June 1975

TR/53

AN INTRODUCTION TO REGULAR SPLINES AND THEIR APPLICATION FOR INITIAL VALUE PROBLEMS OF ORDINARY DIFFERENTIAL EQUATIONS.

by

H. WERNER.

This work was supported in part by the Science Research Council Grant B/RG/74266 made to Brunei University to finance a Symposium on Finite Element Methods during the period January - June 1975 .

The author gratefully acknowledges the excellent research facilities provided by this grant and the dedicated engagement of Dr. J. R. Whiteman. These possibilities lead to the preparation of this report. The calculations were performed on the CDC7600 at the University of London Computing Centre by the courtesy of Brunel University.

W9260530

ABSTRACT

This report describes an application of the general method of integrating initial value problems by means of regular splines for equations with movable singularities. By defining the families of functions that make up the regular splines such that they closely resemble the behaviour of the solutions of the differential equation, it is possible to trace the location of the singularities very precisely.

To demonstrate this we treat Riccati differential equations. These are known to possess solutions with poles, usually of the first order. This type of differential equation or system arises in describing chemical or biological processes or more general control processes.

To make the report self contained it starts with an introduction to regular splines and develops the algebraic tools for the manipulation of rational splines. After the description of the integration procedure, the asymptotic behaviour of the systematic error is investigated. An example exhibits the results obtained from the program given in Appendix A. Then Riccati equations are introduced and methods for the determination of the singularities are developed. These methods are tested numerically with several examples. The results are given in Appendix B.

1. Introduction

The word spline originated from a device used by the draftsmen to obtain graphically smooth interpolations of a given set of points (x_j, y_j), $j=0,\ldots m$ by fitting an elastic rod to these locations on a piece of paper. The rod would then satisfy the physical laws of elasticity, i.e.

$$\int \left(\frac{y''(t)}{\sqrt{1 + y'(t)^2}} \right)^2 dt = \min .$$

and $\quad y(x_j) = y_j \qquad y = 0,\ldots,m.$

Assuming $y'(x)$ to be small, the above variational problem is usually replaced by

$$\int (y'')^2 \, dt = \min \quad .$$

Hence the Euler equation becomes

$y^{IV}(x) = 0$ and it is to hold between the supporting points x_i. Furthermore the rod is linear outside of $[x_0, x_m]$.

Hence the function resulting from the above graphical interpolation under the said simplification - called a <u>natural cubic spline</u> — may be specified as:

(1) i) $u(x) \in C^2(I)$, $I=[x_0, x_m]$.

ii) In each subinterval $I_j = [x_{j-1}, x_j]$ we have
$u(x) = a_j + b_j . z + ½ \; c_j^2 \; z^2(1+d_j z)$,with $z = x - x_{j-1}$,
to be a cubic polynomial.

iii) The function u is <u>interpolating</u>, i.e.

$u(x_j) = y_j$, $j = 0,$ ------, m.

iv) The function u is a <u>natural</u> spline, that is twice continuously differentiable in $(-\infty , + \infty)$, and

$$u''(x) \equiv 0 \quad \text{for } x \leq x_o \text{ and } x_m < x.$$

There are many different ways this concept of spline has been generalised and we refer the reader to the bibliographies on spline literature by Schurer et al.[22, 7 and 28],
Usually u(x) will be a linear combination, depending on a specified number of parameters in each sub-interval I.. In this paper we deviate from almost all of the other generalisations by replacing the linear expression (1 ii) by a nonlinear one. First results in this direction can be found in Arndt [3],Braess-Werner [8], Meder [17], Runge [18], Schaback [19,20],Schomberg [27], Spath[23], Werner [24,25,26].
Schaback found that the interpolating rational splines could be obtained from a variational problem [19].This property was put into an abstract setting by Baumeister [5].
To illustrate this type of generalisation, we will use the example of special rational splines with a quadratic polynomial being the numerator and a linear polynomial being the denominator. In every sub-interval I_j. we may write this function as

(2) $$u(x) = a_j + b_j z + \frac{c_j}{2} z^2 /(1 - d_j z) , \quad z = x - x_j .$$

Before giving the definition of a regular spline, we establish some properties of the rational splines.
Equation (2) may be re-written in the following forms

(3) $$u(x) = a_j + b_j z + \frac{c_j}{2} z^2 + \frac{c_j d_j z^3}{2.(1 - d_j z)}$$

or

(4) $$u(x) = a_j + b_j z_j + \frac{c_j}{2d_j^2}\left[\frac{1}{1 - d_j z} - (1 + d_j z)\right] .$$

The last one is particular ly useful for the calculatio n of the derivative s :

(5) $$u'(x) = b_j - \frac{c_j}{2d_j} + \frac{c_j}{2d_j(1 - d_j z)^2} ,$$

(6) $$u''(x) = \frac{c_j}{(1 - d_j z)^3} ,$$ and more general

(7) $$u^v(x) = \frac{v! c_j d_j^{v-2}}{2(1 - d_j z)^{v+1}} , \quad v = 2,3, \ldots .$$

From (3) respectively (5) (6), (7) we read off

$$(8) \qquad a_j = u_j, \qquad b_j = u'_j, \qquad c_j = u''_j, \text{and} \qquad d_j = \frac{u'''_j}{3u''_j}.$$

Furthermore from (7) and (6) we conclude that the higher order derivatives of u(x) are functions of x and the two parameters u''_j together with either u''_{j+1} or u''_j

2. Regular splines

In [20] Schaback discovered that only few properties of the rational splines were really used in the construction of the interpolating splines and gave an axiomatic formulation. The axioms were further stream-lined in [26] and appended in [25] to suit the need of Tschebyseheff approximation. The properties needed for the application to differential equations are as follows.

Let $I = [\alpha,\beta]$ denote an interval of the real axis R, let $x_0 < x_1 < \ldots, < x_m$ denote points of I and write $I. \;=[x_{j-1}.x_j], h_j \;= x_j - x_{j-1}$.
Furthermore assume $t_j(x,c,d)$ are two-parametric families of functions $c \in D_{1,j}$' $d \in D_{2j}$ .and $x \in I_j$ We assume t_i to he (at least) k-times continuously differentiable with respect to x. Then the following definition is well defined:

$$(9) \qquad S(x_o, \ldots, x_m; t_1, \ldots, t_m) = \left\{ \begin{array}{l} u \mid u(x) \in C^k(I), \\ u(x) = p_j(x) + t_j(x, c_j, d_j) \text{ in } I_j, \\ j = 1, \ldots, m, p_j \text{ being a polynomial} \\ \text{of degree less than } k. \end{array} \right\}$$

In addition we ask for the following axioms to be satisfied;

Axioms

(A1) k - Regularity

For kth order derivates the difference $t_i^k(x,c,d) - t_i^k(x,\bar{c},\bar{d})$ has less than two zeros in I. which are separated by a point in which the difference is different from zero.

This axiom makes it possible to introduce the kth order derivates of two different points of I_j, say x_{j-1} and x_j, or any two analogous expressions (e.g. u''_j and u'''_j) as the natural parametrisations of the families t_j.

Following the notation of cubic splines we may write $M_j \equiv u^{(k)}(x_j)$ and hence $t_j(x, M_{j-1}, M_j)$.

