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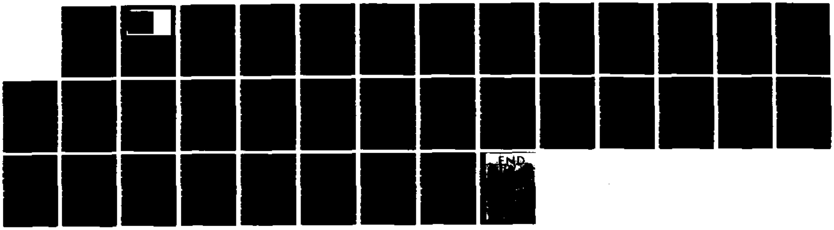

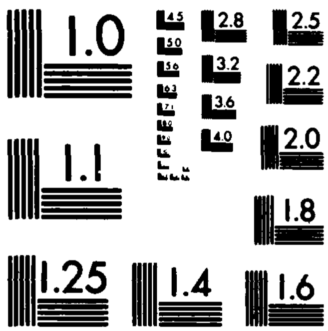

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USING INTERVAL METHODS FOR THE NUMERICAL SOLUTION OF ODE'S

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ABSTRACT

This is a survey article which ~~It~~ deals with the advantages of using interval methods for the numerical solution of initial value problems for ordinary differential equations.

AMS (MOS) Subject Classifications: 34A50, 65-04, 65G10, 65L05

Key Words: Ordinary Differential Equations, Initial Value Problems, Numerical Solution, Interval Methods

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SIGNIFICANCE AND EXPLANATION

Solving differential equations numerically on a computer is not as easy as it seems to be. It is not enough just to write a computer program for the right hand side of the differential equation, define the additional data and then call for a solving subroutine (e.g.: Runge Kutta, Adams-Stormer, Picard-Lindelöf). The numerical results obtained in this way are usually disastrous unless one selects the "correct" step size and a "corresponding" convergence order.

Everybody working in numerical computation knows of this. But it is hardly ever mentioned in detail (if at all) in textbooks.

What most people do not know, however, is the fact that this problem can be solved completely by using interval methods. This is one of the reasons why this paper was written. The above mentioned problem is demonstrated and resolved by using a very simple example.

Unfortunately in interval methods a new problem arises. It is sometimes called the "wrapping effect" and can produce an unwanted explosion of the computed error bounds. This effect is also explained in this paper and a solution to it is presented.

Finally a survey is given to show all the possible numerical interval methods which are known up to now. It is pointed out that as a byproduct of using interval methods the problem of stability just vanishes, if one uses the appropiate interval termination criterium. The list of references given here is, with 123 entries, very long and includes all the relevant work in this field which is known to the author.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

USING INTERVAL METHODS FOR THE NUMERICAL SOLUTION OF ODE'S [1]

Karl L.E. Nickel

1. Introduction

In this paper the initial value problem

(1) $u'(t) = f(t,u(t))$ for $t \in I$,

(2) $u(a) = \alpha$

is treated. Here a,b are real numbers with $a < b$, and $I := [a,b]$. Let n be an integer and $\alpha \in \mathbb{R}^n$, $u : I \to \mathbb{R}^n$, $f : I \times \mathbb{R}^n \to \mathbb{R}^n$. The functions f and u have to satisfy certain regularity conditions.

Let $\hat{u}(t)$ be a solution of (1), (2). Such a solution is not explicitly known in general. Also, it does not have to be uniquely determined. Wanted are explicitly computable error bounding functions

$v,w : I \to \mathbb{R}^n$

such that v and w are respectively lower and upper bounds for $\hat{u}$, i.e.

(3) $v(t) \leq \hat{u}(t) \leq w(t)$ for $t \in I$.

Here and in what follows, the order relation $\leq$ is defined componentwise. In the space of the functions v,w the symbol $\leq$ means the correspondingly induced partial ordering. Using the notation $[v,w]$ for the order interval of the functions v,w, the inequality (3) can be regarded as the inclusion

[1]) This paper is a condensed version of a main lecture given at the Second Seminar On The Numerical Treatment Of Differential Equations in Halle/Saale, DDR (East Germany) at May 16 to 19 of 1983.

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(4) $\hat{u} \in [v,w]$.

Suppose the problem of finding bounds v,w satisfying (3) or (4) has been solved. Then it is quite natural to ask for bounds v,w to all solutions $\hat{u}(t)$ of the same differential equation (1), but with different initial values. Let $A \subseteq \mathbb{R}^n$ be a bounded set. Then one can replace the initial condition (2) by the initial inclusion

(5) $u(a) \in A$

and ask for bounds (3) or (4) to all solutions of (1), (5) .

In general it is quite easy to write down rough bounds which satisfy (3) or (4). It is not as simple, however, to find bounds which are "small", "realistic" or even "optimal". Define the "interval hull" of the set $\{\hat{u}\}$ of all solutions $\hat{u}$ of (1) by

(6) $\text{hull } \{\hat{u}\} := [\inf \{\hat{u}\}, \sup \{\hat{u}\}]$.

If (1), (2) has a unique solution then obviously $\text{hull } \{\hat{u}\} = \hat{u}$. The best one may hope to achieve is to determine v,w such that $[v,w] = \text{hull } \{\hat{u}\}$. There are theoretical investigations of the evaluation of $\text{hull } \{\hat{u}\}$, see Nickel [79] and [80] . Due to the limitations of numerical computations, one normally has to settle for an (outer) approximation of $\text{hull } \{\hat{u}\}$.

