep methods.

These are main numerical methods. They have seen a great deal of attention in literature. A Code based on these methods is available. For these reasons we will confine ourselves only to some practical remarks on them. We have already mentioned above that the essential feature of these methods is the use of several function values to determine a function value at another point. Several formalisms were proposed for that process. Well known are the ADAM-BASHFORTH-MOULTON- and GEAR's methods. Both have been incorporated in the program package called GEAR /HI74/. This Code has a relatively long history. The first version of it was published 1971 under the name DIFSUB. Since then this Code has benefited continually from the basic mathe-

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matical progress and the considerable user experience. The present version (4-th version) of the Code GEAR applies the ADAM-BASHFORTH-MOULTON method up to the order 12 and the GEAR's method up to the order 5. The Code is self-starting and changes automatically step-size and order of method. It is claimed to be particularly well suited to solve stiff problems.

The Code GEAR has since its release been widely used as reference code to test newly developed methods relative to its performance.

PERHAPS, THIS CODE CAN AT PRESENT BE REGARDED AS THE MOST PERFORMANT ODE-SOLVER.

However, as we shall see later, we have treated problems which could not successfully be solved by means of the Code GEAR. More precisely, the Code could either not start or yielded erroneous results.

2.2.3 The RUNGE-KUTTA methods.

We will treat these methods in more detail, because we have implemented a RUNGE-KUTTA solver of systems of ordinary differential equations. The following reasons have prompted the implementation of such a code :

- The Code GEAR could not successfully solve some problems with which we had to deal.
- RUNGE-KUTTA methods are an attractive alternative to multistep methods, because they do not require derivatives of functions involved either.
- Comparison studies of the performance of numerical methods showed that the RUNGE-KUTTA methods are competitive in general and even superior in certain cases /EN75/, /EN76/,

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/HU72/, /SH76/, /G081/, /KA81/ and /G082/.

- Une possibility of controlling the total accumulated error is the comparison of the solution functions obtained with the aid of two different codes each of them based on a different mathematical algorithm , for example, based on RUNGE-KUTTA-- or on multistep methods.

2.2.3.1 Basic notions of RUNGE-KUTTA methods.2.2.3.1.1 The algorithm of these methods.Let us consider the initial value problem

$$dY_{i}(x)/dx = f_{i}(x, Y_{1}, Y_{2}, \dots, Y_{n})$$
, (2.5)
where $i=1,2,3,\dots,n$.

The formal RUNGE-KUTTA approximation of the solution functions reads in vector form

$$Y(x+h) = Y(x)+h \cdot \sum_{j=0}^{s} b_j g_j$$

and the next higher approximation can be written

$$\overline{Y}(x+h) = Y(x)+h \cdot \sum_{j=0}^{\overline{s}} \overline{b}_{j} \overline{g}_{j} , \qquad (2.6)$$

where

h is the increment or step-size,

s is the stage(number of function evaluations) of the method,

$$g_{o} = f(x_{o}, Y(x=x_{o})),$$

 $g_{i} = f(x_{o}+c_{i}h, Y(x=x_{o})+h \sum_{j=0}^{s} a_{ij}g_{j}),$ (2.7)

The determination of these coefficients is in fact the central problem of a RUNGE-KUTTA process of a given order. They are derived in two main steps:

- establishment of the algebraic equations for them,

- solution of these equations with a view to an optimal numerical performance of the RUNGE-KUTTA process.

2.2.3.1.2 Definitions.

If $a_{ij}=0$ for $i \le j$, then the method is said to be explicit. If $a_{ij}=0$ for i < j, then the method is said to be semi-implicit. The method is said to be implicit otherwise.

2.2.3.1.3 Applicability of explicit and implicit methods. Explicit methods are much simpler than implicit methods, because in this case the g_i in (2.7) can be computed in a straightforward manner, i.e., without solving an algebraic system. HOWEVER, SUCH METHODS HAVE TOO LIMITED STABILITY REGIONS (see Chapter 3). The integration of socalled stiff systems of ordinary differential equations with the help of such methods is thus risky, expensive or even impossible, because the step-size is limited to a much too small value. Whereas, THE IMPLICIT METHODS PERMIT A LARGE STEP-SIZE EVEN FOR STIFF PROBLEMS. However, when applying implicit methods, the g_i in (2.7) must be determined via the solution of algebraic equations, which can be non-linear. That requires not only more computational effort in comparison with explicit methods, but introduces also new error sources in the computational procedure.

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2.2.3.2 Brief history of RUNGE-KUTTA methods.

2.2.3.2.1 Generalities.

These methods were invented by the mathematicians C.D.T.RUNGE (1856-1927)/RU95/ and M.W.KUTTA(1867-1944)/KU01/. The basic theory of the remainder of the approximative solution, resulting from these methods, has been developed by L.BIEBERBACH/BI51/. The formal theory of RUNGE-KUTTA processes of any order was published by J.C.BUTCHER /BU63/,/BU642/,/BU64/.

2.2.3.2.2 Explicit methods.

A central problem in numerical analysis is the error estimation. Concerning RUNGE-KUTTA methods, it was R.H.MERSON/ME57/, who made a pioneering work in this field with a view to practical calculations. Although his error estimation was not optimal and led generally to wasteful computation, it provided a fresh impetus to investigate this item. It was R.ENGLAND /EN67/, /EN69/, who proposed a more realistic error estimation along with optimal explicit RUNGE-KUTTA processes. Both are naturally related. Almost at the same time, E.FEHLBERG /FE68/, /FE69/ and /FE70% succeeded in deriving still more optimal RUNGE-KUTTA schemata together with economical error estimations. These error estimations fail, however, for problems of the form Y'(x)=f(x) and a RUNGE-KUTTA process of an order greater than 4 /EN76/. It was J.H.VERNER/VE78/ who developed explicit RUNGE-KUTTA schemata along with error estimations which are claimed to work for any system of ordinary differential equations to be integrated. Recently, J.R.CASH /CA83/ has published a RK-algorithm permitting an automatic change of step-size and order of method.

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2.2.3.2.3 Implicit methods.

These methods evoked interest at a later stage. One reason for that is that implicit methods are more cumbersome algorithms. Furthermore, one has realized rather late that for the solution of certain systems of ordinary differential equations, more precisely, of the so-called stiff systems, methods having large stability regions are required. The integration of stiff systems over a longer path can only be carried out by means of implicit methods, because only they permit an appropriate integration step-size.

The general theory of implicit RUNGE-KUTTA methods of any order has been developed by J.C.BUTCHER/BU64/. An important breakthrough was made by B.L.EHLE/EH69/. HE SHOWED THAT ONE CAN OBTAIN A-STABLE IMPLICIT RUNGE-KUTTA FORMULAE OF ARBI-TRARY ORDER.

Note that multistep methods are only A-stable for orders not larger than 2 / DA63/.

In principle, the implicit RUNGE-KUTTA methods permit thus integration of any system of ordinary differential equations. Unfortunately, to integrate a system of m differential equations, implicit RUNGE-KUTTA methods with a full matrix require the solution of m.q (q-stages) simultaneous implicit (in general non-linear) equations at each integration step. This problem was simplified by S.P.NORSETT/N074/ in that he reduced the full matrix a_{ij} to a triangular matrix, $a_{ij}=0$ for i<j. M.CROUZEIX/CR75/ and R.ALEXANDER/AL77/ continued investigations in this direction. Another important simplification has been proposed by H.H.ROSENBROCK/R063/.

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HIS METHOD CAN BE REGARDED AS A LINEARISATION OF SEMI-IMPLICIT RUNGE_KUTTA METHODS. More precisely, whenever semiimplicit RUNGE-KUTTA methods would require the solution of q non-linear equations, the Rosenbrock-type method calls for the solution of q linear equations. This renders implicit methods more economical and numerically more reliable. C.F.HAINES/HA69/ undertook further researches concerning this method. Later B.A.GOTTWALD and G.WANNER/G081/ and then P.KAPS together with G.WANNER /KA81/ have published RUNGE-KUTTA processes of the Rosenbrock type of orders 4 and 5, 6, respectively. Recently, J.R.CASH/CA83/ and G.J.COOPER together with A.SAYFY/C083/ have published additional implicit RUNGE-KUTTA processes.

2.2.3.3 Status of coefficients of RUNGE-KUTTA methods.

In the subsequent TABLE 2.1 we give a selection of RUNGE-KUTTA processes.

TABLE 2.1: A selection of RUNGE-KUTTA methods for which coefficients are available.

| Explic | it | Impli | cit |
|--------|----------------------|-------|---------------|
| Order | References | Urder | References |
| 1-9 | /FE68/,/FE69/,/FE70/ | 3 | /R063/,/HA69/ |
| 5-9 | /VE78/ | 4 | /G081/ |
| 10 | /CU75/,/HA78/ | 5-6 | /KA81/ |

Observe that there exist additional schemata of RUNGE-KUTTA coefficients, for example, those by ENGLAND /EN67/,/EN69/,

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by SHANK/SH66/, by SARAFYAN /SA72/ and by others. However, it seems that they are not so efficient as those given in TABLE 2.1.

From this Table one can also see that the highest order of explicit RUNGE-KUTTA methods for which coefficients are available in literature is equal to 10, and that the highest order of implicit methods for which coefficients are published is equal to 6.

IT SHOULD BE EMPHASIZED THAT COEFFICIENTS OF STILL HIGHER ORDER RUNGE-KUTTA PROCESSES MIGHT NOT BRING ANY SUBSTANTIAL GAIN ANYMORE.

Besides the question of the usefulness of still higher order RUNGE-KUTTA methods for practical computation, the effort required for the determination of the corresponding coefficients is quite considerable. This is well illustrated in TABLE 2.2, where we list the number of non-linear algebraic equations which must be solved for the computation of the coefficients of an explicit RUNGE-KUTTA process of order p.

TABLE 2.2: The number of non-linear algebraic equations to be solved for the determination of the coefficients of an explicit RUNGE-KUTTA process of order p/HA78/.

| RK-order p | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | |
|------------------|---|---|---|---|-----|----|----|-----|-----|------|--------------|---|
| Number of non- | 1 | 2 | 4 | 8 | 17 | 37 | 85 | 200 | 486 | 1205 | 3047 | - |
| linear equations | • | 2 | - | Ŭ | ± (| 51 | 0) | 200 | 100 | 1209 | J U 1 | |
| to be solved. | | | | | | | | | | | | |

Moreover, the solution of these equations is not unique and a judicious choice with a view to an economical RUNGE-KUTTA process requires skill and experience.

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A measure of such an optimal choice is the number of function evaluations (or stages) for a process of a given order. In TABLE 2.3 we give theoretical lower and upper bounds together with the actual values of the smallest number of function evaluations which are needed for an explicit RUNGE-KUTTA method of a given order. Formulae for the estimation of the bounds of the stages are published in /C072/ and /BU75/.

TABLE 2.3: Bounds of the minimum number of stages s_{min} of explicit RUNGE-KUTTA processes and the corresponding actual values.

| RK-order | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|-----------|------|------------------|-----------------|-----|------|-------------------|-----------------|-------------------|-------|--------|------|----|
| Lower | 1 | 2 | 3 | 4 | 6 | 7 | 9 | 10 | 11 | 12 | ز1 | 14 |
| Actual | 31) | 4 ^{1')} | 5 ¹⁾ | 61) | 82) | 10 ²⁾ | 13 ² |) ₁₇ 2 |) | 184 |) | |
| | | _ | | | 83) | 10 ^{3)} | 13 ³ |) ₁₆ 3 |) | 175 |) | |
| upper | | | | | | | | 11 | 16 | 22 | 29 | 37 |
| 1) /FE68/ | , 2) | /FE6 | 59/, | 3) | /VE7 | 8/, | 4) | /cu7 | 5/, 5 | 5) /H# | 78/. | |

2.2.3.4 Tables of coefficients of RUNGE-KUTTA methods. In what follows we give for convenience a selection of Tables of RUNGE-KUTTA processes. We list only coefficients which deserve particular attention. The notation is that used in (2.6) and (2.7). 2.2.3.4.1 Coefficients of explicit methods.

| i | ° _i | а | b _i | b i | | |
|---|----------------|-----------------|---------------------------|-------------------|-------------------|--|
| i | | 0 | 1 | _ | | |
| 0 | 0 | | | $\frac{1}{250}$ | $\frac{1}{512}$ | |
| 1 | $\frac{1}{2}$ | $\frac{1}{2}$ | | $\frac{255}{256}$ | $\frac{255}{256}$ | |
| 2 | 1 | $\frac{1}{256}$ | $\frac{255}{256}$ | | 1 512 | |
| ſ | | TE | $=\frac{1}{512}(g_0-g_1)$ |) h, | | |

TABLE 2.4: RK-coefficients of order 1(2) by FEHLBERG/FE7o/.

where TE is the truncation error.