We further make some quantitative assumptions;

(A2) k - Smoothness

The functions $t_j(x, M_{j-1}, M_j)$ are $k + \ell$ times continuously differentiable with respect to x, ℓ being ≥ 2, and have continuous partial derivatives with respect to M_{j-1} and M_j.

(A3) k - Boundedness

The derivatives of $t_j(x, M_{j-1}, M_j)$ of order $k+.2. \ldots , k+\ell$ with respect to x depend Lipschitzian on the parameters (M_{j-1}, M_j) or $(M_{j-1}, (M_j - M_{j-1})/h_j)$ or (M_j, u_j'') .

The last property is motivated by what was found for the rational splines at the end of the previous section.

It is left to the reader to find out that

i) $t(x,c,d) = c(x+d)^{\alpha}$, α real

ii) $t(x,c,d) = c.\exp(dx)$

iii) $t(x,c,d) = c.\log(x+d)$

are candidates for regular families. In particular for $\alpha = 3$ we obtain the cubic spline from i) via definition (9).

It might be noted that another property called stiffness is important if one concerns oneself with Tschebyscheff approximation by classes of regular spline functions, compare [24,25].This is important for the closure of the classes of regular splines under uniform convergence in every closed sub-interval of $(\alpha,ß)$.

3. Lemmas on divided differences and applications

Manipulation of regular splines is easily performed by means of divided differences. Hence we collect some formulas for these expressions.

Denote $\Delta^{1}(x_i, x_k)\,u = \dfrac{u_i - u_k}{x_i - x_k}$ and

(**10**) $$\Delta^{k+1}(x_{i_0},\ldots,x_{i_{k+1}})\,u = \Delta^{1}_{c}(x_{i_0}, x_{i_{k+1}})\ \Delta^{k}(c, x_1,\ldots,x_{i_k})\,u\ .$$

Among other properties it is worth noting that the divided differences are invariant under permutations of the arguments $x_{i_0},\ldots,x_{i_{k+1}}$, compare [27].

If the data u_j stem from a function u(x), defined in I having derivatives of sufficiently high order, then limits $x_i \to x_k$ may be considered and the following conventions may he used: $u_j = u(x_i.)$, $u'_i = u'(x_i)$, ... furthermore

$$\Delta^{1}(x_i, x_i)\,u = \lim_{x_k \to x_i} \Delta^{1}(x_i, x_k)\,u = u'_i\ ,$$

(11) $$\Delta^{2}(x_j,\ x_j\ ,\ x_{j+1})u = (\Delta^{1}(x_{j+1,}x_j)u-u_j)/h_{j+1}\ ,$$

(12) $$\Delta^{2}(x_{j-1}\ ,\ x_j\ ,\ x_{j+1})u = (u'_j\ -\ \Delta^{1}(x_{j-1}\ ,\ x_j\ )u/h_j,$$

where we employ the notation $h_j = x_j - x_{j-1}$ already introduced in the previous section.

An immediate consequence of (11) and (12) is:

Lemma **1**: Let $\lambda_j = \dfrac{h_j}{h_j + h_{j+1}}, \mu_j = \dfrac{h_{j+1}}{h_j + h_{j+1}}$, then

(13) $$\lambda_j\ \Delta^2\ (x_j\ ,x_j\ , x_j)u\ +\mu_j\ \Delta^2\ (x_{j-1}, x_j, x_{j+1}\ )u = \ \Delta^2(x_{j-1}\ ,x_{j,}\ x_{j+1}\ )u$$

This formula may be generalised to higher order difference quotients and he applied to solve the interpolation problem, compare Arndt [4].

Lemma 2: Let $u \in C^4 [x_j, x_{j+1}]$. Then

$$(14) \qquad \Delta^2(x_j, x_j, x)u = \frac{2u''_j + u''}{6} + R[u],$$

where $h = x - x_j$, $u'' = u''(x)$ and

$$R[u] = -\frac{h^2}{3}[2\Delta^4(x_j, x_j, x_j, x, x)u + \Delta^4(x_j, x_j, x, x, x)u] = -\frac{h^2}{24}u^{IV}(\xi)$$
$$= -\frac{h^{-2}}{6} \cdot \int_{x_j}^{x} (x-t) \cdot [h^2 - (x-t)^2] \cdot u^{IV}(t)\,dt$$

with some intermediate ξ.

The proof follows from the identity

$$3\,\Delta^2(x_j, x_j., x)u = [2\Delta^2(x_j, x_j, x_j) + \Delta^2(x,x,x)$$
$$+ h(2\Delta^3(x_j, x_j, x_j, x) - \Delta^3(x_j, x_j, x, x) - \Delta^3(x_j, x, x, x))]\,u$$
$$= u''_j + \tfrac{1}{2}u'' - h^2[2\Delta^4(x_j, x_j, x_j, x, x)u + \Delta^4(x_j, x_j, x, x, x)u].$$

The integral representation is obtained from the Peano kernel theorem, as

$$\Delta^4(x_j, x_j, x, x, x)f = \frac{f''}{2h^2} - \frac{(2f' - 3\Delta'(x, x_j)f + f'_j)}{h^3}$$

and $f = (x-t)^3_+$ for $x_j < t < x$ i.e. $f_j = f'_j = f''_j = 0$ imply

$$2\Delta^4(x_j, x_j, x_j, x, x)f + \Delta^4(x_j, x_j, x, x, x)f = \frac{f''}{2h^2} - \frac{3f}{h^4}.$$

Hence the kernel has the form

$$K(t,x) = -\frac{h^2}{3}[z\Delta^4(x_j, x_j, x_j, x, x) + \Delta^4(x_j, x_j, x, x, x)]f = -\frac{1}{6}[(x-t) - \frac{(x-t)^3}{h^2}].$$

In the following the arguments of the divided differences are always points x_j, x_k etc. To simplify notation we write $\Delta^1(j,k)$ instead of $\Delta^1(x_j, x_k)$ etc.

An easy consequence of (11,), (12), (14), is

<u>Lemma 3 ;</u> Let $u \in C^6$, and $h=x_{j+1}-x_j$ the length of the interval $[x_i,x_{i+1}]$then

(15) $$\Delta^2(j,j,j+l)u + \Delta^2(j,j+1,j+l)\,u=(u'_{j+1}-u'_j)\,/h = (u''_{j+1}+u''_j)\,/2+R^*$$

where $$R^* = -\,h^2 \cdot [D^4(j,j,j,j+1,j+1)u +$$

$$+\Delta^4(j,j,j+1,j+1,)u] = -\frac{h^2}{12}\left[u^{IV}\left(\frac{x_j+x_{j+1}}{2}\right)+0(h^2)\right].$$

The result. (15) is obtained by adding (1 4) for j and j+1 with x equal to x_{j+1} or x_j respectively.
One should observe that above error estimate though proved only for $x > x_j$ is independent of this relation and applies for $x < x_j$ also, if the differentiability assumption is satisfied.
As was said before, we use the rational spline for demonstration and as a preparation derive the following formulas.