2. Why Computing Interval Bounds Instead of Approximations ?

It has been exactly 25 years ago since the first electronic computer was installed at the University of Karlsruhe/GERMANY in the summer semester of 1958. The author of this paper was given the responsibility for this machine (Zuse Z 22). One of the very first problems I treated numerically with it was the solution of the following initial value problem (n = 1):

(7) $$u' = |1-u^2|, \; u(0) = 0 \; .$$

The uniquely determined solution of (7) is obviously $\hat{u}(t) := \tanh t$. It has the property $0 < \hat{u} < 1$. Some of the results obtained with a Runge-Kutta method are sketched in Figure 1. The four different step sizes h := 0.85, 0.90, 0.95, 1.0 were used. The values actually computed are denoted by circles. The lines between them are drawn to link up the results with the same step size.

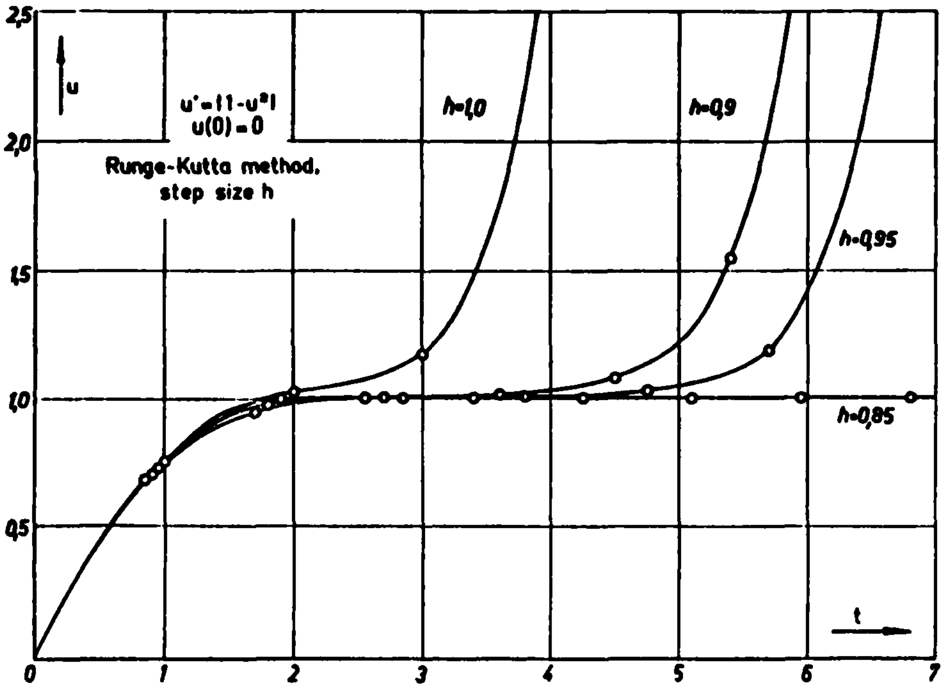


Figure 1. Numerical solution of the initial value problem (7) by using a Runge-Kutta method with the four step sizes h := 0.85, 0.90, 0.95, 1.0.

The numerical result displayed in Figure 1 is rather embarassing and displeasing: three out of four examples enter the "forbidden" region $u > 1$ and there grow exponentially fast toward $+\infty$. Furthermore, the dependence upon the step size parameter h is <u>not</u> monotone, as one would expect.

If one solves this problem (7) using many different methods with many different step sizes, the following occurs (see Figure 2) : One sees a cluster of circles without any indication of the whereabouts of the solution $\hat{u}$. Note that the values high above the "critical line" $u = 1$ belong to both very large <u>and</u> very small step sizes h (!) . As bad as this is, worse is to come: By adding the numerical results of one more method or one more step size <u>no</u> additional information about the solution $\hat{u}$ can be gained !