TABLE 2.5: RK-coefficients of order 2(3) by FEHLBERG/FE70/.

| | c, | | a _{ij} | | ь. | Б. |
|---|-----------------|-------------------------------------|-------------------------------|---------------------------------------|----------------------|----------------------|
| i | | 0 | 1 | 2 | 1 | i |
| 0 | 0 | 0 | | | <u>214</u> 891 | $\frac{533}{2\ 106}$ |
| 1 | $\frac{1}{4}$ | $\frac{1}{4}$ | | | $\frac{1}{33}$ | 0 |
| 2 | $\frac{27}{40}$ | $-\frac{189}{800}$ | 729 800 | | 650 891 | 800 1 053 |
| 3 | 1 | $\frac{214}{891}$ | $\frac{1}{33}$ | 650 891 | | $-\frac{1}{78}$ |
| | TE | $= \left(-\frac{23}{1\ 782}\right)$ | $g_{0} + \frac{1}{33}g_{1} -$ | $-\frac{350}{11583}$ g ₂ - | $+\frac{1}{78}s_3/h$ | |

where TE is the truncation error.

| i / | c, | | ai | b, | б, | | | | | | | |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|----------------------------|-------------------------|-------------------------|-------------------------|-------------------------|--|--|--|--|--|
| 1 L | _ | 0 | 1 | 2 | 3 | 1 | - | | | | | |
| 0 | 0 | 0 | | | | 79 490 | $\frac{229}{1\ 470}$ | | | | | |
| 1 | $\frac{2}{7}$ | $\frac{2}{7}$ | | | | 0 | 0 | | | | | |
| 2 | $\frac{7}{15}$ | 77 900 | <u>343</u> 900 | | | $\frac{2\ 175}{3\ 626}$ | $\frac{1\ 125}{1\ 813}$ | | | | | |
| 3 | $\frac{35}{38}$ | 805 1 444 | $-\frac{77\ 175}{54\ 872}$ | 97 125 54 872 | | 2 166 9 065 | 13 718 81 585 | | | | | |
| 4 | 1 | $\frac{79}{490}$ | 0 | $\frac{2\ 175}{3\ 626}$ | $\frac{2\ 166}{9\ 065}$ | | $\frac{1}{18}$ | | | | | |
| | $T E = \left(\frac{4}{735}\mathbf{s}_{0} - \frac{75}{3\ 626}\mathbf{s}_{2} + \frac{5\ 776}{81\ 585}\mathbf{s}_{3} - \frac{1}{18}\mathbf{s}_{4}\right)h.$ | | | | | | | | | | | |

TABLE 2.6: RK-coefficients of order 3(4) by FEHLBERG/FE7o/.

where TE is the truncation error.

. .

TABLE 2.7: RK-coefficients of order 4(5) by FEHLBERG/FE70/.

.

| ī/ | | | | aij | | | Ь. | б. |
|----|-----------------------|------------------------|-----------------------------------|----------------------------------------------------------------|----------------------------------------------------|------------------|-----------------------------------------|-----------------------------------------------------------|
| i\ | ° i | 0 | 1 | 2 | 3 | 4 | 1 | i |
| 0 | 0 | 0 | | | | | $\frac{25}{216}$ | $\frac{16}{135}$ |
| 1 | $\frac{\tilde{l}}{4}$ | $\frac{1}{4}$ | - | | | | 0 | 0 |
| 2 | $\frac{3}{8}$ | $\frac{3}{32}$ | $\frac{9}{32}$ | | i | | $\frac{1\ 408}{2\ 565}$ | $\begin{array}{r} 6 \ 656 \\ \hline 12 \ 825 \end{array}$ |
| 3 | $\frac{12}{13}$ | $\frac{1932}{2197}$ | $-\frac{7\ 200}{2\ 197}$ | $\frac{7\ 296}{2\ 197}$ | | | $\frac{2 197}{4 104}$ | $\frac{28}{56} \frac{561}{430}$ |
| 4 | 1 | $\frac{439}{216}$ | - 8 | $\frac{3\ 680}{513}$ | $-\frac{845}{4\ 104}$ | | $-\frac{1}{5}$ | $-\frac{9}{50}$ |
| 5 | $\frac{1}{2}$ | $-\frac{8}{27}$ | 2 | $-\frac{3\ 544}{2\ 565}$ | $\frac{1859}{4104}$ | $-\frac{11}{40}$ | | $\frac{2}{55}$ |
| | | $T E = \left(-\right)$ | $-\frac{1}{360}g_{0}+\frac{1}{2}$ | $\frac{128}{4\ 275}$ ^g ₂ + $\frac{2}{7}$ | $\frac{197}{5\ 240}$ g ₃ $-\frac{1}{5}$ | 0 ⁸ 4 | $\frac{2}{55}$ ^g 5) h , | |

where TE is the truncation error.

| | °i | | | a | | ^b i | 5 _i | | | |
|------|----------------|--------------------|------------------|-------------------|--------------------|------------------|----------------|---|------------------|-----------------|
| i \' | | 0 | 1 | 2 | 3 | 4 | 5 | 6 | | |
| 0 | 0 | 0 | | | | | | | <u>31</u> 384 | 7 1408 |
| 1 | <u>1</u> 6 | 1 6 | | | | | | | | 0 |
| 2 | $\frac{4}{15}$ | $\frac{4}{75}$ | <u>16</u> 75 | | | | | | <u>11</u> 28 | <u>25</u> 16 |
| 3 | 2 3 | <u>5</u> 6 | _ <u>8</u> 3 | <u>5</u> 2 | | | | | _1 3 | 2 |
| 4 | <u>4</u> 5 | - <u>1</u> 5 | <u>144</u> 25 | -4 | <u>16</u> 25 | | | | <u>12</u> 76 | <u>5</u> 8 |
| 5 | 1 | <u>361</u> 320 | - <u>18</u> 5 | <u>407</u> 128 | - <u>11</u> 80 | <u>55</u> 128 | | | <u>5</u> 66 | 0 |
| 6 | 0 | - <u>11</u> 640 | 0 | <u>11</u> 256 | - <u>11</u> 160 | $\frac{11}{256}$ | 0 | | | <u>5</u> 66 |
| 7 | 1 | <u>93</u> 640 | - <u>18</u> 5 | <u>803</u> 256 | - <u>11</u> 160 | <u>59</u> 256 | 0 | 1 | | <u>5</u> 66 |

TABLE 2.8: RK-coefficients of order 5(6) by FEHLBERG/FE68/ and /FE69/.

The truncation TE reads

$$TE = \frac{5}{66} (g_0 + g_5 - g_6 - g_7)h$$

| $\overline{\langle}$ | 4 | 1 | 2 | 3 | ey 4 | 5 | 6 | 7 | 8 |
|----------------------|-------------------|--------------------------|--------------------|----------------|---------------------|------------------|-----------|------|----|
| 1 | -0 | | | | | | | | |
| 2 3 | 1 1 1 1 | · 규 권 | 14 | | | | | | |
| 4 | - 2 | | 4 27 -4 | # #1 ~16 | 54 | | | | |
| 5 6 | ⁵ 1 | 55 = <u>369</u> 73 | 77 73 | 5380 219 | 11 =12285 384 | 2695 1752 | | | |
| 7 | Ş | <u>-8716</u> #91 | 63 <u>6</u> 297 | 39520 891 | <u>-416</u> 11 | 52 27 | 0 | 601 | |
| 8 | 1 | 236 | 7 | 78 | 128 | 384 | 0 | 3328 | |
| ō, | | 1 80 57 | 0 | 4 25 | 243 1120 1377 | 77 160 171 | 73 700 | #91 | 2 |
| Ь, | | 640 | 0 | 65 | 2240 | 320 | 0 | 8320 | 33 |

TABLE 2.9: RK-coefficients of order 5(6) by VERNER /VE78/.

with the truncation error

 $TE = \left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix} _{-10}^{11} g_1 - \begin{smallmatrix} 1 \end{smallmatrix} _{-12}^{12} g_3 + \begin{smallmatrix} g g g \\ 22 \end{smallmatrix} _{-10}^{11} g_4 - \begin{smallmatrix} -1 \\ -12 \end{smallmatrix} _{-10}^{11} g_5 - \begin{smallmatrix} -1 \\ -7 \end{smallmatrix} _{-10}^{11} g_6 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_7 + \begin{smallmatrix} 2 \\ -3 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ -12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g g \\ +12 \end{smallmatrix} _{-12}^{11} g_8 + \begin{smallmatrix} g$

TABLE 2.10: RK-coefficients of order 6(7) by VERNER /VE78/.

| X | c; | 1 | 2 | 3 | 4 | ^a ii 5 | 6 | 7 | 8 | 9 | 10 |
|----|--------|----------------------|---|--------------------------|------------------------|--------------------------|------------------------------|----------------------|------|---------------------|---------------------|
| ĩ | 0 |] | | | | | | | _ | | |
| 2 | 112 | | | | | | | | | | |
| 3 | ł | 0 | ł | | | | | | | | |
| 4 | ł | 16 | O | 16 | | | | | | | |
| 5 | 2 | 21 | 0 | <u>-81</u> 16 | 2 | | | | | | |
| 6 | 16 | 1344688 250563 | 0 | <u>=1709184</u> 83521 | 1365632 83521 | -7 <u>8208</u> 250563 | | | | | |
| 7 | 1 2 | <u>559</u> 384 | 0 | 6 | <u>-204</u> 47 | 14 39 | -4913 78208 | | | | |
| 8 | 1 | <u>-621</u> 224 | 0 | 12 | <u>-456</u> 47 | 48 91 | 14739 | 67 | | | |
| 9 | 3 | -12253 99144 | 0 | 16 27 | 459 | 29072 161109 | <u>-2023</u> 75816 | <u>112</u> 12393. | Э | | |
| 10 | 1 | <u>30517</u> 2512 | 0 | -7296 157 | 2 <u>68728</u> 7379 | <u>2472</u> 2041 | <u>-3522621</u> 10743824 | 132 157 | 0 | =12393 4396 | |
| Б, | | 7 40 | 0 | 0 | 16 43 | 16 45 | 0 | 215 | 7.90 | | |
| ь, | | <u>2881</u> 40320 | 0 | 0 | 1216 2961 | <u>-2624</u> 4095 | 2 <u>4137569</u> 57482880 | 4 21 | 0 | <u>4131</u> 3920 | <u>-157</u> 1260 |

with the truncation error

 $\Gamma E = (\frac{-17}{26\pi\pi}g_1 + \frac{272}{4935}g_4 - \frac{272}{273}g_5 + \frac{24137599}{57442840}g_6 - \frac{14}{105}g_7 - \frac{7}{90}g_8 + \frac{4131}{3920}g_9 - \frac{157}{1260}g_{10})\ln \ ,$

| ם. ס | н н | 77 1440 864 | • | 0 | <u>1771561</u> 6289920 | <u>32</u> 105 | 2 43 2580 | <u>16807</u> 74880 | 270 0 | 270 | <u>11</u> 270 |
|----------------------|--------|----------------|---------------|----------|---------------------------|------------------|---------------------|------------------------|------------------|--------------------------|------------------------|
| | 80 | | <u> </u> | <u> </u> | | | | | | | |
| | - | | | | | | | | | 0 | 0 |
| | ø | | | | | | | | 7203 9152 | 1029 18304 | <u>1029</u> 1408 |
| | s | | | | | | | <u>1053</u> 2401 | - 4617 - 2816 | | - <u>729</u> - 512 |
| aij | 4 | | | | | | 2176 1701 | 16807 | 71 | :16 | 1 18 |
| | 8 | | | | | 813 | | <u>116359</u> 16807 | 335765 23396 | - <u>5115</u> - 46552 | <u>- 51237</u> 3584 |
| | 3 | | | | 기지 | - 165 | <u>1067</u> 54 | 888 888 | 131 | 0 | Ŧ |
| | 1 | | | -18 | • | • | • | 0 | 0 | 0 | • |
| | 0 | • | 64 5 3 | • | ᅴ컶 | 치고 | 2383 | <u>10077</u> 4802 | | 역왕 | 1833 |
| ا ن ان | | 0 | 20 | 4 3 | 2 | | cd t es | ~ 10 | | 0 | |
| | 1 / | 0 | -4 | 5 | 3 | 4 | uð. | 8 | ۲ | 6 0 | ۵ |

TABLE 2.11: RK-coefficients of order 6(7) by FEHLBERG /FE68/.