let $v(x) = \dfrac{1}{1-dx}$ then

(**16**) $$\Delta^1(i,k)\,v = \frac{1}{(1-dx_i)(1-dx_k)}$$ and by induction

$$\Delta^k(0,\ldots,k)v = \frac{d^k}{(1-dx_0)\ldots(1-dx_k)} .$$

In particular ,if

$$u(x) = a + bc + \frac{c}{2d^2}\left(\frac{1}{1-dz} - 1 - dz\right) \quad , \; z = x - x_j ,$$

and $N = 1 - d\,.(x_{j+1} - x_j)$,

then e.g.

$$\Delta^2(j,j,j)\,u = \frac{c}{2} ,$$

$$\Delta^2(j,j,j+1)\,u = \frac{c}{2N} ,$$

$$\Delta^2(j,j+1,j+1)\,u = \frac{c}{2N^2} ,$$

$$\Delta^2(j+1,j+1,j+1)\,u = \frac{c}{2N^3} ,$$

$$\Delta^3(j,j,j+1,j+1)\,u = \frac{cd}{2N^2} \bullet$$

In general

$$(17) \qquad \Delta^k(j,\ldots,j,\underbrace{j+1,\ldots,j+1}_{r})u = \frac{c}{2}\frac{d^{k-2}}{N^r} \text{ for } k \geq 2 .$$

Since u''_j and u''_{j+1} apparently determine c,d and N these quatities determine every derivative and divided difference of higher order in a very simple manner.
Hence we note for further use that

$$(18) \qquad N = \Delta^2(j,j,j+1)u / \Delta^2(j,j+1,j+1)u$$

$$c = 2\ (\Delta^2(j,j,j+1)u)^2 / \Delta^2(j,j+1,j+1)u$$

$$d = \Delta^3(j,j,j+1,j+1)u / \Delta^2(j,j+1,j+1)u .$$

These formulas describe c,d,N in terms of u and its first derivative at x_j and x_{j+1} .

4. Some remarks on interpolation

The interpolation problem for rational splines was first treated by Schaback when k=2 in his Dissertation [19]. The generalisation to regular splines and some improvements were given in [20], and this approach was generalised by Arndt[4] to $k > 2$.
We consider here the case $k = 2$ only, i.e. splines that are twice continuously differentiable.

Problem: Given interpolation data $(x_j, y_j), j = 0,\ldots, m$ and boundary data M_o or u'_o and M_m or u'_m, find $u(x) \in S$ satisfying these conditions.

We try to represent u(x) by means of $y_o, \ldots, y_m$ and $M_o, \ldots, M_m$ and derive the determining equations from this representation.
It is immediately seen that

$$(19) \qquad u(x) = t_j(x, M_{j-1}, M_j) + y_j + z\,\Delta^1(j-1,j)y - t_j(x_j, M_{j-1}, M_j)$$

$$- z.\Delta^1(j-1,j)\,t_j(\bullet, M_{j-1}, M_j) \text{ in } I_j \text{ , again } z = x - x_j \ \bullet$$

Application of Lemma 1 furnishes the equations

$$\lambda_j \ \Delta^2(j-1, j, j) t_j(\bullet, M_{j-1}, M_j) + \mu_j \ \Delta^2(j,j,j+1) t_{j+1}(\bullet, M_j, M_{j+1})$$

$$= \Delta^2(j-1,j,j+1)y, \ j = 1, \ldots, m-1,$$

which transform to

$$(20) \quad \lambda_j \ M_{j-1} + 2M_j + \mu_j \ M_{j+1} = 6 \cdot \Delta^2(j-1,j,j+1)y + R^{(j)} \ j = 1, \ldots, m-1,$$

The boundary data either enter by giving M_o (resp.M_m)explicitly or by providing Δ^2 (0,0,l)y, $h_o = \lambda_o = 0$, $\mu_o = 1$, i.e. adding another one to the above equations and similarly for $j = m$.
$R^{(j)}$may be obtained from Lemma 2. It is of order h^2 if the M_j and $\Delta^2 (j,j^+1)M$ are in a closed bounded region such that the fourth order derivatives of u(x) stay bounded.
Now the left hand side of (20) is of the form

$$A \cdot \begin{bmatrix} M_o \\ \cdot \\ \cdot \\ \cdot \\ M_m \end{bmatrix}$$ with a matrix A which has a bounded inverse.

If the fourth order derivatives of $t_j(x,M_{j-1},M_j)$ depend Lipschitzian on M_{j-1} and M_j , say, the right hand side of (20) constitutes a contracting operator in some norm with respect to the vector of the M_j if h is sufficiently small; that is, the mesh generated by $\{x_j\}$ in I is sufficiently fine. Hence one may solve for the M_j by iteration, if the values of M_j are admissible as parameters of the families t_j. Assuming this assumption to be met, which may be a restriction on $y(x) \in C^5$, one can see that the interpolating splines and their derivatives converge to y(x),due to the formula

$$u^{(v)}(x)-y^{(v)}(x)= 0(h^{4-V}) \qquad \text{for} \quad v=0,1,2,3,$$

uniformly in each I_j. That is to say the convergence of the third order derivative is uniform in each subinterval and although there may be discontinuities at the knots x_j, the jumps there are small since at the left side and right side of x_j the values of $u'''(x)$ are close to that of the continuous function $y'''(x)$.

For a complete proof the reader is referred to [26].

5. Integration of initial value problems.

In this section we consider the classical initial value problem for ordinary differential equations.

Given

$f(x,y)$ in a domain G, sufficiently smooth, say four times differentiable,

$(x_o,y_o) \in G$,

find $x_+ > x_o$ and $y(x) \in C^4[x_o, x_+]$ such that

$y'(x) = f(x,y(x))$ and

$y(x_o) = y_o$.

Here we report on a method for the numerical solution of this problem by regular splines as worked out in the Dissertation of Runge C183 . It has already been used by Loscalzo-Talbot in the special case of the cubic spline [16] . Lambert & Shaw [12,13,14] used rational and more general expressions to find a solution of the initial value problem, but in an explicit way that proved cumbersome in its application. We give an explicit set of formulas for the rational splines to demonstrate the ease of application of this method and also discuss its remarkable accuracy.
For stability reasons we use $k = 2$. Higher k require additional efforts for numerical stabilisation and will be dealt with in another paper.

Method: (a) To initialise the solution we need u_o , u'_o u''_o.
We may take

(21) $u_o = y_o$, $u_o' = f(x_o, y_o)$, $u_o'' = f_x(x_o, y_o) + f_y(x_o, y_o) \cdot u'_o$.

If it is inconvenient to calculate f_x and f_y , any other initialisation will also do.

(b) Recursive definition of $u(x)$ in I_{j+1} for $j = 0,1,...$.

Prescribe step size h, let $x_{j+1} = x_j + h$.

Given u_j, u'_j, u''_j determine u''_{j+1} such that

(22) $$u'_{j+1} = f(x_{j+1}, u_{j+1})$$

holds. Determine $u_{j+1}, u'_{j+1}, u''_{j+1}$ from $u(x)$, $x \in I_{j+1} = [x_j, x_{j+1}]$ to get data for next step.
This now has to be turned into a numerical procedure.
Example:

First we will set up the algorithm for the rational splines.