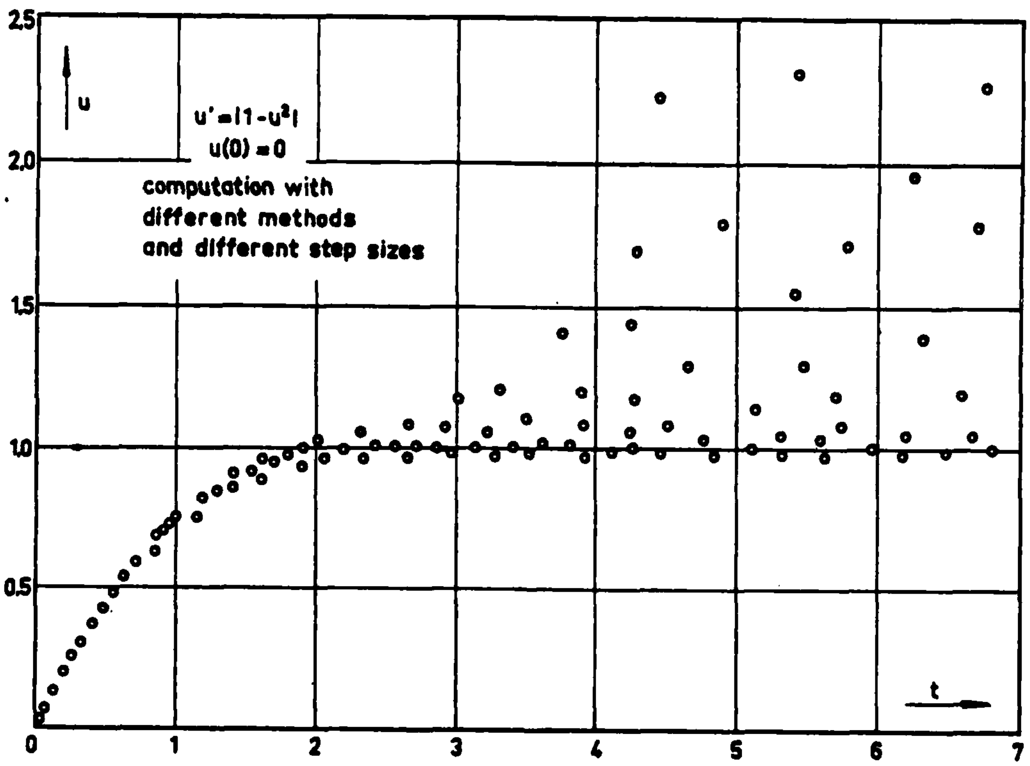


Figure 2. Sketch of numerical results of solving the initial value problem (7) by using different methods and different step sizes. This sketch is schematic, <u>not</u> actually computed.

For the "normal" user of a computer and of the numerical methods praised in mathematical textbooks such a situation is a nightmare and most certainly intolerable. By doing calculations over and over again, nothing is learned about the values of the desired solution $\hat{u}(t)$. I myself have, therefore, used this special example (7) and Figure 1 in classes over the years again and again to teach my students a sound distrust of the "usual" textbook methods.

By using interval methods for solving (7) the whole conception changes. This is illustrated in Figure 3. An interval method produces bound functions v,w such that (4) is valid. A first very rough inclusion to the solution of (7) is $\hat{u}(t) \in [v,w] := [1 - e^{-t}, 1]$. This can be found easily with the aid of differential inequalities (see W. Walter [117]). A second inclusion is computed by using a power series method (see Section 5) on a coarse grid with the step size $h := 0.5$. These two interval bounds are combined in Figure 3. The first one is realistic for large values of t, while the second gives

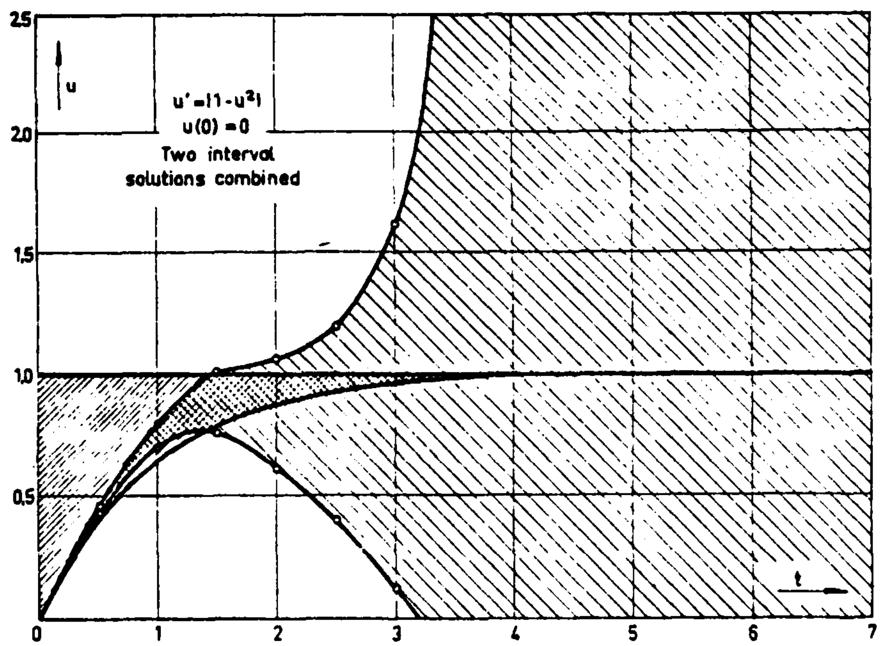


Figure 3. Combination of two interval bounds to the solution of problem (7) .

very pessimistic results. For $0 \leq t \leq 1$ the opposite is true. There are two very pleasant and surprising results :

i) The bounds are valid for <u>all</u> values of t, not only at the grid points.

ii) The intersection of the two inaccurate interval inclusions gives a much better result in the whole line $0 < t < \infty$ than each one produces alone.

Hence, by taking into account the results of more and more interval computations, one gets more and more information about the solution $\hat{u}$. This result is completely contrary to the result gained in the non-interval numerical computation (see Figures 1 and 2).

3. Blowing-Up Of Intervals; A Difficulty Inherent In All Computations Involving Sets .

There is a certain built-in difficulty in solving initial value problems with inclusions using general sets. Sometimes it is called the "wrapping effect". It has first been noticed with interval methods by R. E. Moore [69], but this difficulty arises also even more drastically when using norm bounds. It is best explained by Moore's own example. Considered is the system of two linear differential systems $(n = 2)$

$$(8) \qquad \begin{aligned} u_1' &= u_2 , \\ u_2' &= -u_1 . \end{aligned}$$

The solutions are concentric circles around the origin in the u_1,u_2- plane. Suppose the initial values for $t = 0$ lie in a (small) square $A = [\alpha]$, see Figure 4. Then for $t > 0$ this square is rotated around the origin. Bounding this square by an interval according to (3) and (4) has the