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with the truncation error TE

$$TE = \frac{11}{270} (g_0 + g_7 - g_8 - g_9) h .$$

.

- 23 -

| .,т о | | 0 | | | | | -100 | | 1 | | 10 | ° | 41 | 198 |
|----------|----|----|------|------|-----|----------------|------|-------------------|-----------|---------------|------------------------------|---------------------|----------|------------------------|
| ٦. م | | 17 | | 0 | 0 | 0 | 10 | 9 2 | ရန | 5 0 00 | 0 6 | 17 28 | | |
| | 11 | | | | | | | | | | | | | 1 |
| | 10 | | | | | | | | | | | | 0 | o |
| | ი | | | | | | | | | | | 41 18 | 4 | 12 |
| | 80 | | | | | | | | | | 12 | 42 164 | en 14 | 33 164 |
| | 7 | | | | | | | | | 3 | <u>17</u> 6 | 8 2 87 | 5 | <u>51</u> 82 |
| | 9 | | | | | | | | <u>13</u> | 67 | - <mark>19</mark> | 2133 | 3 205 | 2193 |
| أنا | 5 | | | | | | | <u>125</u> 54 | 8 6 | 9 | 311 | 301 | 8 7 | - 289 82 |
| | 4 | | | | | | 5 | 8 5 | 61 225 | <u>5</u> 5 | - <u>976</u> - <u>135</u> | 4496 1025 | 0 | <u>1496</u> 1025 |
| | 3 | | | | | <u>8</u> 19 | -14 | <u>125</u> 108 | 0 | 20 | 23 108 | 181 | • | 18 |
| | 8 | | | | ∞ | 16 16 | 0 | 0 | 0 | 0 | 0 | • | 0 | • |
| | ٦ | | | - 2 | 0 | • | 0 | 0 | 0 | • | 0 | 0 | 0 | 0 |
| | • | 0 | ~ 5 | -199 | -12 | 이업 | - 2 | <u>श्र</u> थि | 50 F | 61 | 108 | 4100 | 5 m | - <u>1777</u> -4100 |
| ч. | | 0 | 2 23 | - 0 | ~ ~ | 5 | 0 | olo | -10 | 00 m | - 6 | T | 0 | 1 |
| | 2 | 0 | - | 8 | e | 4 | ۍ | 9 | 7 | 90 | a | 10 | 3 | 12 |

TABLE 2.12: RK-coefficients of order 7(8) by FEHLBERG /FE68/.

$$fE = \frac{41}{840} (g_0 + g_{10} - g_{11} - g_{12})h.$$

- 24 -

, ∆_{ij} 6 ¢, 븄 뉴 걪 <u>-408</u> 125 $\frac{352}{125}$ 造 328 ļ -1263 2401 37 392 26411 $\frac{-64125}{26411}$ 2401 ş 9408 73 6720 <u>-47104</u> 25515 <u>1325</u> 504 -41792 23515 145800 6075 -23814 180075 -77824 1980825 <u>-636635</u> 633864 300125 -183 7000 ŧ. ;}}} 7600 -20032 5225 80256 -42599 912000 <u>-1029</u> 4180 1408 <u>}</u> <u>-27061</u> 204120 -1353775 1197504 40448 280665 $\frac{17667}{25515}$ -71687 1166400 <u>98</u> 225 11503 458304 <u>-1029</u> 992 -38144 -84046 16275 8525 10912 341 ō, <u>2401</u> 12375 14080 <u>2401</u> 19200 450 <u>32</u> 125 79200 1760 쁐 쁐 1760 b, ¥

with the truncation error

t

.

 $\Gamma \dot{E} = \left(\frac{-1}{480}g_1 - \frac{16}{375}g_6 - \frac{2401}{528000}g_7 + \frac{2401}{132000}g_8 + \frac{243}{14080}g_9 - \frac{2401}{19200}g_{10} - \frac{19}{450}g_{11} + \frac{243}{1760}g_{12} + \frac{31}{720}g_{13}\right)h .$

•

- 25 -

TABLE 2.14: RK-coefficients of order 8(9) by FEHLBERG /FE68/.

c(1) = 0.4436 8940 3764 9818 3109 5994 0428 1370c(2) = 0.6655 3410 5647 4727 4664 3991 0642 2055c(3) = 0.9983 0115 8471 2091 1996 5986 5963 3083 c(4) = 0.3155 0000 0000 0000 0000 0000 0000 0000 c(5) = 0.5054 4100 9481 6906 8626 5161 2673 7384c(6) = 0.1714 2857 1428 5714 2857 1428 5714 2857c(7) = 0.8285 7142 8571 4285 7142 8571 4285 7143c(8) = 0.66543968121011562534953769255586c(9) = 0.2487 8317 9680 6265 2069 7222 7456 0771 $c(1o) = 0.1090\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000$ $c(11) = 0.8910\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000$ $c(12) = 0.3995\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000$ $c(13) = 0.6005\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000\ 0000$ c(14) = 1c(15) = 0c(16) = 1a(1, o) = 0.4436 8940 3764 9818 3109 5994 0428 1370a(2, 0) = 0.1663 8352 6411 8681 8666 0997 7660 5514a(2,1) = 0,4991 5057 9235 6045 5998 2993 2981 6541a(3,o) = 0,2495 7528 9617 8022 7999 1496 6490 8271a(5,2) = 0.7487 2586 8853 4068 3997 4489 9472 4812a(4, 0) = 0.2066 1891 1634 0060 2426 5567 1039 3185a(4,2) = 0.17707880377986347040380997288319 $a(4,3) = -0.6819 7715 4138 6949 4669 3770 7681 5048 \cdot 10^{-1}$ $a(5, o) = 0.1092\ 7823\ 1526\ 6640\ 8227\ 9038\ 9092\ 6157$ $a(5,3) = 0.40215962642367995421990563690087 \cdot 10^{-2}$ a(5,4) = 0.3921 4118 1690 7898 0444 3923 3017 4325 $a(6, o) = 0.9889 9281 4091 6466 5304 8447 6543 4355 \cdot 10^{-1}$ a (6,3) = 0.3513 8370 2279 6396 6951 2044 8735 6703 · 10~2 a(6, 4) = 0.1247 6099 9831 6001 6621 5206 2387 2489 $a(6,5) = -0.55745546834989799643742901466348 \cdot 10^{-1}$ a(7, o) = -0.3680 6865 2862 4220 3724 1531 0108 0691 a (7,4) =-0.2227 3897 4694 7600 7645 0240 2094 4166 · 10+1 $a(7,5) = 0.1374 2908 2567 0291 0729 5656 9124 5744 \cdot 10^{+1}$ $a(7,6) = 0.20497390027111603002159354092206 \cdot 10^{11}$ $a(8, \circ) = 0.45467962641347150077351950603349 \cdot 10^{-1}$

TABLE 2.14 (cont.).

a(14,6) =-0.6557 0189 4497 4164 5138 0068 7998 5251 a (14,7) =-0.3908 6144 8804 3986 3435 0255 2024 1310 a(14,8) = 0.2679 4646 7128 5002 2936 5844 2327 1209a (14,9) =-0.1038 3022 9913 8249 0865 7698 5850 7427 · 10+1 $a(14, 10) = 0.1667 2327 3242 5867 1664 7273 4616 8501 \cdot 10^{+1}$ a (14, 11) = 0.4955 1925 8553 1597 7067 7329 6707 1441 $a(14, 12) = 0.11394001132397063228586738141784 \cdot 10^{+1}$ $a(14, 13) = 0.5133 6696 4246 5861 3688 1990 9719 1534 \cdot 10^{-1}$ a(15,0) = 0.1046 4847 3406 1481 0391 8730 0240 6755 · 10a (15,8) =-0.6716 3886 8449 9028 2237 7784 4617 8020 · 10-2 a(15,9) = 0.8182 8762 1894 2502 1265 3300 6524 8999 • 10a(15,10) =-0.4264 0342 8644 8334 7277 1421 3808 7561 · 10-2 $a(15, 11) = 0.2800 9029 4741 6893 6545 9763 3) 15 3703 \cdot 10^{-3}$ $a(15, 12) = -0.8783 5333 8762 3867 6639 0578 1314 5633 \cdot 10^{-2}$ $a(15, 13) = 0.1025 4505 1108 2555 8064 2177 6968 4009 \cdot 10^{-1}$ a(16,0) =-0.1353 6550 7861 7406 7080 4421 6888 9966 · 10+1 a (16,5) =-0.1839 6103 1448 4827 0375 0441 9898 8231 a (16,6) =-0.6557 0189 4497 4164 5138 0068 7998 5251 a (16,7) =-0.3908 6144 8804 3986 3435 0255 2024 1310 a(16,8) = 0.2746 6285 5812 9992 5758 9622 0773 2989a(16,9) =-0.1046 4851 7535 7191 5887 0351 8857 2678 · 10⁺¹ a (16, 10) = 0.1671 4967 6671 2315 5012 0044 8830 6588 . 10" a (16, 11) = 0.4952 3916 8258 4180 8131 1869 9074 0287 $a(16, 12) = 0.1148 1836 4662 7330 1905 2257 9595 4930 \cdot 10^{+1}$ $a(16, 13) = 0.4108 2191 3138 3305 5603 9813 2752 7525 \cdot 10^{-1}$ a(16,15) = 1 $h(o) = 0.3225 6083 5002 1624 9913 6129 0096 0247 \cdot 10^{-1}$ b(8) = 0.2598 3725 2837 1540 3018 8870 2317 1963 $b(9) = 0.92847805996577027788063714302190 \cdot 10^{-1}$ b(1o) = 0.1645 2339 5147 6434 2891 6477 3184 2800b(11) = 0.1766 5951 6378 6007 4367 0842 9839 7547 b(12) = 0.2392 0102 3203 5275 9374 1089 3332 0941

 $b(13) = 0.3948 4274 6042 0285 3746 7521 1882 9325 \cdot 10^{-3}$ $b(14) = 0.3072 6495 4758 6064 0406 3683 0552 2124 \cdot 10^{-1}$

with the truncation error

 $TE = b(14)(g_0 + g_{14} - g_{15} - g_{16})h$.