Apparently from (2) and (8) the equation

$$u(x) = u_j + u'_j z + \frac{u''_j}{2} \cdot \frac{z^2}{1 - dz}$$

is to hold in I_{j+1} and d has to he chosen to satisfy (22).
One will try to solve (22) by an iteration, starting with

$d^{(0)} = 0$ if $j = 0$ or a value $d^{(0)}$ derived from d_j that was obtained in I_j. Since for this interval the denominator vanishes at

$$z = x_{pol} - x_{j-1} = 1/d_j ,$$

one would try

$$1/d^{(o)} = x_{pol} - x_j = 1/d_j - h = (1 - hd_j)/d_j ;$$

i.e. we take

(23) $$d^{(o)} = d_j / N_j .$$

(here again $N_j . = 1 - hd_j$ is used).

The value $d^{(0)}$ is iteratively improved by means of equation (22).Since

$$u'(x)\Big|_{x=x_{j+1}} = u'_j + \frac{u''_j}{2} \frac{2z - z^2 \cdot d}{1 - dz^2}\Big|_{z=h} = u'_j + \frac{u''_j}{2} h \left[\frac{1}{1 - dh} + \frac{1}{(1 - dh)^2} \right]$$

and

(24) $$\frac{\partial u'_{j+1}}{\partial d} = \frac{u''_j \cdot h^2}{2} \left[\frac{1}{(1 - dh)^2} + \frac{2}{(1 - dh)^3} \right] \approx \frac{u''_j}{N_j^2} 1.5 . h^2 ,$$

we may calculate the change δ of $d^{(0)}$ by (almost) Newton's method

$$(2.5) \qquad h \cdot \delta = \frac{N}{1.5 \cdot u''_j} \left[\frac{N}{h} \left[f(x_{j+1}, u(x_{j+1}, d^{(0)})) - u'_j \right] - \frac{1}{2} h''_j \left(1 + \frac{1}{N} \right) \right] .$$

We may now continue with this iteration until the change is less

than a prescribed tolerance. One should observe that $\frac{\partial f(x, u(x, d))}{\partial d}$ is small if h is small. If h is not very small it may, however, be advisable to use another method, e.g. Regular Falsi (Secant rule). See Appendix A for a program.

In numerical experiments it proved better to use the above crude value of $\frac{\partial u'_{j+1}}{\partial d}$ instead of the precise one. In fact, if $d > 0$ we take a value of the derivative that will be slightly smaller than the correct one. This implies we are getting a value of δ from (24) that has too large an absolute value. If $\delta > 0$, that is d becomes larger, then the exact value of the derivative is increasing. If $\delta < 0$, d becomes smaller. Then the value of the derivative is decreasing and our approach tries to compensate for that.

Since we switch to Regular Falsi in the next step it is better in any case to overshoot the solution d and this tends to happen with the above approach.

6. Rate of convergence of integration scheme

Numerical results (compare Appendix B) indicate that fourth order convergence of the method of integration described by (25) is expected. To prove this fact we first show that we may view the method as a non-linear two step method by establishing a relation between the values u_{j-1}, u_j, u_{j+1} of the approximating regular spline.

If u_j is known, then $u'_j = f(x_j, u(x_i))$ is also available. Hence in each subinterval I_j and I_{j+1} the spline u(x) can be represented by

$$(26) \qquad u(x) = u_j + z \bullet u'_j + z^2 \bullet \Delta^2 (j, j, j \pm 1) u + z^2 (z \mp h) \bullet \Delta^3 (j, j, j\pm1, j\pm1) u +$$

$$+ z^2 (z \mp h)^2 \bullet \Delta^4 (j, j, j \pm 1, j \pm 1, x) u , \qquad z = x - x_j .$$

The last term describes the remainder term. It is twice continuously differentiable with respect to x between x_j and $x_{.j\pm 1}$.

We differentiate (26) twice and let x tend to the limit $x=x_{j,}$ $(z \to 0)$, Then every term containing a factor z will disappear so that

$$(27)\ \tfrac{1}{2}\, u''(x_j \pm 0) = \Delta^2(j,j,j\pm 1)u + (\mp h)\,\Delta^3(j,j,j\pm 1,j\pm 1)u +$$

$$+ \quad h^2 \bullet \Delta^4(j,j,j,j\pm 1,j\pm 1)u$$

$$= 2\,\Delta^2(j\,,j\,,j\pm 1\,)u - \Delta^2(j\,,j\pm 1,\,j\pm 1)u + h^2 \bullet \Delta^4(...)u\,.$$

We may resolve that identity to get an expression in terms of u and its first derivative

$$(28) \qquad \tfrac{h^2}{2}\ u''(x_j\pm 0)= 2[u_{j\pm 1} - u_j - (\pm h) - u'_j]-[(\pm h)u_{j+1} - u_{j\pm 1} + u_j]$$
$$+\ h^4 \bullet \Delta^4(\ldots)u \ ,$$

keeping in mind $x_{j\pm 1} - x_j = \pm h$.
The connection between the two restrictions of u(x) to I_j and I_{j+1}, respectively, is given by

$$u''(x_j-0) = u''(x_j+0)\ .$$

Substitution of (28) into this equation and rearranging terms results In

$$(\mathbf{29})\quad \mathbf{3}(u_{j+\mathbf{1}} - u_{j-\mathbf{1}}) = h\cdot\left[f(x_{j+\mathbf{1}},u_{j+\mathbf{1}}) + \mathbf{4}f(x_j,u_j) + f(x_{j-\mathbf{1}},u_{j-\mathbf{1}})\right] + A[u],$$

where

$$A[u]=h^4\,[\Delta^4(j,j,j,j-1,j-1)u - \Delta^4(j,j,j,j+1,j+1)u].$$

We observe that the term A[u] on the right hand side looks like a perturbation term to the linear recurrence relation which happens to be the Milne-Simpson rule.

If $y(x)$ Is an exact solution to the given differential equation and is five times continuously differentiable, then $y'(x_i) = f(x_i, y(x_i))$, for $i = j-1, j, j+1$ and (29) becomes an identity from which we conclude that

$$(30) \quad A[y] = \frac{h^4}{24}\left[y^{IV}(t_-) - y^{V}(t_+)\right] = \frac{\theta . h^5}{12} . y^{V}(t), \theta \ \varepsilon \ (0,1) \ ,$$

with intermediate points t, t_-, t_+ of $I_J \cup I_{J+1}$.

To get some preliminary information about the convergence of $u(x,h)$ we Start from identity (28) to obtain

$$(29') \qquad 3(u_{j+1} - u_{j-1}) = h(u_j' + 4u'_j + u'_{j-1}) + h^4 . [\Delta^4 (j,j,j,j-1,j-l) \ u \ - \Delta^4 (j,j,j,j+1,j+l)u] \ ,$$

which holds for any twice continuously differentiable function.

In contrast to (29) the first derivatives are retained.

We apply (29') to the difference

$$w(x,h) = u(x,h) - y(x)$$

and use $w_j := w(x_j, h)$ etc. That is.we do not indicate the dependence on h explicitely although h will be varied in the sequel.