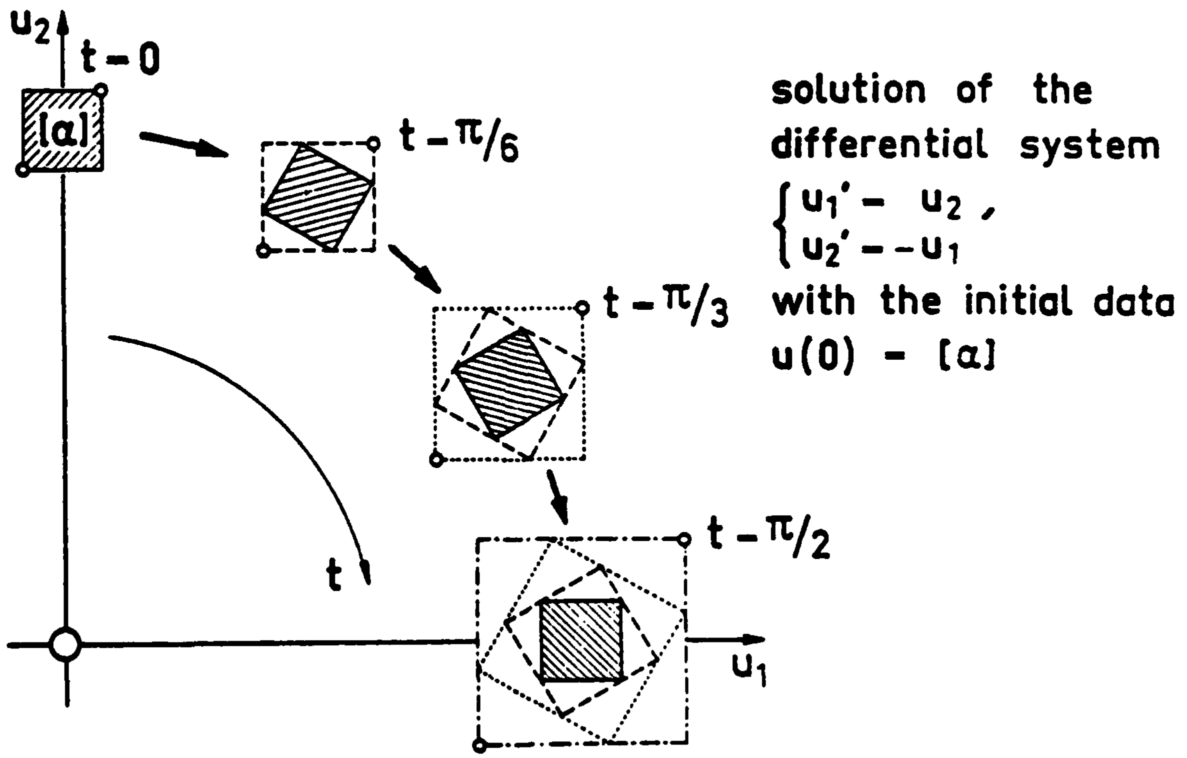


Figure 4 . Interval blow-up, exemplified at the solution of the system (8).

following meaning in the u_1,u_2-plane: One has to find a new enclosing rectangle (a square) with sides parallel to the coordinate axes. In Figure 4 this is first done at $t = \pi/6$, producing a larger square. Now this new and larger square also rotates for $t > \pi/6$ and has to be bounded again by a rectangle (square) parallel to the axes. By repeating this, the enclosing squares become larger and larger, independently of the fact that the image of the initial set $[\alpha]$ keeps its size. It can be seen easily that the original square is blown up by a factor of $e^{2\pi} \approx 535$ (!) after only <u>one</u> revolution $(t = 2\pi)$ as the step size h vanishes. This is the price to be paid for bounding the solutions of (8) with initial values in $[\alpha]$ by rectangles parallel to the axes, i.e. intervals.

Obviously this problem with the special system (8) could be resolved by using a disc to enclose the initial data instead of the square $[\alpha]$. Such a disc keeps its shape and size while rotating for $t > 0$. Generalizing this idea to arbitrary systems would mean replacing interval bounds by norm bounds (spheres). Unfortunately, this is even more likely to produce exploding bounds, as can be seen by very simple examples, even with linear differential systems (1).

In the past 15 years several ideas have been invented to overcome that difficulty:

i) Moore [69] uses local coordinate transformations.

ii) Kahan [44] bounds the solutions by ellipsoids with axes not nessessarily parallel to the coordinate axes.

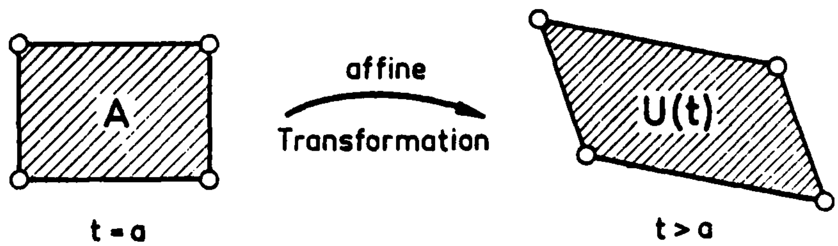
iii) Walzel [118] uses a pretransformation to get (hopefully) a "better" differential equation.

iv) Eijgenraam [26] uses a solution set which has built-in coordinate transformations.