| X | 9 | 1 | 2 | 3 | 4 | 3 | • | •ıj 7 | | , | 10 | u't | 12 | 13 | 14 | 15 | 16 |
|------------|-------------------|----------------------------|---|-----------------|----------------------------|----------------------------|--------------------------|-------------------------|--------------------|-----------------|------------------------|-----------------|--------|------|-----|-----|----|
| | 0 | | | | | | | | | | | | | | | _ | |
| z | 4 | 4 | | | | | | | | | | | | | | | |
| 3 | i | 1 | à | | | | | | | | | | L K./Z | | | | |
| 4 | 1 | <u></u> | 0 | 1 | | | | | | | | | | | | | |
| 5 | 22 | 4 94 | 0 | -94 - 14 133 | 22 <u>893</u> 00 | | | | | | | • | • | | | | |
| 6 | 6 <u>.1</u> 15 | <u>91</u> 150 | 0 | 0 | 212.32 | 43,32 | | | | | | | | | | | |
| 7 | * ₁₃ 1 | <u>927 - 147</u> 1230 | 0 | 0 | <u>=16248,7328</u> 9375 | -4193878 | <u>142685798</u> 9375 | | | | | | | | | | |
| 8 | 3 | 3 | 0 | 0 | 0 | 0 | 14 <u>,-1</u> 34 | 18-1 | | | | | | | | | |
| 9 | | 林 | 0 | 0 | 0 | 0 | 111-21 | 11,21 | 734 | | | | | | | | |
| 10 | | | 0 | 0 | 0 | 0 | 2661 | 2 <u>46 1</u> 864 | 냙 | 커 | | | | | | | |
| 11 | | <u>5034 - 271</u> 61440 | 0 | 0 | 0 | 0 | 0 | 7859 - 1626 10240 | -2232.413 | =394,271 960 | <u>517-513</u> 3120 | | | | | | |
| 12 | 5 | 403 | 0 | 0 | 0 | 0 | -1347-2334 | 134921 -40538 | -9710-9710-9 | 405 | 43 | =24424 | | | | | |
| 13 | i | 103680 | 0 | 0 | 0 | 0 | 13434 | -231278, 40717 49120 | 19472168 | 403 | =1113, 343 | 1811 | 144 | | | | |
| 13 | 1 | 1296 | 0 | 0 | 0 | 0 | 864 | 364 | - <u>299</u> 48 | 114 | -4 | 1053 | 藏 | ų | | | |
| 15 | | 318400 | 0 | 0 | 0 | 0 | = 11111 | 3+3600 | 57600 | 2075 | -1797-542 5400 | 347 | 1000 | 103 | 0 | | |
| 16 | 1 | 279600 | 0 | 0 | 0 | 0 | 7436 | 186400 | #3200 | -132192.121401 | 5825 | -169984 9047 | 30240 | 1123 | 0 | 333 | |
| б, | | 101 | 0 | 0 | 0 | 0 | 0 | 0 | -22 | 74 103 | -201 240 | 1924 | 7360 | Ħ | 283 | | |
| <i>b</i> , | | អ | 0 | 0 | 0 | 0 | 0 | 0 | ·120 | 111 111 | 9 <u>3</u> 2=0 | -2048 4823 | ain a | *** | 0 | * | 썘 |

with the truncation error

 $\mathrm{TE} \ = \ \left(\begin{array}{c} \frac{-7}{409} g_1 + \frac{43}{210} g_8 - \frac{14}{23} g_9 + \frac{14}{10} g_{10} - \frac{1024}{973} g_{11} - \frac{21}{3400} g_{12} - \frac{1}{12} g_{11} - \frac{9}{100} g_{14} + \frac{9}{23} g_{11} + \frac{211}{4100} g_{14} \right) \mathbf{h} \quad .$

TABLE 2.15: **RK-coefficients** °F, order 8(9) by VERNER /VE78/.

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TABLE 2.16: RK-coefficients of order 10 by CURTIS /CU75/.

| a2. | = +0.14525 18960 31615 05176 | $a_{11,2} = 0$ |
|---------------------------|---------------------------------------|---------------------------------------------------------------------|
| ¢2 | = +0.14525 18960 31615 05176 | $a_{11,1} = 0$ |
| a3. | = +0.07262 59480 15807 52588 | $a_{11,4} = 0$ |
| <i>a</i> ₃ , | ≠ +0.07262 59480 15807 52588 | $a_{11,3} = 0$ |
| C, | = +0.14525 18960 31615 05176 | $a_{11.6} = +0.39460\ 08170\ 28556\ 18607$ |
| 94.1 | = +0.05446 94610 11855 64441 | $a_{117} = +0.34430 11367 96333 34877$ |
| GA .7 | = 0 | $a_{11} = -0.07946\ 68266\ 42926\ 61291$ |
| <i>Q</i> ₄ , 3 | +0.16340 83830 35566 93323 | $a_{11} = -0.39152 18947 89596 61238$ |
| E4 | = +0·21787 78440 47422 57764 | $a_{11,10} = 0$ |
| 84.1 | = + 0·54469 46101 18556 44411 | $c_{11} = +0.35738 42417 59677 45184$ |
| <i>a</i> . , | = 0 | $a_{121} = +0.03210.00687.79632.09213$ |
| <i>a</i> ., | = - 2·04260 47879 44586 66540 | $a_{112} = 0$ |
| | = +2.04260 47879 44586 66540 | $a_{12,3} = 0$ |
| c | = +0·54469 46101 18556 44411 | $a_{124} = 0$ |
| α, , | = +0.06536 33532 14226 77329 | $a_{115} = 0$ |
| -0,1 Q4 7 | = 0 | $a_{114} = 0$ |
| -0,4 Gr 3 | = 0 | $a_{112} = 0$ |
| -0.J | = +0·32681 67660 71133 86646 | $a_{1,1} = -0.00018463759975120501$ |
| - 0.4 04 6 | = +0.26145 34128 56907 09317 | $a_{110} = +0.15608940253132198608$ |
| ~••.> C | = +0.65363 35321 42267 73293 | $a_{11,0} = +0.19344968576545602528$ |
| a | = +0.08233 70775 74827 16585 | $q_{11,10} = +0.26116 12387 63663 64969$ |
| 7 | ⇒ 0 | $c_{12} = \pm 0.64261 57582 40322 54816$ |
| -7.2 (7- x | = 0 | $a_{11} = \pm 0.04423749328524996327$ |
| s | = +0.21191719632028035617 | $a_{11,1} = 0$ |
| -7,4 0- / | = -0.03997 34350 80542 18312 | $a_{13,1} = 0$ |
| -1.3 //- / | = +0.02037 (-531, 75960, 06198) | |
| G- | = +0.27465949199052540088 | $a_{13,1} = 0$ |
| C7 | = +0.08595305779007343812 | $a_{13,3} = 0$ |
| 48,1 | | $a_{13,6} = 0$ |
| 48.2 | = 0 | $a_{13,7} = 0$ $a_{13,7} = \pm 0.00464.07744.34539.03964$ |
| 46.3 | = 0 | $a_{13,8} = \pm 0.04704 \ 66028 \ 26151 \ 36532$ |
| u 8.1 | 0 0 | $a_{13,9} = \pm 0.08620$ 74994 80114 88160 |
| 48,5 | | $a_{13,10} = +0.00020140014 00100$ |
| a 8,6 | = +0.2911/ 094/8 05885 09003 | $a_{13,11} = -0.03858 07017 43966 71537$ |
| a _{8,7} | $\approx +0.39644 / 5145 14/02 41049$ | $a_{13,12} = -0.03030.02017.43500.21552$ |
| C 8 | ≈ +0.77337 73201 10000 94484 | |
| a9,1 | $\approx +0.03012 09348 30009 07330$ | |
| a9,2 | = 0 - | $u_{14,2} = 0$ |
| a _{9,3} | = 0 | a _{14,3} - 0 |
| a9.4 | <i>≈</i> 0 | $a_{14,4} = 0$ |
| a9.5 | | $a_{14,5} = 0$ |
| 29.6 | = + 0.137/4 04820 82444 20890 | $a_{14,6} = 0$ |
| a9,7 | = +0.39510 98495 81567 43999 | a - ± 0.31978 56784 11636 70673 |
| a9.8 | | |
| Cg | = +0.58018 31400 82995 70863 | $a_{14,9} = -0.11171 77912 33452 87347$ |
| a10,1 | $\approx +0.0/233$ 14442 23379 48078 | |
| a10.2 | ≈ U | |
| a10,3 | = 0 | (14,12) = -0.43390 14298 65722 07269 |
| a10,4 | ≈ 0 | (14,13) = +0.33233 13400 00130 30384 |
| a10.5 | = 0 | $v_{14} = + 0.00232 / 0019 04/32 34043 = 0.002634 26423 5708 05923$ |
| a10.6 | $= +0.22002\ 76284\ 68999\ 81021$ | $a_{15,1} = +0.02024 \ 30432 \ 3/981 \ 03892$ |
| a10.7 | = +0.08789533425436734013 | $a_{13,2} = 0$ |
| a10,8 | | $a_{13,1} = 0$ $a_{13,1} = 0$ |
| a10,9 | = -0.21832 82289 48875 46891 | 115,4 ~ U |
| c10 | = +0.11747 23380 35267 65357 | $q_{11} = 0$ |
| a11.1 | = +0.08947 10093 67311 14229 | (1, 1, 2, 1) = 0 (1, 1, 2, 1) = 0 |
| | | ··· • • • • • • • • • • • • • • • • • • |

.

 $a_{15,0} = +0.04863 \ 13942 \ 38672 \ 66107$ $a_{15,2} = +0.04274 38253 83464 78868$ a11,10 = -0.15575 14733 74349 19785 $a_{15,11} = +0.13260 47194 91765 23318$ $a_{15,12} = -0.09402\,96215\,29465\,15652$ $a_{15,13} = +0.36891 19544 21896 67414$ $a_{15,14} = -0.01197\ 02001\ 30288\ 60976$ $c_{15} = +0.35738 42417 59677 45184$ $a_{16,1} = +0.10284$ 18616 86822 30957 $a_{16,2} =$ ٥ $a_{16,3} =$ 0 n a16.4 = 0 $a_{16,5} =$ a_{16,6} = 0 a_{16,7} = 0 $a_{16,8} = -1.29708\ 67206\ 53005\ 11984$ $a_{16,9} = -3.30609\ 69033\ 14255\ 58655$ $a_{16,10} = -0.06747\ 08496\ 92334\ 33385$ $a_{16,11} = -3.59679 \ 15480 \ 63726 \ 08732$ $a_{16,12} = +4.00369$ 56199 26740 87775 $a_{16,13} = +0.04100574882612781166$ $a_{16,14} = +0.26978 32108 90450 67539$ $a_{16,15} = +4.49273533863350200133$ $c_{16} = +6.64261 57582 40322 5481\vec{6}$ $a_{171} = +0.00876\ 60933\ 97736\ 46361$ 0 $a_{17,2} =$ n a17.3 = a17,4 = 0 a17,5 = 0 0 a_{17,6} = a17,7 == 0 $a_{17,8} = +0.58404 29244 96019 59632$ $a_{17,9} = +1.29877 96899 66251 57393$ $a_{17,10} = -0.05854751882306637183$ $a_{17,11} = +0.96649 29364 08446 17558$ $a_{17,12} = -1.41862\ 48359\ 70972\ 65394$ $a_{17,13} = +0.32460 19941 17747 10444$ $a_{17,14} = -0.05497 11264 10616 89342$ $a_{17,15} = -0.91544 14072 48110 49093$ $a_{17,16} = +0.14742\ 89120\ 31297\ 84267$ $c_{17} = +0.88252\ 76619\ 64732\ 34643$ $a_{18,1} = +0.10173\ 66974\ 11157\ 66388$ $a_{13,2} = 0$ 0 $a_{18,3} =$ ۵ a18.4 = 0 a13.5 = a18.6 = 0 $a_{1\,8.7} = 0$

 $a_{18,8} = -1.69621\ 75532\ 09432\ 81071$ $a_{18,9} = -3.82523584621162425452$ $a_{15,10} = -0.05854751882306637183$ $a_{18,11} = -2.52076\ 77892\ 27152\ 29120$ $a_{18,12} = +5.06895 15710 79828 19146$ a18.13 = +0.03221 83852 50196 89969 $a_{1+,14} = +0.09661 35792 25014 27296$ $a_{10,15} = +3.44722703652775671816$ a18,16 = -0.20173 27870 73975 92774 $a_{1b,17} = +0.55575 42250 51297 90987$ $= +1.00000\ 00000\ 00000\ 00000$ C1 8 = +0·03333 33333 33333 33333 b. b2 0 b3 0 ---- b_4 0 = b 5 = 0 b₆ 0 = b, ≓ n δ. 0 = b. -----0 610 = 0 b11 0 = $b_{12} = +0.23119\ 09904\ 31452\ 64709$ b13 = +0.18923747814892349016614 = +0.03153957969148724836= +0.27742918851774317651b15 = +0.04623 **8**1980 86290 52942 b16 = +0.15769 78984 57436 24180 b17 b18