Since

$$(31) \qquad w'_j = u'(x_j,h) - y'(x_j)$$

$$= f(x_j, u_j) - f(x_j, y_j)$$

$$= f_y(x_j, y_j) \cdot w_j \quad ,$$

we write

$$(32) \quad f_{y|j} := f_y(x_j, \tilde{y}_j), \ A_j := \Delta^4 (j,j,j,j-1,j-1)\,w - \Delta^4 (j,j,j,j+1,j+1)w$$

and obtain

$$(33) \quad 3(w_{j+1} - w_{j-1}) = h\,(f_{y|j+1} w_{j+1} + 4 f_{y|j} w_j + f_{y|j-1} w_{j-1}) + h^4 \cdot A_j .$$

We assume that $x_+ > x_0$ and $h_0 > 0$ are such that for $x_0 \le x \le x_+$, $h \le h_0$ the solution $y(x)$ exists and has derivatives $y''(x)$ and $y'''(x)$, such that $t(x;x_j,h,y''(x_j),y'''(x_j))$ are defined and that also $u(x,h)$ exists in $[x_0, x_+]$. Under these assumptions we derive certain a priori estimates.

We introduce

$$(34) \qquad v_j = w_j \cdot h^{-K}$$

with an integer k to be specified later, insert v_j into (32) and add up for j =1,3,..., 2v-1, to find

$$(35) \qquad v_{2v} = v_0 + \frac{h}{3} \cdot (fy\,|_{2v} + 4 f_{y|2v-1} v_{2y-1} + 2 f_{y|2v-2} v_{2v-2} + \ldots + 2 f_{y|2} v_2 + 4 f_{y|1} v_1 + f_{y|0} v_0) + \frac{1}{3} h^{4-k} \cdot \sum A_j .$$

Approximately the second term on the right hand side looks like Simpson's rule for numerical integration of $\int_{x_0}^{x_n} f_y(t, y(t)) \cdot v(t)\,dt$, f_y (t,y(t))-v(t)dt, if y is replaced by y and v tends to an integrable function for $h \to 0$. One can invoke the theory of compact; operators (compare Werner-Schaback [27] Chapter IV to derive estimates for v from (35), if the behaviour of $h^{4-k} \cdot \Sigma A_j$ is known. This is related to the proper choice of k.

If u_j'' and u_j''' are close to y_j'' and y_j''' there is control of their magnitude and by Axiom A3 the fourth (and fifth) order derivatives of $w(x,h)$ are bounded in each interval I_j. This implies a uniform bound for the quantities A_j and since their number grows like $\frac{1}{h}$, the expression $h \cdot \Sigma A_j$ is bounded. From this consideration one expects to get an estimate of v for k =3 at least.

To improve the order k of convergence a sharper estimate for ΣA_j is needed.

If w were five times continuously differentiable, A_j would be of order O (h) as is seen by (32). In general, however, w is only twice continuously differentiable. Hence

$$A_j = \Delta^4 (j,j,j,j-1,j-1)\,w - \frac{w^{IV}}{4!}(x_j-0) + \frac{w^{IV}}{4!}(x_j+0) \tag{36}$$
$$- \Delta^4 (j,j,j,j+1,j+1)\,w - jp\,(w_j^{IV})$$
$$= -\theta_1 \cdot h \cdot w^V(\tilde{x}_{j-}) - \theta_2 \cdot h \cdot w^V(\tilde{x}_{j+}) - jp\,(w_j^{IV})$$

where we introduced the jump of the fourth order derivative of w in x_j, i.e.

$$jp\,(w_j^{IV}) := w^{IV}(x_j+0) - w^{IV}(x_j-0).$$

This jump is directly related to the values of the second and third order derivatives of u(x,h) by the parameter is ation of the generating family $t(x_j, x_j, h, u''_j, u'''_j)$. Since $u''(x,h)$ is continuous,the problem reduces to the estimation of the jump for u''' at the knots. The next section is devoted to this task.

7. Asymptotic expansion of the error.

Again we use the above representation of the generating function of the splines, that is $t(x; x_j, h, t''_j, t'''_j)$,and assume differentiability with respect to x and the parameters of sufficiently high order (that is we use now the left end point x_j and the length h of the interval I_{j+1} and the second and third derivative for the parameterisationy. Also we assume that in all of $[x_o, x_+]$ the same generating functions are used, since we will have to compare

$$t^{IV}(x_j-0\,; x_{j-1}, h, t''_{j-1}, t'''_{j-1}) \quad\text{and}\quad t^{IV}(x_j+0\,; x_j, h, t''_j, t''_j)\ .$$

We observe that u(x,h) and its derivatives at the knots are (recursively) defined functions of h. It is left to the reader to verify that they depend continuously differentially on h.
For $j = 0$ by construction

$$w(x_0, h) = w'(x_0, h) = w''(x_0, h) = 0.$$

We procede by induction to show

$$\frac{d^i}{dx^i} w(x_j, h) = \mathbf{0}(h^{4-i}), \qquad i = \mathbf{0}, \mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4} \tag{37}$$

to hold uniformly in $[x_0, x_+]$.
Assume (37) to hold for $j < n$ and also for $j = n$ and $i = 0,1,2$.
In I_{j+1} the spline is determined from the data at x_j and equation (22).
this implies that $w(x_{j+1}, h)$ satisfies (31).

Let $x = x_0 + sh$, and (with $k=4$ in (34))

$$v(s, h) = w(x, h) \bullet h^{-4} \bullet \tag{38}$$

Hence

$$\frac{d^i}{ds^i} v(s, h) = \frac{d^i}{dx^i} w(x, h) \bullet h^{i-4} \bullet \tag{39}$$

In I_{j+1}, we have

$$h \cdot \frac{d}{dx} v(s, h)\Big|_{s = j+1} = v'(s, h)\Big|_{s = j+1} = h.f_y(x_o + (j+1)h, \tilde{y}_{j+1} \tag{40}$$

and

$$\begin{aligned} v(s, h) &= v_j + v'_j(s - j) + \frac{1}{2} v''_j (s - j)^2 + \frac{1}{6} \cdot v'''_j (s - j)^3 \\ &+ \frac{1}{24} \cdot v^{IV}_j (s - j)^4 + (s - j)^5 \cdot \Delta^5 (j, j, j, j, j, s) v \end{aligned} \tag{41}$$

$$\begin{aligned} v'(s, h) &= v'_j + v''_j (s - j) + \frac{1}{2} v'''_j (s - j)^2 + \frac{1}{6} v^{IV} (s - j)^3 \\ &+ 5 (s - j)^4 \Delta^5 (j...,) v + (s - j)^5 \cdot \Delta^6 (... , s, s) v . \end{aligned}$$

This yields

$$(42)\qquad v'_j + v''_j + \frac{1}{2} v'''_j + \frac{1}{6} v^{IV}_j + 5\, w^{V}_j \cdot h + w^{VI}_j \cdot h^2 = h \cdot f_y(x_{j+1}, \tilde{y}_{j+1})\,[v_j + v'_j + \frac{1}{2} v''_j + \frac{1}{6} v'''_j + \frac{1}{24} v^{IV}_j + \dots].$$

For $h \to 0$ this frunishes

$$(43)\qquad v'_j + v''_j + \frac{1}{2} v'''_j + \frac{1}{6} v^{IV}_j = 0\,;$$

i.e. v'''_j becomes a function of. v'_j, v''_j, v^{IV}_j It should he observed that boundedness of v'''_j implies $w'''_j \to 0$ and thus the last two arguments. u''_j, u''_j of $w^{IV} = v^{IV} = t^{IV}(x_{j+1}; x_j, h, u''_j, u''_j) - y^{IV}$ tend to y''_j, y'''_j respectively.