Some years ago R. Lohner [59] and the author [79] solved this problem independently of each other at least for linear systems (1), by using the following facts: If the right hand side f in (1) is linear then the mapping from the initial value $\hat{u}(a) = \alpha \in R^n$ to $\hat{u}(t) \in R^n$ for a fixed value of $t > a$ is obviously an affine transformation. Now take any $m > n$ points α_i in the u-space and let $\hat{u}_i(t)$ be the solutions of the differential equation (1) for the initial conditions $\hat{u}_i(a) = \alpha_i$ for $i = 1(1)m$. Let A be the set spanned by the $\{\alpha_i\}$, i.e. the convex hull of the points α_i for $i = 1(1)\ m$. Let U(t) be the set spanned similarily by the $\{\hat{u}_i(t)\}$ for a fixed value of $t > a$. Then, obviously,

$$\hat{u}(t) \in U(t) \qquad \text{for } t \in I$$

for <u>any</u> solution $\hat{u}(t)$ of (1) and (5), see the Figures 5 and 6. If the



<u>Figure 5</u>. Affine transformation of the initial interval set $A = [\alpha]$ to $U(t)$ for $t > a$.

initial set A is an n-dimensional interval defined by the $2n$ "upper" and "lower" corners, then the transformed set $U(t)$ is in general <u>not</u> an interval (see Figure 5). But it can be described completely by using only the $2n$ points of the values $\hat{u}_i(t)$. If one starts with a simplex A, then $U(t)$ is also a simplex defined by $m = n + 1$ points, see Figure 6. Hence for linear differential equations it suffices to solve $n+1$ initial value problems (1), (2) in order to bound all the infinitely many solutions $\hat{u}(t)$ of (1) with initial values (5). After getting such simplex bounds, it poses no problem to transform them into interval bounds by taking hull $U(t)$ for any $t \in I$, see Figure 6.

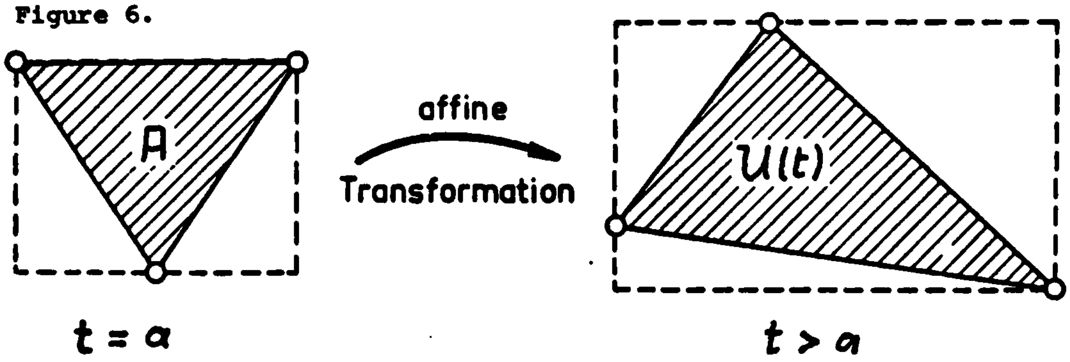


Figure 6. Affine transformation of the initial simplex set A to the new simplex $U(t)$ for $t > a$ together with the two intervals hull A and hull $U(t)$ (dashed lines).

In general, the functions $\hat{u}_i(t)$ cannot be evaluated explicitly. Hence they have to be computed numerically by using interval methods. By moving from t to $t+h$, therefore, a (small) interval containing $\hat{u}_i(t+h)$ is produced. Hence the "corners" of $U(t)$ have to be redefined at each h-step, see Figure 7. This gives a "computable" set $\tilde{U}(t)$ instead of the optimal set $U(t)$ for which inclusion $U(t) \subseteq \tilde{U}(t)$ is satisfied.

These ideas have been outlined and elaborated in a paper of J. Conradt [19]. The method worked well, beyond all expectations. Results are given in the next section.

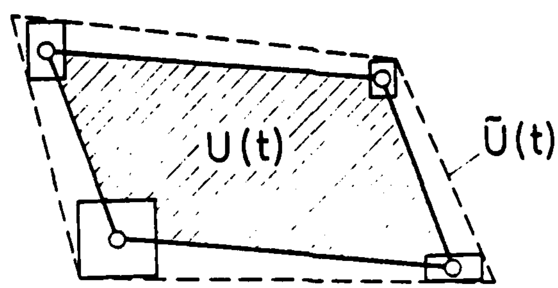


Figure 7. The computable set $\tilde{U}(t)$ (dashed lines) containing $U(t)$.

4. A Posteriori Bounds.

In this Section it is assumed that an approximation $\tilde{u}$ to the solution $\hat{u}$ of (1), (2) is known. Two error bounding functions $\underline{\sigma}, \bar{\sigma} : I \to \mathbb{R}^n$ which are computed from $\tilde{u}$ are wanted such that the following inclusion is true for the error $\hat{u} - \tilde{u}$:

$$(9) \qquad \underline{\sigma}(t) \leq \hat{u}(t) - \tilde{u}(t) \leq \bar{\sigma}(t) \quad \text{for} \quad t \in I \, .$$

To get such a function $\tilde{u} : I \to \mathbb{R}^n$ (which has to be defined for <u>all</u> values of $t \in I$) one usually takes a pointwise approximation for a certain step size h and transforms it to $\tilde{u}(t)$ by using spline interpolation. Once that $\tilde{u}$ is known, the error bounds $\underline{\sigma}$, $\bar{\sigma}$ can be computed by using known theorems from the theory of differential inequalities (see W. Walter [117]). This method has been worked out first by Markowitz [61], [62]. Later Conradt [19] made improvements, gave complete interval programs and computed several examples.