TABLE 2.17: RK-coefficients of order 10 by HAIRER /HA78/.

| A(11, 1) - 2-34065736913354493717-002 |
|-------------------------------------------------------------------------|
| A(11, 2) = 0.0000000000000000000000000000000000 |
| A(11, 3) = 0.0000000000000000000000000000000000 |
| A(11, 4) = 0.0000000000000000000000000000000000 |
| A(11, 5) = 0.0000000000000000000000000000000000 |
| A(11, 6) = 9.44931301894961802240 - 002 |
| A(11, 7) = -2.72872055901956419006-001 |
| A(11, 8) = 2.24072046115592207410 = 001 |
| A(11, 0) = 6.0438(44)075(350054)6 - 001 |
| |
| A(12, 1) = A(44)(25)(32)(25)(35)(35)(35)(35)(35)(35)(35)(35)(35)(3 |
| |
| A(12, 2) = 0.0000000000000000000000000000000000 |
| A(12, 3) = 0.0000000000000000000000000000000000 |
| (12, 3) = 0.0000000000000000000000000000000000 |
| A(12, 5) = 0.0000000000000000000000000000000000 |
| A(12, 0) = -1.18799007180441007723 - 003 |
| A(12, 7) = 7.2030049909281134803-002 |
| A(12, 0) = 1.93209029870479240397 - 002 |
| X(12, 5) = -1.62205240586643050412 - 002 |
| A(12,10) = -2373326340640630426333-004 |
| A(12,11) = 4.33207837134829383300 - 003 |
| $\mathcal{A}(13, 1) = 1^{-78401080400430429292 - 001}$ |
| A(13, 2) = 0.0000000000000000000000000000000000 |
| A(13, 3) = 0.0000000000000000000000000000000000 |
| A(13, 4) = 1.10154439538638507040 - 001 |
| A(13, 5) = 5.25186129370448772884 - 001 |
| A(13, 6) = -4.89148591820436212803 - 001 |
| A(13, 7) = 9.32443612635135733038 - 001 |
| $\mathcal{A}(13, 8) = -7.74475053439839525409 - 001$ |
| A(13, 9) = -1.05490217813935824270 + 000 |
| A(13,10) = 1.31046712034157154509 - 001 |
| $\mathcal{A}(13,11) = 5 \cdot 870 \cdot 49777599 \cdot 487392267 - 001$ |
| A(13,12) = 6.20898052074878791881 - 001 |
| $\mathcal{A}(14, 1) = 1.30220806600497793496 - 001$ |
| A(14, 2) = 0.0000000000000000000000000000000000 |
| A(14, 3) = 0.0000000000000000000000000000000000 |
| A(14, 4) = 6.96088703288076908079 - 001 |
| A(14, 5) = 2.50497721570339375352 - 001 |
| A(14, 6)7.58948987129607342662-001 |
| A(14, 7) = -1.71517208463488383577 - 001 |
| A(14, 8) = -3.70217673678906704688 - 001 |
| A(14, 9) = 1.2498[008574747347802 - 001] |
| A(14,10) = 3-35310924837267073965-003 |
| $\mathcal{A}(14,11) = -6.63254613676153581907 - 003$ |
| $A(14,12) = 4 \cdot 29116573121617904714 - 001$ |
| $\mathcal{A}(14,13) = -3.71778567824697893108 - 002$ |
| A(15, 1) = 2.49297267609681978013 - 001 |
| A(15, 2) = 2.77211832531930184738 - 001 |
| A(15, 3) = 0.0000000000000000000000000000000000 |
| A(15, 4) = 0.0000000000000000000000000000000000 |
| A(15, 5) = 0.0000000000000000000000000000000000 |
| A(15, 6) = -1.45940595936085218185 - 001 |
| A(15, 7) = -7.99015893511029475358 - 001 |
| A(15, 8) = 0.0000000000000000000000000000000000 |
| A(15, 9) = 0.0000000000000000000000000000000000 |
| $\mathcal{A}(15,10) = 0.000000000000000000000000000000000$ |
| $\mathcal{A}(15,11) = 0.0000000000000000000000000000000000$ |
| $A(15,12) \Rightarrow 0.0000000000000000000000000000000000$ |
| A(15,13) = 1.45940595936085218185-001 |
| A(15,14) = 7.99015893511029475358 - 001 |
| A(16, 1) = 5.00000000000000000000000000000000000 |
| A(16, 2) = 0.0000000000000000000000000000000000 |

| C(1) = 0.0000000000000000000000000000000000 |
|----------------------------------------------------------------------------------|
| C(2) = 5.00000000000000000000000000000000000 |
| $C(3) = 5 \cdot 26509100141612162751 - 001$ |
| C(4) = 7.89763650212418244126-001 |
| C(5) = 3.93923570125671611283 - 001 |
| C(6) = 7.66653986253548800000-001 |
| $C(7) = 2 \cdot 89763650212418244126 - 001$ |
| C(8) = 1.08477689219566212940 - 001 |
| C(9) = 3.57384241759677451843-001 |
| C(10) = 8.8232/661964/32346426-001 |
| C(12) = 0.42013738240322340157001 C(12) = 1.17472338035267653574001 |
| C(12) = 7.66653986253548800000 - 001 |
| C(14) = 2.89763650212418244126-001 |
| C(15) = 5.26509100141612162751 - 001 |
| C(16) = 5.00000000000000000000000000000000000 |
| C(17) = 1.00000000000000000000000000000000000 |
| A(2, 1) = 5.00000000000000000000000000000000000 |
| A(3, 1) = 2.49297267609681978013 - 001 |
| A(3, 2) = 2.77211832531930184738-001 |
| $A(4, 1) = \frac{1.97440912553104561032 - 001}{100}$ |
| A(4, 2) = 0.0000000000000000000000000000000000 |
| A(4, 3) = 5.92322737659313683095 - 001 |
| A(5, 1) = 1.97320548628702140900 - 001 |
| A(5, 2) = 0.0000000000000000000000000000000000 |
| A(5, 3) = 2.95083334092671853711-001 |
| A(5, 4) = -9.84803125957023833277-002 |
| A(0, 1) = 0.0000000000000000000000000000000000 |
| A(6, 2) = 0.0000000000000000000000000000000000 |
| A(6, 4) = 1.10154439538638507040 = 001 |
| A(6, 5) = 5.25186129370448772884 - 001 |
| A(7, 1) = 1.34200341846322406193 - 001 |
| A(7, 2) = 0.0000000000000000000000000000000000 |
| A(7, 3) = 0.0000000000000000000000000000000000 |
| A(7, 4) = 6.96088703288076908079 - 001 |
| A(7, 5) = 2.50497721570339375352-001 |
| A(7, 6) = -7.91023116492320445498-001 |
| $A(8, 1) = 7 \cdot 22182741896621454448 - 002$ |
| A(B, 2) = 0.0000000000000000000000000000000000 |
| $A(8, 3) \approx 0.0000000000000000000000000000000000$ |
| A(8, 4) = 0.0000000000000000000000000000000000 |
| $A(8, 5) \Rightarrow -5.85363229364550369120 - 002$ |
| A(8,0) = 5.04/35/0005/44945/925 = 0.05 |
| A(0, 1) = 3.12550081251656170620 - 002 |
| A(9, 7) = 0.0000000000000000000000000000000000 |
| A(9, 1) = 0.0000000000000000000000000000000000 |
| A(9, 4) = 0.0000000000000000000000000000000000 |
| A(9,5) = 0.0000000000000000000000000000000000 |
| A(9, 6) = 1.09123821542419946873 - 004 |
| A(9,7) = 1.56725758630995015164 - 001 |
| A(9, 8) = 1.69294351171974399670 - 001 |
| A(10, 1) = 1.19066044146750321445 - 002 |
| A(10, 2) = 0.0000000000000000000000000000000000 |
| $\mathcal{A}(10, 3) = 0.0000000000000000000000000000000000$ |
| A(10, 4) = 0.0000000000000000000000000000000000 |
| A(10, 5) = 0.0000000000000000000000000000000000 |
| A(10, 0) = 2.8343/082024606548112 - 001 |
| A(10, 1) = -9.1210(2)(0.00131000-000) $A(10, 0) = -2.4444533204034034034037-001$ |
| A(10, 0) = 2.04040333949743004037-001 $A(10, 0) = 7.38840800146360076388-001$ |
| 1.200430031402030/0300-001 |

TABLE 2.17 (cont.).

| A(16, 3) 8-07097076095341093251-001 |
|----------------------------------------------------|
| A(16, 4) = 0.0000000000000000000000000000000000 |
| A(16, 5) = 0.0000000000000000000000000000000000 |
| A(16, 6) = 0.0000000000000000000000000000000000 |
| A(16, 7) = 0.0000000000000000000000000000000000 |
| A(16, 8) = 0.0000000000000000000000000000000000 |
| A(16, 9) = 0.0000000000000000000000000000000000 |
| A(16,10) = 0.000000000000000000000000000000000 |
| A(16,11) = 0.0000000000000000000000000000000000 |
| A(16,12) - 0-000000000000000000000000000000000 |
| A(16,13) = 0.0000000000000000000000000000000000 |
| A(16,14) = 0.0000000000000000000000000000000000 |
| A(16,15) - 8-07097076095341093251-001 |
| A(17, 1) = 5.73207954320575412321 - 602 |
| A(17, 2) = -5.000000000000000000000000000000000000 |
| A(17, 3) = -8.97470163394855120846-001 |
| A(17, 4) = 0.0000000000000000000000000000000000 |
| A(17, 5) = 0.0000000000000000000000000000000000 |
| A(17, 6) = -1.03991004922695343354 + 000 |
| A(17, 7) = -4.07357014288385809022 - 001 |
| A(17, 8) = -1.82830236640741849663 - 001 |
| A(17, 9) = -3.33659270649225021137 - 001 |
| A(17,10) = 3.95648542376057924001 - 001 |
| |

| A(17,11) = | 6-95057049459982281780-001 |
|-----------------|------------------------------------------|
| A(17.12) = | 2.71487376457383239111-001 |
| A(17.13) m | 5-85423734866589756811-001 |
| A(17.14) - | 9-58819077713235370479-001 |
| A(17,17) | 9.07/701/220/#EE19/306 001 |
| A(17,15) = | 8.97470103339653184200-001 |
| A(17,16) 🖛 | 5-000000000000000000-001 |
| B(() = | 3-3333333333333333333333333333-002 |
| B(2) = | -3-33333333333333333333333-002 |
| R(3) - | |
| | 0.0000000000000000000000000000000000000 |
| | |
| B(5) = | 0-0000000000000000000000000000000000000 |
| B(6) 🖛 | -1-300000000000000000000000000000000000 |
| B(T) = | -1.8000000000000000000000000000000000000 |
| R(8) = | 0-0000000000000000000000000000000000000 |
| | 7.77470189517743176508-001 |
| | 2.77429100317743170300-001 |
| $B(10) \approx$ | 1-89237478148923490136-001 |
| B(11) == | 2-77429188517743176508-001 |
| B(12) = | 1-89237478148923490158-001 |
| B(13) 🛥 | 1-3000000000000000000000000000000000000 |
| B(14) | 1,8000000000000000000000000000000000000 |
| | 1 2000000000000000000000000000000000000 |
| <i>B</i> (15) ≈ | 1-2000000000000000000000000000000000000 |
| B(16) ≈ | 3-3333333333333333333333333333 |
| B(17) ⇒ | 3-33333333333333333333333333333 |
| | |

4

we take here over the formulae and the notations from /KA81/. Given the initial value problem

$$y'(x) = f(y(x)), y(x_0) = y_c$$
 (autonomeous system) (2.8)

then the approximate solution y_1 of the exact solution $y(x_1 + h)$ reads

$$y_1 = y_0 + h \sum_{i=1}^{S} m_i k_i$$
, with (2:9)

$$Ek_{i} = f(y_{0} + h \sum_{j=1}^{i-1} a_{ij}k_{j}) + \sum_{j=1}^{i-1} c_{ij}k_{j}, \quad (i=1,2,3,\ldots,s), \quad (2.10)$$

and

$$E = I - \gamma_{nf}'(y_{0}), f' = \partial f / \partial y, I is the unit matrix. (2.11)$$

The coefficients a_{ij} , c_{ij} , m_i and γ are constant.