The equations (41) also yield the recurrence relations for the derivatives of lower order. In the limit $h \longrightarrow 0$, we have

$$(44)\qquad \begin{aligned} v_{j+1} &= v_j + v'_j + \frac{1}{2} \cdot v''_j + \frac{1}{6} v'''_j + \frac{1}{24} v^{IV}_j + 0(h) \\ v'_{j+1} &= v'_j + v''_j + \frac{1}{2} v'''_j + \frac{1}{6} v^{IV}_j + 0(h) \quad = 0(h), \text{because of (43)}, \\ v''_{j+1} &= v''_j + v'''_j + \frac{1}{2} v^{IV}_j + 0(h) \\ v'''_{(j+1-0)} &= v'''_j + v^{IV}_j + 0(h) \end{aligned}$$

and from (43)

$$(45)\qquad v'''_{j+1} := v'''_{(j+1+0)} = -2\, v'_{j+1} - 2 v''_{j+1} - \frac{1}{3} v^{IV}_{j+1} + 0(h)\ .$$

Therefore

$$(46) \qquad jp\,(v'''_{j+1}) = -2v'_j - 4v''_j - 4v'''_j - \frac{8}{3}v^{IV}_j + 0(h) .$$

Omitting the terms 0(h), using $v'_j = 0$ and (43) we find the recurrence relations

$$v_{j+1} = v_j + \frac{1}{6}v''_j - \frac{1}{72}v^{IV}_j$$

$$(47) \qquad v''_{j+1} = -v''_j + \frac{1}{6}v^{IV}_j$$

$$v'''_j = -2v''_j - \frac{1}{3}v^{IV}_j$$

for the leading terms of the error w(x,h) and its derivatives at $x = x_{j+1}$.

This proves the assertion made above about the "behaviour of the error.

Since we are interested in $j \to \infty$, $h \to 0$ such that $x_0 + h \to x$ (fixed),

we consider the solution of (47) for $j \to \infty$.

This is an inhomogeneous system of difference equations, multiples of v^{IV}_j being the inhomogeneous parts. The general solution is given by

$$(48) \qquad v_j = v_0 + \frac{1}{12}[1-(-1)^j]v''_0 + \frac{1}{72}\cdot B_j$$

$$v'_j = 0$$

$$v''_j = (-1)^j\cdot v''_0 + \frac{1}{6}\cdot B_j$$

$$v'''_j = -(-1)^j.2.v''_0 - \frac{1}{3}v^{IV}_j - \frac{1}{3}B_j$$

$$B_j = (-1)^{j-1}\left[v^{IV}_1 - v^{IV}_1 + \ldots + (-1)^{j-1}.v^{IV}_{j-1}\right].$$

The proof is immediate by induction.

From (48) we conclude that the B_j are uniformly bounded for $h \to 0$, $0 \le j \cdot h \le x_+ - x_0$, since the difference $v_j^{IV} - v_{j+1}^{IV} = h \cdot w^V(\tilde{x}_j)$ taking appropriate points $\tilde{x}_j$.
This in turn implies the boundedness of the v_j and v_j'', v_j'''.
Also $\Sigma\, jp(w_j''') = h \cdot \Sigma\, jp(v_j'')$ is bounded.

Using interpolation to express w(x,h) in each I_j and the estimates derived from (37), (44), (48) for w(x,h) and its derivatives in the knots, one easily finds $w^{(i)}(x,h) = 0(h^{4-i})$ to hold uniformally in $[x_o, x_+]$, if u(x,h) exists.
These a priori estimates show that any solution u(x,h) and its derivatives up to the third order are close to the corresponding values of y(x) if h is sufficiently small.
In the usual way one can specify closed domains for the parameter t''_j, t'''_j containing $y''(x_j)$ and $y'''(x_j)$ to get a priori estimates for the fourth and fifth order derivatives of t and from this fix h_o and $[x_o, x_+]$ so as to guarantee that u(x,h) and its derivatives lie in the said domains such that the a priori estimates apply. Hence one can finally conclude existence of the spline approximations u(x,h).
Thus we obtained all the properties that were needed to prove 4th order convergence, where we leave technicalities such as selecting a proper sub-interval $[x_0, x_+]$, h_0 and controlling the influence of the 0(h) terms to the reader.
It is worth pointing out, that $w'(x,h)=0(h^4)$ holds at the knots because of (31), but only $0(h^3)$ within the intervals I_j as can be seen from (41).

8. Numerical Application

The foregoing considerations have practical consequences also.
First we observe that the boundedness of the solutions of the homogeneous system to (47) will prevent numerical instability.
We need not be afraid of having accumulation of round off errors.
Secondly, the errors w, w'', w''' show an oscillatory behaviour by (48) which is also visible in applications.

Nevertheless, <u>Richardson Extrapolation</u> is possible, if only values with even indices j are used. This is illustrated by the following examples, taken from Appendix B.
In-the first example the exact solution is tan x.
We get the following table

x	h	j	u(x,h)	w = u(x,h) - tan x	w. h^{-4}
1.5	.4	3	13.6056	-.4958	- 19.4
	.2	6	14.1521	.0508	31.7
	. 1	12	14.1049	.0035	34.9
1. 1	.4	2	1.978163	0.01340	.5236
	.2	4	1.965815	0.00106	.6597
	. 1	8	1.964833	0.00007	.7347

This shows that for even j the convergence is of fourth order, while for odd j the expected difference arises.
In the next table we use numbers from the third example and apply <u>Richardson Extrapolation</u>.

x	h	j	u(x,h) .	extrap.values
0.9	. 1	6	1.03771496	
	.05	12	1.03758845	
	.025	24	1.03758023	1.03758002
				1.03757968 ± 4.10^{-8}
1.3	0. 1	10	3.3398534	
	0.05	20	3.3376001	
	0.025	40	3.3374549	3.3374499
				3.3374452± $7\text{-}10^{-7}$
1.4	0.1	11	8.856543	
	0.05	22	8.875228	
	0.025	44	8.874017	8.876473 (poor since j is odd!)
				8.873936 ± 6.10^{-6}

For ease of comparison the extrapolated value of the first two lines is placed adjacent to the computed value of the third line.
The fourth line contains the extrapolated value of the second and third line.
Some estimated error bounds are added.

9. An Application to differential equations with moveable singularities :
Riccati equations.

The solutions of non—linear differential equations may become infinite in places where the differential equation is given by a perfectly smooth right hand side. Furthermore, the singularity depends on the individual solution, and there may be others behaving in a very regular fashion.

As an example consider the problem

(49) $$y' = 1 + y^2 , \qquad y(x_0) = y_0,$$

with the solution

$$y = \tan (x - x_0 + \arctan y_0) .$$

Obviously the poles are dependent on the initial data.
It is, however, remarkable that the analytical form of the singularity is well determined - it consists of 1st order poles only. This property is shared(under mild assumptions) by all so-called Riccati differential equations, characterised by a right hand side

(50) $$f(x,y) = f_0(x) + f_1,(x)\cdot y + f_2(x)\cdot y^2 .$$

For simplicity we assume $f_0(x)$, $f_1(x)$, $f_2(x)$ to be holomorphic functions of x.
These equations or systems of such equations frequently arise in applications to chemistry, biology and more general control theory.