A very important property of (9) is that it gives an improvement (!) of the approximation $\tilde{u}$ if the two bounds $\underline{\sigma}$ and $\bar{\sigma}$ both have the same sign. Experience shows that this can often be accomplished !

In his paper Conradt [19] treated the differential equation (8) as an example for his method. The initial values $u_1(0) := 0$, $u_2(0) := 1$ were chosen. This gives the solution $\hat{u}_1(t) = \sin t$, $\hat{u}_2(t) = \cos t$. An approximation $\tilde{u}$ was evaluated by using a 4th order Runge-Kutta method and by interpolating with 4th order splines. The following two results are typical. They where obtained by using the step size $h := 0.125$ with single precision ($\approx$ 7 decimal digits) on a UNIVAC 1110 computer.

i) Naïve interval method : At $t = 52$ he got very pessimistic bounds with

$$\bar{\sigma}_1 - \underline{\sigma}_1 = \bar{\sigma}_2 - \underline{\sigma}_2 = 8.4_{10}{+16} \, .$$

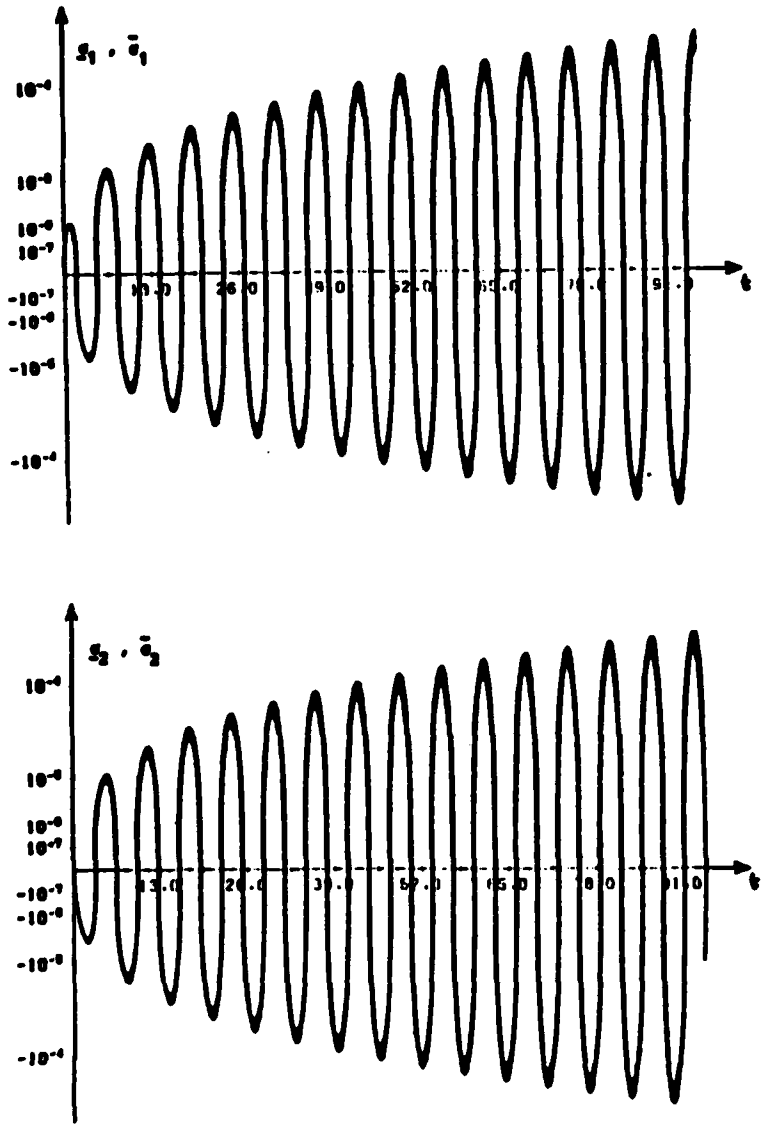
ii) Point enclosure method from Section 3 : At $t = 2152$ (an argument, more than 41 times larger than in i)) he found the much better values

$$\underline{\sigma}_1 = 1.03_{10}{-3} \, , \qquad \bar{\sigma}_1 = 2.31_{10}{-3} \, ,$$

$$\underline{\sigma}_2 = -4.66_{10}{-3} \, , \qquad \bar{\sigma}_2 = -3.46_{10}{-3} \, .$$

Note that these two pairs of bounds $\underline{\sigma}_1$, $\bar{\sigma}_1$ and $\underline{\sigma}_2$, $\bar{\sigma}_2$ each have the same sign. Hence his computed bounds give a considerable improvement of his approximations $\tilde{u}_1$ and $\tilde{u}_2$!!!

In Figure 8 the two strips $\bar{\sigma}_1$, $\underline{\sigma}_1$ and $\bar{\sigma}_2$, $\underline{\sigma}_2$ are sketched for the case ii). They contain the two errors $\hat{u}_1 - \tilde{u}_1$ and $\hat{u}_2 - \bar{u}_2$ for $0 \leq t \leq 94$. Note that the error terms are periodic and change sign as the solution does. This Figure was taken from Conradt [19].



<u>Figure 8</u>. See text. The blackened area contains the two error components $\hat{u}_1 - \tilde{u}_1$ and $\hat{u}_2 - \tilde{u}_2$.

5. Which Interval Methods Are Available To The User ?

There are 3 classes of methods for proving the existence of a solution to the initial value problem (1), (2). With any one of these, a class of corresponding numerical approximation methods can be associated. This correspondence is shown in Table 1.

Table 1.