Given the initial value problem

$$y'(x) = f(x;y(x)), y(x_0)=y_0$$
 (non-autonomeous system) (2.12)
then by putting $x'=1$, the differential equation
becomes autonomeous and the foregoing formalism applies.
However, if one leaves (2.12) non-autonomeous then the

following formalism is valid

$$y_{1} = y_{0} + h \sum_{i=1}^{s} m_{i}k_{i} , \qquad (2.13)$$

$$Ek_{i} = f(x_{0} + A_{i}h, y_{0} + \sum_{j=1}^{i-1} a_{ij}k_{j}) + B_{i}hr_{x}(x_{0}, y_{0}) + \sum_{j=1}^{i-1} c_{ij}k_{j} , \qquad (2.14)$$

$$(i=1,2,...,s),$$

$$E = I - \gamma hf_{y}(x_{0}, y_{0}) , \qquad (2.15)$$

where

$$B_{1} = \gamma, \quad B_{i} = \gamma + \sum_{j=1}^{i-1} c_{ij} B_{j}, \quad (i=2,s),$$

$$A_{i} = \sum_{j=1}^{i-1} a_{ij} B_{j} / \gamma \quad (i=1,s) \quad .$$
(2.16)

We will now give the tables of these RUNGE-KUTTA processes of the orders 4, 5 and 6.

TABLE 2.18: RK - coefficients of order 4 by GOTTWALD-

WANNER /GO81/.

| γ = "395 | |
|------------------------------|------------------------------|
| a ₂₁ == 438 | $c_{21} = -1.94347441894707$ |
| a31 =.938948678483428 | $c_{31} = .416957530989189$ |
| $a_{32} = .0730795420615381$ | $c_{32} = 1.32396782072923$ |
| $b_1 = .729044879960308$ | $c_{41} = 1.5(951325778448)$ |
| $b_2 = .0541069773272405$ | $c_{42} = 1.35370815030093$ |
| $b_3 = .281599362440017$ | $c_{43} =854151495257539$ |
| $b_4 = e_4 = .25$ | $e_1 =0190858871999474$ |
| e, =.255608791716455 | $e_3 =0863816280897592$ |

with the error estimator

 $EST = Max\left(U_{round}, Max_{i=1, w}\left(\left|\sum_{j=1}^{4} e_{j} k_{j}(i)\right| / Max(1, |y_{i}|, |y_{arw}(i)|)\right)\right)$

TABLE 2.19: RK-coefficients of order 5 by KAPS-WANNER /KA81/.

v = 0.141127125787

| | r — 4 |)• · · · · · · · · · · · · · · · · · · · |
|------------------|-------|------------------------------------------|
| a21 | - | 0.28225425157410630D+00 |
| c21 | - | -0.81524951688460885D+00 |
| a31 | - | 0.57116380169300584D + 00 |
| c31 | - | 0.81127189717323099D+01 |
| a32 | 35 | 0.12386230035678339D+01 |
| c32 | = | 0.64300627424554704D+00 |
| a41 | | 0.72285966684392441D+00 |
| C41 | - | 0.18891319022399990D - 01 |
| a42 | - | 0.97672836707474073D+00 |
| C42 | - | -0.37493862667874616D +01 |
| a43 | - | -0.32856006264202144D -01 |
| C43 | - | 0.95094153717403742D - 01 |
| ⁽¹ 51 | = | 0.67849717523250110D + 00 |
| c 51 | = | 0.53507619725099805D + 01 |
| a,2 | = | 0.20208927497707465D+01 |
| c 3 2 | * - | -0.25460873945213962D+01 |
| a 5 3 | - | -0.10701369811124179D + 00 |
| | | |

 $c_{11} = 0.41864844423231233D + 00$ $a_{54} = 0.66019768386713535D + 00$ $c_{54} = -0.33062805583808154D + 01$ $m_1 =$ 0.77900694405566295D+00 0.37121621947171690D+01 $m_2 =$ $m_3 = -0.73417673328703555D + 00$ $m_{\star} = 0.24040545624571883D + 01$ $m_s = 0.59299247626627483D + 00$ $B_1 = 0.14112712578705315D + 00$ $A_2 = 0.28225425157410630D + 00$ $B_2 = 0.26073304669844646D - 01$ $B_3 = 0.13028171350787572D + 01$ $B_{\star} = 0.16992460579297673D + 00$ $A_{1} = 0.85887287421294685D + 00$ $B_5 = 0.81348381758071946D + 00$

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with the truncation error

$$TE = \max(|y_{2,i} - \hat{y}_{2,i}| / (2^{p} - 1) \max(1, |y_{2,i}|)),$$

i=1,n

where

$$y_1 = y_0 + h \sum_{i=1}^{s} m_i k_i$$
, $y_2 \approx y_1 + h \sum_{i=1}^{s} m_i k_i$, $\hat{y}_2 = y_0 + 2h \sum_{i=1}^{s} m_i k_i$.

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TABLE 2.20: RK-coefficients of order 6 by KAPS-WANNER /KA81/.

γ=0**.**17315586842719120

| = 0.34631173685438241D + 000 | a, 3 | = -(| 0.54599770789200043D+000 |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| = -0.63453397891179372D +000 | C 63 | = (| 0.24468706426428219D+001 |
| = 0.51484422823733024D+000 | a | = - (| 0.42431494939094088D+000 |
| = 0.36437911365480913D + 001 | CAA | - (| 0.28555063127446144D+001 |
| = 0.61607853745814515D + 000 | a | = (| 0.27503664994042264D + 001 |
| = 0.12945713592535053D + 001 | C | =(| 0.12600541876984773D + 002 |
| = 0.42083594880532555D + 000 | <i>m</i> , | =(| 0.67246858827422954D + 001 |
| = 0.69161953050956585D - 001 | <i>m</i> , | = -(| 0.12998203944959025D + 002 |
| = 0.12398256101276536D + 000 | <i>m</i> , | = −(| 0.41709683120954452D+001 |
| = -0.12905884218846234D + 000 | , m, | = -(| 0.20786455336141339D + 001 |
| = -0.43663557947609954D - 002 | <i>m</i> . | = (| 0.15638447165125274D + 002 |
| = -0.40532167899763093D - 001 | m, | - (| 0.10493031673621379D + 001 |
| = 0.44508808952624152D + 000 | A . | = (| 0.0000000000000000000000000000000000000 |
| 0.17583309748309236D + 001 | B. | - (| 0.17315586842719120D + 000 |
| 0.14790956438776313D + 000 | <u>.</u> | = (| 0.34631173685438241D+000 |
| = 0.17092158755220803D + 001 | B | - 0 | .63282586262158533D - 001 |
| = -0.10863189236472590D - 001 | A | = 0 | .74000000000000000D+000 |
| ≈ -0.54015868028686558D - 001 | В, | = 0 | .88602351075795778D+000 |
| 0.16749655714649715D + 000 | Ă. | = 0 | 44380509942047506D+000 |
| = -0.14204573489819585D + 001 | B, | = 0 | .14105203545498545D+000 |
| = -0.78286965861140857D + 000 | A | = 0 | .5800000000000000D+000 |
| = 0.92366768689092273D+001 | <i>B</i> , | = 0 | .33756706706153310D+000 |
| = -0.16763611643856503D + 001 | A | = 0 | .82684413157280881D+000 |
| = 0.11681533450127634D+002 | ₿, s | = 0 | 82901025130889673D+000 |
| | = 0.34631173685438241D + 000 = -0.63453397891179372D + 000 = 0.51484422823733024D + 000 = 0.36437911365480913D + 001 = 0.61607853745814515D + 000 = 0.12945713592535053D + 001 = 0.42083594880532555D + 000 = 0.69161953050956585D - 001 = 0.12998256101276536D + 000 = -0.12905884218846234D + 000 = -0.43663557947609954D - 002 = -0.43663557947609954D - 002 = -0.44508808952624152D + 000 = 0.17583309748309236D + 001 = 0.17992158755220803D + 001 = -0.10863189236472590D - 001 = -0.5401586802868558D - 001 = -0.14204573489819585D + 001 = -0.78286965861140857D + 000 = 0.92366768689092273D + 001 = -0.16763611643856503D + 001 = -0.16763611643856503D + 001 = -0.1676361164385653D + 001 = -0.16763611643856502 + 002 = -0.16763611643856502 + 002 = -0.16763611643856502 + 002 = -0.16763611643856 | $ = 0.34631173685438241D +000 a_{63} a_{63}$ | $ = 0.34631173685438241D + 000 \qquad a_{6,3} = -0 \\ = -0.63453397891179372D + 000 \qquad c_{6,3} = 0 \\ = 0.51484422823733024D + 000 \qquad a_{6,4} = -0 \\ = 0.36437911365480913D + 001 \qquad c_{6,4} = 0 \\ = 0.61607853745814515D + 000 \qquad a_{5,5} = -0 \\ = 0.42083594800532555D + 001 \qquad c_{6,5} = -0 \\ = 0.42083594800532555D + 000 \qquad m_1 = -0 \\ = 0.69161953050956585D - 001 \qquad m_2 = -0 \\ = 0.12398256101276536D + 000 \qquad m_4 = -0 \\ = -0.43663557947609954D - 002 \qquad m_5 = 0 \\ = 0.4508808952624152D + 000 \qquad m_4 = -0 \\ = 0.17583309748309236D + 001 \qquad m_6 = 0 \\ = 0.17583309748309236D + 001 \qquad m_6 = 0 \\ = 0.17992158755220803D + 001 \qquad B_1 = 0 \\ = 0.17992158755220803D + 001 \qquad B_2 = 0 \\ = -0.401586802868558D - 001 \qquad B_3 = 0 \\ = -0.142045773489819585D + 001 \qquad B_4 = 0 \\ = 0.16749655714649715D + 000 \qquad A_4 = 0 \\ = 0.1778286965861140857D + 000 \qquad A_5 = 0 \\ = 0.9236676868092273D + 001 \qquad B_5 = 0 \\ = 0.16763611643856503D + 001 \qquad B_5 = 0 \\ = 0.16763611643856503D + 001 \qquad B_6 = 0 \\ = 0.16763611643856503D + 001 \qquad B_6 = 0 \\ = 0.16763611643856503D + 001 \qquad B_6 = 0 \\ = 0.16763611643856503D + 001 \qquad B_6 = 0 \\ = 0.16763611643856503D + 001 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ = 0.11681533450127634D + 002 \qquad B_6 = 0 \\ \end{bmatrix}$ |

with the same error estimator as for the process of

TABLE 2.19

2.2.3.5 Concluding remarks.

The derivation of a performant RUNGE-KUTTA method is centered on two main themes:

- the choice of optimal coefficients, i.e., they should permit economical computation, which is to say, there should be a minimum number of function evaluations (stages). In addition, the estimated error should be close to the true error and its computation should require little effort.
- the stability of the methods. THE FACT THAT ALL ERROR ESTIMATIONS OF AVAILABLE RUNGE-KUTTA PROCESSES ARE ONLY LOCALLY VALID RENDERS CONSIDERATIONS ON STABILITY PARTICU-LARLY IMPORTANT.

If the integration takes place outside or close to the boundary of the stability region the solution risks destabilisation. The knowledge of the stability region of a method is thus crucial. Moreover, knowing this region one can estimate, using a stiffness diagnostic of the system to be solved, prior to the integration, the total computational effort required for the solution.

Stability considerations assume thus a prominent position in numerical integration. Therefore, we will now explore this important field with a view to our needs.

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3.0 ON THE STABILITY OF THE METHODS.