Theorem : Let f(x,y) have the form (50) with holomorphic functions $f_j(x)$ and assume $f_2(x) \neq 0$ in $(\alpha , ß)$. Then every solution y(x) of the differential equation $y' =f(x,y)$ is holomorphic in $(\alpha , ß)$ or has poles of tho first order. If $y(x)$ has a pole at x^* the residue is given by

(51) $$c_{-1} = - 1/f_2(x^*).$$

Proof : It is. proved in standard text books on differential equations that solutions of ordinary differential equations with analytic $f(x,y)$ are locally analytic. To consider the totality of the solutions in a neighbourhood of x^*, assume $\bar{y}(x)$ to be a solution with $\bar{y}(x^*) = 0$, and hence regular analytic for x sufficiently close to x^* . Let $y(x)$ be any second solution different from $\bar{y}(x)$. Let

(52) $$v(x) = 1/(\bar{y}(x) - y(x))$$

such that

(53) $$y(x) = \bar{y}(x) - 1/v(x)$$, where we assume $v(x) \neq 0$ for the derivation

$$y'(x) = \bar{y}'(x) + v'/v^2$$ and by means of the differenta l equations ,

$$= f_0 + f_1 y + f_2 y^2$$

$$= f_0 + f_1\bar{y} + f_2\bar{y}^2 - f_1/v - 2f_2\bar{y}/v + f_2/v^2 .$$

Hence after multiplication with v^2 and appropriate cancellations:

(54) $$v' = f_2 - (f_1 + 2f_2 y)\cdot v .$$

Now assume $y(x) \to \infty$ for $x \to x^*$. By (52) this implies $v(x) \to 0$ and by (54) we find

(55) $$v^1(x^*) = f_2(x^*).$$

This proves,in view of (53),the statement on the residue. ■

If we dispense with the assumption $f_2(x) \neq 0$, the solution y may have poles of order m.

Then $v(x) = (x-x^*)^m \bullet q(x)$, $q(x^*) \neq 0$ and from (54) we find

(56) $f_2(x) = m(x-x^*)^{m-1} .[q(x^*) + 0(|x-x^*|)].$

Hence a pole of order m of a solution of the differential equation at x* may only arise if f_2 has a zero of order m-1 at x*.

It is obvious that one can get the expansion of v(x) from (54) of $\bar{y}(x)$ from the differential equation and $\bar{y}(x) = 0$ and hence of y(x), at the pole x*.

For example

$$v''(x^*) = f'_2(x^*) - f_1(x^*)\cdot v'(x^*)$$
$$= f^1{}_2(x^*) - f_2(x^*)\cdot f_1(x^*)$$

and hence

(57)
$$y(x) = -1/v(x) + 0(|x-x^*|) = \frac{-1}{(x-x^*)f_2(x^*) + \frac{u''}{2}(x-x^*)^2 + \ldots} + 0(|x-x^*|)$$
$$= -(f_2(x^*)(x-x^*))^{-1} + \frac{f'_2(x^*) - f_2(x^*)\cdot f_1(x^*)}{2f_2(x^*)} + 0(|x-x^*|) .$$

Needless to say, rational splines should provide a good type of approximation to the solutions of the Riccati equations. The quality of the approximation obtained in the examples given in Appendix B will become apparent from the application in the next section.

10. The estimation of location of poles for solutions of Riccati equations

To find the movable singularities of a solution of an initial value problem we propose two methods. The first one is general and can

be used whenever a pole (of first order) is expected.
The second one uses the special properties of Riccati equations.

Method I : We use the pole of the rational spline solution in the interval I_j. closest to this pole as an estimate for the pole of exact solution.
That is, if u(x) is given by (2) in I_j, then we estimate

(58) $$x_{pole} = x_{j-1} + 1/d_j .$$

To get an appraisal of the error assume that the exact solution has a simple pole at x* .
Let $t = x - x^*$ and in particular $t_j = x_j - x^*$,... and $w = u - y$,
then,

(59) $$y(x) = \frac{c_{-1}}{t} + c_0 + c_1 t + c_2 t^2 + \ldots \quad .$$

Hence

$$\Delta^2(x_{j-1}, x_j, x_j)u = \Delta^2(\ldots)y + \Delta^2(\ldots)w$$
$$= \frac{c_{-1}}{t_{j-1}t_j^2} + c_2 + 0(|t_{j-1}|) + 0(\|w\|\cdot h^{-2})$$
$$+ 0(\|w'\|\cdot h^{-1})$$

and

$$\Delta^3(x_{j-1}, x_{j-1}, x_j, x_j)u = \Delta^3(\ldots)y + \Delta^3(\ldots)w$$
$$= \frac{-c_{-1}}{t_{j-1}^2 \cdot t_j^2} + c_3 + 0(|t_{j-1}|) + 0(\|w\|\cdot h^{-3})$$
$$+ 0(\|w'\|\cdot h^{-2}) .$$

By (18) we obtain

(60) $$\frac{1}{d_j} = \frac{\Delta^2(x_{j-1},x_j,x_j)u}{\Delta^3(x_{j-1},x_{j-1},x_j,x_j)u}$$

$$= -\frac{t_{j-1}^2 \cdot t_j^2}{t_{j-1}\cdot t_j^2} \cdot \frac{c_{-1}+c_2\cdot t_{j-1}\cdot t_j^2+0(t_{j-1}^2\cdot t_j^2) + 0(\|w\|\cdot h^{-2}\cdot |t_{j-1}|\cdot t_j^2 + \ldots}{c_{-1}+c_3\cdot t_{j-1}^2\cdot t_j^2+0(|t_{j-1}^3|\cdot t_j^2) + 0(\|w\|\cdot h^{-3}\cdot t_{j-1}^2\cdot t_j^2+\ldots}$$

$$= -t_{j-1}(1+\frac{c_2}{c_{-1}}\cdot t_{j-1}\cdot t_j^2+0(t_{j-1}^2\cdot t_j^2)+0[(\|w\|\cdot h^{-3}+\|w'\|\cdot h^{-2})\cdot t_{j-1}^2\cdot t_j^2]).$$

This formula expresses $x_{pole}- x_{j-1}$ by means of $x^* - x_{j-1}$ plus error terms.

Method II From (59) we obtain

$$y_j'' = \frac{2c_{-1}}{t_j^3} + 2c_2 + 0(|t_j|) ,$$

hence

$$t_j^3 = \frac{2c_{-1}+2c_2 t_j^3+0(|t_j^4|)}{y_j''}$$

$$= \frac{2c_{-1}+2c_2 t_j^3+0(|t_j^4|)}{u_j'' - w_j''} .$$

Now one may eliminate c_{-1} by (5) i.e. the coefficient $f_2(x)$ of y^2 on the right hand side of the Riccati equation and use the numerically obtained value of u''_j to express t_j:

(61) $$-t_j^3=\frac{2}{f_2(x^*)\cdot u_j''}\left(1-c_2\cdot f_2(x^*)\cdot t_j^3+0\left(\left|\frac{w_j''}{u_j''}\right|\right)+0(|t_j^4|)\right) .$$

The pole will thus be approximated by solving the equation

(62) $$(x_{pole}-x_j)^3 = \frac{2}{u_j''\cdot f_2(x_{pole})} .$$

Equation (61) gives an appraisal of the error.