Existence Theorem	Numerical Method	Problems / Advantages
Peano	Finite Differences	Stability ? / Any (high) order of stability possible
Picard-Lindelöf	Numerical Quadrature and Iteration	Only linearly convergent / Always stable
Power Series Method	Taylor Series	f has to be analytic / Automatic generation of coefficients

In what follows the expression "point-method" will be used to distinguish between the usual methods producing points and interval methods which produce inclusions (3) or (4) as results. During the last years some progress has been made in transforming some of the existing point-methods into interval methods or in creating new interval procedures. This progress is, however, still much too slow. One reason for this may be that far too few people are working in this field. If only 10% of the many mathematicians working with numerical methods for solving ODE 's would choose interval methods much more could be achieved in a very few years.

5.1 Finite Differences

Nearly no interval difference methods have been published up to now. One of the few exceptions is the paper of Shokin [103] who gives an interval Runge-Kutta method; see also Oelschlaegel and Nitsche [81] on this paper.

One of the easiest-to-generate methods is an interval extension of Euler's method which is repeatedly mentioned in the literature. Because of a poor convergence rate (only linear) it is, however, hardly ever used for practical purposes.

5.1,1 Stability

In difference methods stability is the most important problem. Dahlquist and Rutishauser detected this independently of each other in 1951. If a point-method is unstable, then no convergence of the approximation to the solution can be expected. Surprisingly enough the same is not true for interval methods ! This has been shown by the author [77], provided that the natural termination criterion for interval sequences is used. Hence with interval methods one can use unstable difference schemes and still have convergence ! The only effect is that the rate of convergence will slow down. More precisely : In interval computation combined with a termination criterion the order of convergence is the difference between the order of consistency and the order of (in-) stability.

5.2 Picard-Lindelöf Iteration

This is one of the "classic" methods which use Interval Analysis. The two equations (1), (2) are written as one Volterra integral equation and then solved iteratively by

$$
(10) \quad \begin{cases} u_0(t) \quad \text{arbitrary} , \\ u_{\nu+1}(t) := \alpha + \int_0^t f(s,u_\nu(s))\, ds \quad \text{for} \quad \nu = 0, 1, \ldots . \end{cases}
$$

In interval methods all the functions u_ν, f in (10) are regarded as interval functions (interval extensions of the point-functions). There are three steps to be taken :

i) Find a priori bounds v,w for the solution $\hat{u}$ of (1), (2), such that $\hat{u} \in u_0 := [v, w]$. Sometimes it is not easy to find close bounds. If u_0 is pessimistic, more iterations are necessary.

ii) Find an interval extension to f which is "close". If f is rational this can be done automatically.

iii) Perform the integration in (10) as interval integration using one of many known procedures.

One big advantage in using (10) is that no stability problems occur. One of the disadvantages, however, is the slow (linear) convergence. This may be the reason why, up to now, this class of methods have been used only occasionally.

Quite recently, however, a new approach to (10) has been published by Raith [84]. He generates a method of arbitrarily high (!) order of convergence. A big advantage of his method is that the regularity assumptions imposed on the right hand side f of (1) are very weak (continuity normally suffices). Experiments show good results.

5.3 Power Series Method

Let f be analytic in $I \times \mathbb{R}^n$. Then (1), (2) has a unique solution which is also analytic. Assume that it exists for all $t \in I$. Let $m > 1$ be an integer number and $0 < h \leq b-a$ a fixed step size. Then by Taylor's Theorem, $\hat{u}(t)$ satisfies the recurrence relation

$$(11) \qquad \hat{u}(t+h) = \sum_{\mu=0}^{m-1} \frac{\hat{u}^{(\mu)}(t)}{\mu!} h^\mu + \frac{\hat{u}^{(m)}(\xi)}{m!} h^m \quad \text{with} \quad t < \xi < t+h .$$

Assume that intervals $U_\mu(t)$ can be computed for all $t \in I$, $\mu = 0(1)m$, such that the following inclusions are true:

$$(12) \qquad \hat{u}^{(\mu)}(t) \in U_\mu(t) \quad \text{for } \mu = 0(1)\, m-1$$

and

$$(13) \qquad \hat{u}^{(m)}(\xi) \in U_m(t)$$

for all $t \in [a,b-h]$, $t < \xi < t+h$, $0 < h \leq b-a$.

Define for simplicity $U(t) := U_0(t)$ and the grid $t_\nu := a + \nu h$ for $\nu = 0(1)k$ with $k-1 < (b-a)/h < k$. Then by (11), (12) and (13) the following interval method is suggested for solving (1), (5) recursively:

$$
(14)\quad \begin{cases} U(a) := A, \\[2ex] U(t_{\nu+1}) := \sum\limits_{\mu=0}^{m} \dfrac{U_\mu(t_\nu)}{\mu!} h^\mu , \\[2ex] U(t_\nu+\tau) := \sum\limits_{\mu=0}^{m} \dfrac{U_\mu(t_\nu)}{\mu!} \tau^\mu \qquad \text{for } 0 < \tau < h \\[2ex] \text{for all } \mu = 0(1)k-1. \end{cases}
$$