A basic problem of the numerical solution of ordinary differential equations is the stability of the method applied. Approximately speaking, the question is, which step-size is permitted for the integration of a given system without risking destabilisation of the solution functions. This problem is nowadays well studied and the so-called stability regions are for the numerical methods well known /LA73/, and /HA76/.

FOR PRACTICAL CALCULATIONS THE FOLLOWING RULE IS HELPFUL,

 $h\lambda = \bar{h} \in \mathbb{R}$, (3.1)

where R is the stabilty region of the method considered, h is the step-size, λ is the maximal value of all λ_i , and λ_i are the eigenvalues of the matrix

$$\partial \mathbf{f}_{i} / \partial \mathbf{y}_{j} = \partial \mathbf{y}_{i} / \partial \mathbf{y}_{j}, \quad (i, j=1, 2, ..., n)$$
 (3.2)

(see (2.11)).

Note that λ can be complex.

Eq.(3.1) says simply that the step-size h must be chosen such that h does not lie outside the stability region. We give here for convenience stability regions which are relevant in the context of our work. The stability intervals for explicit RUNGE-KUTTA methods are /LA73,p139/ given in TABLE 3.1.

TABLE 3.1: Stability intervals $Re(\vec{h})$ of explicit RUNGE-

KUTTA methods.

| RK-order | · 1 | 2 | 3 | 4 | 7 | |
|-----------------------------------------|------|------|-------|-------|------|--|
| Interval $Re(\overline{h})$ of absolute | -2.0 | -2.0 | -2.51 | -2.78 | -5.× | |
| stability | | | x heu | value | | |

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The graphical representation of the corresponding stability regions in the \bar{h} -plane is given in FIG. 3.1 /LA73, p.227/.



FIG.3.1: Stability regions of explicit RUNGE-KUTTA methods of orders p: 1,2,3,4.

The stability values $Re(\bar{h})$ of the ADAM-BASHFORTH-MOULTON methods /LA73,p.107/, which are applied in the CODE GEAR, are listed in TABLE 3.2.

TABLE 3.2: Stability intervals $Re(\overline{h})$ of the ADAM-BASHFORTH-MOULTON methods.

| Order | 4 | 5 | 6 | 7 | 8 | |
|------------------------|------|------|------|------|------|--|
| Stability intervals | -1.3 | -1.0 | -0.7 | -0.5 | -0.4 | |

From TABLE 3.1 and TABLE 3.2 follows that the stability , interval $\operatorname{Re}(\overline{h})$ is shrinking with increasing order of the

ADAM-BASHFORTH-MOULTON methods, whereas it is extending with increasing order of explicit RUNGE-KUTTA methods. The implicit RUNGE-KUTTA process of the Rosenbrock type of order 4 published by GOTTWALD-WANNER /GO81/ is A-STABLE. The corresponding stability region is indicated in FIG.3.2.



FIG.3.2: Stability region of A-STABLE methods.

The implicit RUNGE-KUTTA process of the Rosenbrock type of order 6 published by KAPS-WANNER /KA81/ under the designation ROW6B is A($\alpha = 85.74^{\circ}$)-STABLE. The A(α)-STABILITY region is sketched in FIG.3.3. Note that several RUNGE-KUTTA processes of the Rosenbrock type of order 5 and 6 are published together with their stability regions in /KA81/.



FIG.5.3: $A(\alpha)$ -STABILITY region.

The so-called GEAR's method, which is used in the CODE GEAR, is STIFFLY-STABLE. The corresponding stability regions are sketched in FIG.3.4. For further details see /LA73,p.234/.



FIG.3.4: Stability regions R_1 and R_2 of STIFFLY-STABLE methods.

From the above considerations we can conclude the following with a view to practical computations:

- The step-size decreases when the order of the ADAM-BASHFORTH-MOULTON methods increases.
- Conversely, the step-size can increase when the order of the explicit RUNGE-KUTTA methods increases.
- If $\lambda = \max(\lambda_i)$ is very large and the path of integration is not very short then neither the ADAM-BASHFORTH-MOULTON methods nor the explicit RUNGE-KUTTA methods can successfully solve the system, because the number of steps required for the integration exceeds any tolerable computational time as well as any acceptable error propagation. In such a case METHODS WITH LARGE ABSOLUTE STABILITY REGION MUST BE USED.
- To solve such problems, the Code GEAR uses the GEAR's method, which is stiffly stable (see FIG. 3.4). We will in that case apply the implicit RUNGE-KUTTA methods of the Rosenbrock type of order 4 and 6. They are A-stable (see FIG. 3.2)

and $A(\alpha)$ -stable (see FIG.3.3), respectively.

- Generally speaking, any performant ODE-solver should thus apply two classes of methods, such with large stability regions for the integration of stiff problems, i.e., implicit methods, and such with smaller stability regions for the integration of non-stiff problems. Recall that the latter requires much less computational effort per step

than the former and is moreover numerically safer. STABILITY CONSIDERATIONS GIVE THUS A VALUABLE INSIGHT WITH REGARD TO APPLICABILITY OF THE VARIOUS NUMERICAL METHODS OF SOLUTION OF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS.

4.0 THE RUNGE-KUTTA SOLVER OSIRIS OF SYSTEMS OF ODES.

4.1 CRITERIA OF THE CHOICE OF RUNGE-KUTTA METHODS.

To make a choice among the variety of available RUNGE-KUTTA processes we applied the following criteria:

- The RUNGE-KUTTA solver should permit integration of systems of ordinary differential equations of the types characterized in TABLE 4.1.
- The RUNGE-KUTTA solver should enable an automatic optimization of the computational time of an integration.
- TABLE 4.1: Characteristics of systems of ODEs which we wish to integrate.

| W | 10 ² -10 ⁴ | 10 ⁴ -10 ⁶ | 10 ⁶ -10 ⁷ | 10 ⁸ -10 ²⁰ |
|-------------------------------------|----------------------------------|----------------------------------|----------------------------------|-----------------------------------|
| RUNGE-KUTTA method applicable | explicit | explicit (implicit) | implicit (explicit) | implicit |

W = Path of integration $x |\text{Re}(\lambda_{\text{max}})|$. $|\text{Re}(\lambda_{\text{max}})/\text{Re}(\lambda_{\text{min}})|$: $10^6 - 10^{18}$. Number of ODEs : 10-100. λ_i are eigenvalues of the Jacobian matrix (3.2).

According to the first criterion, we have to use both explicit as well as implicit RUNGE-AUTTA methods. The 2-nd criterion calls for RUNGE-AUTTA methods of low order (for low precision computation) and of high order (for high precision computation). Results of performance comparison calculations using the various methods which are published in /SH76/, /EN76/, /FE69/, /FE70/, /VE78/, /G081/, /KA81/ and /HA78/ together with our own experience have led us to incorporate in our RK-solver code the methods which we list in TABLE 4.2.

| TABLE 4 | 4.2: | RUNGE- | -KUTTA | methods | applied | in | our | ODE-solver | code. |
|---------|------|--------|--------|---------|---------|----|-----|------------|-------|
|---------|------|--------|--------|---------|---------|----|-----|------------|-------|

| Author(s) | Ref. | Order | Local error estimator |
|------------------|------------------|--------------|-----------------------|
| Explicit methods | | | |
| FEHLBERG | /FE70/ /FE69/ | 4(5) 7(8) | given given |
| VERNER | /ve78/ | 8(9) | given |
| HAIRER | /на78/ | 10 | by step-size division |

Implicit methods (of the Rosenbrock type):

| GOTTWALD-WANNER | /G081/ | 4 | given(by step-size division) |
|-----------------|--------|---|------------------------------|
| KAPS-WANNER | /KA81/ | 6 | given |

Comments on TABLE 4.2:

- We found that the FEHLBERG RK-processes are more efficient than those by VERNER. We have included the process 8(9) by VERNER in our RK-solver, because FEHLBERG's processes of orders > 4 fail when applied to solve problems of the kind y'=f(x) (see in 2.2.3.2.2).
- We have included HAIRER's process also, because this is the highest order of explicit RK-processes which is available at present.
- Among the implicit RUNGE-KUTTA processes, those of the Rosenbrock type are the most efficient and the safest, because they offer the advantage of linearizing a problem (see in 2.2.3.2.3).

Moreover, the application of RUNGE-KUTTA processes of low and high order is appropriate for integration with low and high precision.

4.2 DETERMINATION OF THE STIFFNESS OF A SYSTEM.

In addition to the integration methods listed in TABLE 4.2, a diagnosis of the difficulty(stiffness) of the problem is helpful and instructive. To make such a diagnosis, the eigenvalues of the matrix $\partial y'_i / \partial y_j$ must be determined (see 3.2). They give information about the stiffness and offer in principle a criterion to select dynamically the most appropriate integration method.

4.3 THE ERROR CONTROL.

we estimate the uncertainty caused by a single integration step (local error) and verify the total accumulated error (global error).

4.3.1 The local error.

An estimation of the local error is available for each RUNGE-KUTTA process mentioned in TABLE 4.2, except for the process by HAIRER. For this process we estimate the local error by step-size division.

4.3.2 The total accumulated error.

Essentially, we verify this kind of error with the aid of an additional integration imposing a different tolerance. Another possibility to verify this error is a supplementary integration using a code which is not based on RUNGE-KUTTA methods, but, for example, on the multistep methods. In other words, we can compare results obtained independently with the help of both codes, the RK-solver as well as the Code GEAR.

In some cases, conservation laws can be used to check the accuracy of the computed functions. This is of course the ideal way to determine the total accumulated error.

4.4 THE IMPLEMENTATION OF THE RUNGE-KUTTA SOLVER OSIRIS. The general structure of the program OSIRIS is schematized in the following FIGURE 4.1.



FIGURE 4.1: Scheme of the program OSIRIS.

والمتحريرين المركب والمتحين المستحد بكام الأ

<u>RKUN</u>: In this subroutine the appropriate algorithm for the integration is chosen. To this end the performance of the various algorithms is memorized: the integration step-sizes h_i (of i-th method) and the number of operations n_i required to perform one iteration $(n_i$ is constant for a given method) are stored and the efficiency $= h_i/n_i$ is determined for each method i.

when the integration starts, the efficiency of each explicit RUNGE-KUTTA method is evaluated with the constrain of maximal 50 iterations per step. Then the integration is continued with the most efficient method until it needs more than 50 iterations per integration step. Then the method previously memorized as the 2-nd most efficient method is applied, etc.. If all explicit RUNGE-KUTTA methods fail to integrate one step with maximal 50 iterations then if the number of iterations> N>50, and in any case if the estimated total number of integratio n steps is too high, then implicit methods are called for. The program is returning to explicit methods whenever they are judged to be enough efficient. The criterium for such a switch is based on the eigenvalues of the Jacobian matrix.

F5, F8, Hairer, V9, ROW4A: Designate the subroutines of the algorithm RUNGE-KUTTA-FEHLBERG 4(5), RUNGE-KUTTA-FEHLBERG 7(8), RUNGE-KUTTA-HAIRER (10), RUNGE-KUTTA-VERNER 8(9) and RUNGE-LUTTA-4 implicit of the Rosenbrock type, respectively. The latter subroutine is that developed by "ANNER. (DEC and SOL are subroutines of ROw4A solving a linear algebraic system; FAS and FDAS render a non-autonomeous system automatically autonomeous).

<u>PILOT:</u> This subroutine varies instantaneously the integration step-size in dependence on:

the ration R=local error/required precision,
the acceptance of the preceding step-sizes(R<1).
Furthermore, PILOT is estimating continuously the total number of integration stepsneeded. Firs number affects the choice of the algorithm to be used.

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Users of OSIRIS must furnish the subroutines FCT and FCD. FCT: FCT(T,Y,DY) defines the system of ODE to be solved, where

 $DY(I) = dY_{i}(t)/dt = f_{i}(t, Y_{1}(t), \dots, Y_{T}(t)).$

<u>FCD:</u> FCD(T,Y,dF) or DF(I,J) denotes the Jacobian of the system

dri /gr .

Users of OSIRIS must furthermore supply the following input data:

- the initial values,

- the precision to which the solution functions should be computed(common relative error for all unknowns),
- the maximal number N of iterations permitted per integration step,
- the upper bound of the integration.