Note that $U(t)$ is defined by (14) for <u>all</u> $t \in I$. By (11), (12), (13) and (14) the following (desired) inclusion is guaranteed:

$$\hat{u}(t) \in U(t) \quad \text{for all} \quad t \in I.$$

If all intervals $U_\mu(t_\nu)$ are globally bounded, then method (14) obviously defines a convergent sequence with

$$\lim_{h\to 0} U(t) = \hat{u}(t) \quad \text{for all} \quad t \in I .$$

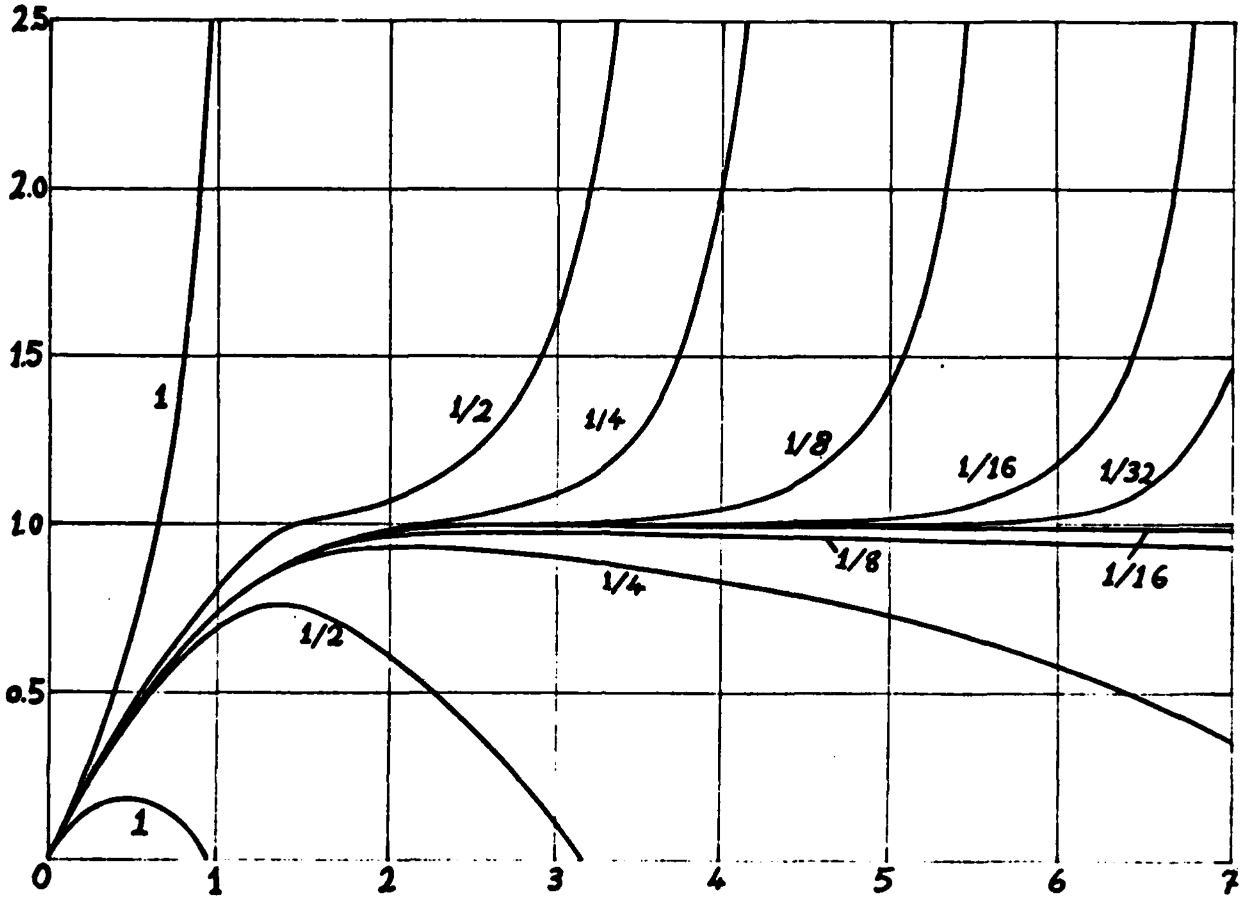
It seems at first that the conditions imposed on f and u are very strict and that, moreover, the assumptions concerning the computability of the intervals U_μ by (12) and (13) can rarely be met. Unfortunately, this wrong opinion is still believed by most numerical analysts. It has been shown, however, by people working in interval analysis that the opposite is true and that the method presented in (14) has nearly no limitations on it. There are two reasons for this:

i) In numerical analysis any function f has to be evaluated by a program on a computer. Any program, however, can only produce the values of a piecewise rational function, and so any "usable" function f is piecewise analytic.

ii) It can be shown that the computation of the intervals $U_\mu(t)$ in (12) and (13) can be carried out automatically by software using the compiler of the computer, if only f is given as a program with no jumps. This is known as " automatic differentiation ", see R. E. Moore [68], L. B. Rall [87] and others.

As an Example the initial value problem (7) was treated with that method, using $m = 5$ (convergence order $m-1 = 4$) and using different step sizes $h := 1, 1/2, 1/4, 1/8, 1/16, 1/32$. The results are shown in Figure 9. There only the bounds are sketched. In order not to overload the picture the computed interval strips have not been hatched as in Figure 3. The bounds shown in Figure 3 have been computed with this method, too, using the step size $h := 0.5$.

This method and Raith's method described in Section 5.2 both work remarkably well. Up to now, no data are available which favor one method over the other.



<u>Figure 9</u>. Solution of problem (7) by using the power series method with the different step sizes h := 1, 1/2, 1/4, 1/8, 1/16, 1/32.

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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Ordinary Differential Equations, Initial Value Problems, Numerical Solution, Interval Methods

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This is a survey article. It deals with the advantages of using interval methods for the numerical solution of initial value problems for ordinary differential equations.

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