The initialisation of the step-size is automatically done. For this purpose the eigenvalues of the Jacobian matrix are used.

The global error is estimated by means of two integration runs with different tolerance.

5.0 APPLICATION :.

We consider the following system of differential equations

$$dY_{i}(t)/dt = \sum_{j}^{J} (\sum_{k}^{K} b_{ijk}g_{k}(t) + c_{ij})y_{j}(t),$$
 (5.1)

where

b_ijk and c_ij are constants, i=1,2,3,...,I .
 j=1,2,3,...,J ,
 k=1,2,3,...,K .

 $g_k(t) = p_k(t).C.e^{\alpha t}$, where α and C are constants.

In the following we give a representative example of problems which we have solved with the aid of OSIRIS.

Input data:

 $\alpha = 0.3.10^6$.

 $C=0,43.10^9$ for $t \le 10^{-6}$; C=0 for $t > 10^{-6}$.

Values of $p_{k}(t)$, k=1,2,3,4:

 K=1
 K=2
 K=3
 K=4

 0.1000E
 00
 0.2000E
 00
 0.3000E
 00
 0.4000E
 00

 0.4000E
 00
 0.3000E
 00
 0.2000E
 00
 0.2000E
 00

They have to be interpolated (in log(t)) between $t=10^{-20}$ (values in first line) and $t=10^{-6}$ (values in 2-nd line).

Initial values $Y_i(t=t_0)$, $i=1,2,3,\ldots,13$:

I Y(I)

9 1.E 20 Y(1) =0 else.

13 1.E20

| v | Val alu | ues es c | of c | ij' | i,j= | 1,2 | ,3, | ,1 | 3: | c=1, | 1 4 7 8 10 5 4 8 8 12 | J 13 13 13 13 13 13 13 12 6 7 11 | C(1 1.48 2.31 4.95 4.33 1.4 7. 7. 7. 7. | J) 11E 06 05E 07 11F 05 22E 07 E 08 E 04 E 03 E 06 E 06 E-02 |
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| 1 | 2 | 6.2 | 230E | . 01 | 0,57 | E | 00 | 0.9 | E | -01 | 0.2 | 450) 70 | E=02 | |
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| 2 | 6 | 4.3 | OUOE | 00 | 0.16 | 10E | 00 | 0.04 | 25E | 00 | 0.2 | 4 : | E-02 | |
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| 6 | 4 | 0. | E | 00 | 0. | E | 00 | 0. | ε | 00 | 0.7 | 51 8 | E 00 | |
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| 7 | 4 | 0. | E | 00 | 0. | ε | 00 | 0. | £ | 00 | 0.66 | 53 E | 00 | |
| 7 | 6 | 0.5 | 060E | 00 | 0,19 | 7 E | 00 | 0.5 | Ë | 00 | 0.10 | 37 8 | 00 | |
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| 8 | 2 | 0. | ٤ | 00 | 0. | E | 00 | 0. | Ε | 00 | 0.10 |)5 E | 00 | |
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| 8 | 7 | 2.6 | 000E- | -08 | 1.4 | , E- | 0.7 | 1.2 | , E- | 03 | 1.48 | 6 E | -02 | |
| 8 | 9 | 0.2 | 300E | 00 | 0.002 | ιE | 00 | 0.001 | E | 00 | 0.00 | 01E | 00 | |
| 8 | 10 | 1.2 | 2005 | 00 | 0,163 | Ε | 00 | 0.019 |) E | 00 | 0.00 | 196 | 00 | |
| 9 | 7 | U. U. | <u>ک</u> | 00 | 0. | F | 00 | 0. | F | 00 | 0.00 | 94 E | 00 | |
| 9 | 8 | Ŭ. | Ē | 00 | υ, | Ē | ů0 | 0. | Ē | 00 | 0.13 | 2 2 | 00 | |
| 9 | 10 | 0. | E. | 00 | 0. | E | 00 | 0.090 | 17E | υŨ | 0.48 | 2 E | 00 | |
| 9 | 11 | 1.21 | 100E | 00 | 0.131 | 5£ | 00 | 0,004 | ITE | 0Ú | 1.38 | E | -03 | |
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| 10 | 8 | 0. | Ł | 00 | 0. | Ë | 00 | 0. | ε | 00 | <i>ü</i>.41 | E | 00 | |
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| 11 | 10 | 0. | F. | 40 | 9. | t. | 0.0 | 9. | t. | 00 | 0.93 | 1 E | 00 | |
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- the numbers on the scale are exponents, for example, -11 means 10^{-11} .
- the eigenvalues of the Jacobian matrix remain constant in the interval $t=10^{-0}$ to 10^{6} .

The calculations for this particular example have been carried out on a NITRA-125. Computing time: 216 minutes. This corresponds to about 1 minute on a CDC-7600.

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ACKNOWLEDGEMENTS

We are much indebted to Professor Gerhard WANNER for his program ROW4A (implicit RUNGE-KUTTA method of the Rosenbrock type of order 4). We are very grateful to Olivier BERSILLON for the program EIGENP (calculation of eigenvalues and eigenvectors of real matrices) and we thank Roger PERRIER and Denise COTTEN for computing assistance. <u>ANNEX 1</u>: An Algorithm to solve Systems of non-linear, coupled Ordinary Differential Equations.

We consider the system (1.2) which we repeat here for the sake of convenience

$$dY_{i}(t)/dt = \sum_{s=1}^{S} g_{is}(t) \prod_{j=1}^{I} Y_{j}^{r_{isj}}(t) , \qquad (A.1)$$

where i=1,2,3,...,I · r are integers. isj

$$Y_{i}(t) = \sum_{n=0}^{\infty} \frac{(t-t_{0})^{n}}{n!} \sum_{H,K} (a_{i,H,K} G^{H})_{n} \prod_{j=1}^{I} y_{j}^{k_{j}},$$
 (A.2)

where

$$K = k_1 k_2 k_3 \cdots k_1$$
, $H = \begin{pmatrix} h_{q11} h_{q12} \cdots h_{q18} \\ h_{q21} h_{q22} \cdots h_{q28} \\ \cdots \\ h_{q11} h_{q12} \cdots h_{q18} \end{pmatrix}$
(A.3)

with $q=0,1,2,3,\ldots,n-1$ for a term of order n.

If the g_{is} are constants, then q=0 for terms of any order.

$$(G^{H})_{n} = \prod_{q=0}^{n-1} \prod_{i=1}^{I} \prod_{s=1}^{S} g_{is}^{h_{qis}}$$
, here q symbolizes the (A.4)

number of derivations of g_{is} , for example, $g_{is}^{h_{3is}=7} = (\frac{d^3}{dt^3} g_{is})^7$ and $y_j = Y_j(t=t_0)$. (A.7)

Evidently, for the computation of the solution functions Y_i one has first to know the coefficients

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 $a_{i,H,K}$. By means of mathematical induction one can show that the following recurrence relation is valid

$$(a_{i,H,K})_{n+1} = \sum_{i=1}^{I} \sum_{s=1}^{S} ((k_{i}+1-r_{isi})a_{i,K_{1}}+D_{1}-r_{is1},k_{2}+D_{2}-r_{is2}),$$

$$(k_{3}+D_{3}-r_{is3})\cdots (k_{I}+D_{I}-r_{isI};H_{ois}) +$$

$$+ \sum_{q=1}^{n} \sum_{i=1}^{I} \sum_{s=1}^{S} (h_{q-1,is}+1)a_{i,H_{qis}},K)_{n}$$
(A.6)

- It permits calculation of the solution functions

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to any order of approximation and thus to any accuracy desired. - The coefficients $a_{i,H,K}$ have only to be computed once for a given system (A.1). They are neither dependent on the initial values nor on the g_{is} . They can, therefore, be stored on a permanent file. As the labels H,K are known automatically with the coefficients, the quantity G^{H} in (A.2) is also known and can equally be stored on a permanent file, if the g_{is} are constants. In this latter case the whole integration process is simply reduced to the formation of the initial value dependent part k_{j}^{j} in (A.2) and the summation of the power series. This renders the present method economical.

- If the g_{is} are constants, then only terms with H_{ois}; i.e. only the first two lines of (A.6) remain active. In this case (A.6) is substantially simpler.
- Finally, the recurrence relation (A.6) generates curiously in certain cases, i.e. for certain systems (A.1), number sequences which are known from other mathematical disciplines, for example, from combinatorial theory /SC76/, /DU79/, /SC05/.

To illustrate this algorithm we apply it to solve EULER's equations of motion in a force-free field. They read

 $dY_{1}(t)/dt = b_{1}Y_{2}Y_{3},$ $dY_{2}(t)/dt = b_{2}Y_{1}Y_{3},$ $dY_{3}(t)/dt = b_{3}Y_{1}Y_{2}, \text{ where } b_{1}, b_{2}, b_{3} \text{ are constants.}$ (A.1.1)

Comparing (A, 1, 1) with (A, 1) one obtains

$$b_1 = g_{11}, b_2 = g_{21}, b_3 = g_{31}, and$$

 $r_{112} = r_{113} = 1, r_{211} = r_{213} = 1, r_{311} = r_{312} = 1, and r_{isj} = 0$ else.

Eq.(2) becomes thus

$$Y_{i}(t) = \sum_{n=0}^{\infty} \frac{(t-t_{0})^{n}}{n!} \sum_{H,K}^{(a_{i},H,K} G^{H})_{n} y_{1}^{k_{1}} y_{2}^{k_{2}} y_{3}^{k_{3}}, \qquad (A.2.1)$$

where

$$H=h_{11}h_{21}h_{31}$$
, $K=k_1k_2k_3$, and (A.3.1)

$$(G^{H})_{n} = b_{1}^{h_{1}} b_{2}^{h_{2}} b_{3}^{h_{3}}.$$
 (A.4.1)

(A.6) becomes

$$(a_{1,H=0,100})=(a_{2,H=0,010})=(a_{3,H=0,001})=1$$
, and with
 $H_{011}=h_{11}-1,h_{21}h_{31}, H_{021}=h_{11}h_{21}-1,h_{31}, H_{031}=h_{11}h_{21}h_{31}-1.$
(A.C.1)

We can make the following concluding remarks:

- By means of the here presented method the solution functions of a system of type (A.1) can be computed directly, which is to say, without being obliged to pass by the intermediate step of determining schemata, up to any approximation desired.
- The new method is economical. This is due to the fact that the computation is split-up into three parts:
 - The determination of the coefficients a_{11,K}, which are independent of the initial values, i.e. they are constant for a given system (A.1).

- The calculation of the quantity G^{H} which is also variable independent, if the g_{is} are constants.
- The formation of the initial value dependent part consisting of the y_i.

A substantial part of the computation has thus only to be done once for a given system (A.1), more precisely, the coefficients $a_{H,K}$ and the quantity G^H can be stored on a permanent file, if the g_{is} are variable independent.

Consequently, the integration is essentially reduced to the summation of the terms of the power series. This results, of course, in a considerable gain of execution time.

- The application of the newly developed algorithm does not involve the solution of algebraic equations at each integration step as this is, for example, the case when applying implicit methods.
- According to our experience the here presented method seems to be particularly efficient for solving non-linear systems of type (A.1) with g_{is} constant.
- The method which has been developed in this ANNEX 1 should be regarded as being complementary to RUNGE-KUTTA and multistep methods.

Finally, we summarize for convenience in TABLE A.1 some characteristics of the numerical methods discussed in this work. TABLE A.1: Characteristics of numerical methods.

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| Method | Order of approximation for which coefficients are available | Comment |
|-------------|-------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
| RUNGE-KUTTA | explicit implicit up to 10 up to 6. | Schemata prior to compu- tation have to be estab- |
| Multistep | ADAM-BASHFORTH-MOULTON up to 12, GEAR's method up to 5. | lished for each order. Algebraic equations have to be solved, when applying implicit methods. |
| This work | unlimited (recurrence relation for coefficients). | No schemata prior to its usage needed. No algebraic equations to be solved. |

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