From (62) we obtain

(63) $$x_{pole} = \phi(x_{pole}) := x_j + \sqrt[3]{\frac{2}{u_j''}} \cdot f_2^{-\frac{1}{3}}(x_{pole}) .$$

Since

$$\frac{\partial\phi}{\partial x_{pole}} = \left(-\frac{1}{3}\right) \cdot \sqrt[3]{\frac{2}{u_j'' f_2}} \cdot \frac{f_2'(x_{pole})}{f_2(x_{pole})} = -\frac{(x_{pole} - x_j) \cdot f_2'(xpole)}{3f_2(xpole)}$$

becomes small for x_j close to x_{polo} equation (63) may be solved. by iteration in the usual fashion.

Appendix A: Program for rational spline approximation for solution of initial value problem. The program has to be called by a driver program and the right hand side of the differential equation has to be available as a function subroutine.

It is assumed that the resulting rational spline has positive second order derivatives throughout the interval of integration, (It is also easy to adapt it to the case that this derivative is always negative.) If this derivative changes sign it could be appropriate to switch to cubic splines. No provision has been made for this case except the printing of an error message.

If no convergence occurs in the evaluation of d within MAXIT iterations (counter ITER),the step size will be halved and evaluation of d starts again. If MHALB step size halvings have been performed(counter ITERA) without successful calculation of d,the program will terminate the integration of the differential equation. The program should be self explanatory in view of the foregoing text.

```
   SUBROUTIN    NLINT   ( XANF , XEN D ,  YOA , Y2A , F, EPS , HA, MAXIT ,HALB )
   SOLVES    THE    INITIAL   VALUE   PROBLEM
        Y'   =   F ( X , Y )   ,      Y( X A N F )    =    YOA   .
   IF POSSIBLE THE INTEGRATIONEXTENDSUP TO THE  POINT XEND.
   RATIONAL    SPLINE    FUNCTIONS    ARF    USED.
   NOT A T ION :
         XANE     =    INITIAL    VA LUE    OF    X
         XEND     =   ENDPOINT  OF  INTEGRATION UNLESS A PULE  ARISES
         YOA      =   Y(XANF)
         Y2A      =   Y"  (  XANF )
         HA       =    INITIAL    STEP    SIZE
         MAXIT   =   MAXIMAL NUMBER OF  ITERATIONS ALLOWED IN  ONE    STEP
         EPS      =   THE    ACCURACY    USED    IN    VARIOUS    PLACES
         MHALB =   MAXIMAL    NUMBER    OF    HALVING    OF    STEP    SIZE
         NI         =   NUMBER  OF  DIFFERENT  STEP   SIZES   FOR   INTEGRATION

       WRI TE(  6, 1  )

           H0        =   H A    *    4.
           N I       =   3
       D0  100              I=1.    NI
           H0        =   H0/ 2.
           H         =   H0
           ITERA  =   0
    I N I T I A L   VALUES
           X         =   XANF
           Y0        =   Y0A
           Yl        -   F  (  X,Y0)
           Y2        =   Y2A
C                                                              GO  TO  98
C  INTEGRATION
C    5    CONTINUE
        IF ( ITERA    .GE . MHALB )
            ITERA =  ITERA   +   1
            DH       =  0.
            H        =  H/2.
         WRITE  ( 6 , 2 )    H
C
     10    CONTINUE
            INTER=0
            GN      =0.
            XX      =X + H
            YN      =1. - DH
  REGULA FALSI
  20.CONTINUE
      IF (MAXIT    .LT . ITER )                   GO TO 5
           ITER   =   ITER    +    1
           W0      =    YO    +   H * (Y) +H*Y2/YN/2. )
           W1      =    F(XX,W0 )
           G       =    (W1 – Y1 ) /H – Y2* (1. +DH/YN/2.)/YN
       IF( ABS(G-GM) .LE.EPS)                  GO TO 30
       IF (ABS(G) . GE. 10000000.)             GO TO 96
       IF (ITER .EO. 1)
             ZE    = YN*YN*G /Y2/1.5
       IF (ITER    .GT.1)
             ZE    = G*(DHN – DH)/(G – GN )
             DHN = DH
```

```
            ZF     = G
            DH     = DH + ZF
            YN     = 1. - DH
         IF( ABS(ZF) .GE. EPS)                         GO TO 20
C
      30 CONTINUE
            D      = DH/H
         WRITE(6,3)  X,Y0,Y1,Y2,D
C
C     DATA FOR NEXT STEP
C
      X      =   XX
      YO     =   Y0  + H* ( Y1  +  H*Y2/YN/2. )
      Y1     =   F( X , Y0 )
   IF ( YN   .LE.  EPS )                              GO  TO   96
      Y2     =  Y2/YN/YN/YN
   IF(Y2.LE. EPS)                                     GO  TO  94
      DH     =   DH/YN

   IF( ( DH. LT. 1. ) .AND. ( X . LE . XEND-EPS ) )
 1                                                    GO  TO   10

            D      =  DH/H
         WRITF(6,3)   X,Y0,Y1,Y2,D
                                                      GO  TO  100

   ERROR MESSAGES

  94    WRITE (6, 95)
                                                      GO  10   100
  96    WRITE(6,97)
                                                      GO  10   100
  98    WRITE(6,99) ITERA
 100    CONTI NUE

      1. FORMAT ( *0*,T8,*X* ,T19,*U(X) *, T33,*U1 ( X ) * , 147 , *U0 (X)*,T61,*D*)
      2  FORMAT (*0    H   =*,    F6.4/)
      3  FORMAT (    F12.5,    4F14.8,    15,    F20.8,    F14.8)
     95  FORMAT (*0    Y2   BECOMES   ZERO   OR   NEGATIVE*)
     97  FORMAT ( *0   G   BECOMES   TO   LARGE*)
     99  FORMAT (*0    FINISHED BECAUSE*, 15,  *  HALVINGS  OF  STEP  SIZE* )

         RFTURN
         END
```

Remark: For practical purposes it is useful to replace

DH.LT.1. by

DH.LT.0.8 ,

say, to avoid overflow in case the pole almost coincides with a grid point.

Appendix B: The following numerical examples are obtained by means of the above program. Calculation was started at x = 0.3 and continued with the step size H until x. + H would transgress the estimated pole. Listed are the data x_j, u_j, u'_j, u_j'' and d_J such that u(x) is easily calculated in any intermediate point.

The program was modified so as to give some additional information that demonstrates the performance of the method.

The integer following d gives the number ITER of iterations in solving for d_j. The two last columns give the estimated values of the pole of the solution. In the last column the theory of Riccati equations based upon the value of u_j'' is used. In the foregoing column the pole was determined as the zero of the denominator, hence it depended essentially on d_j with its oscillatory behaviour and linear convergence (from the convergence of the third order derivative).

Obviously in the first case the exact solution is y = tan x and hence x_{pole}= 1,57079633.

GIVEN THE FOLLOWING INITIAL VALUE PROBLEMS

Y1 = 1 + Y.Y , Y(θ,3) = TAN(θ,3)

H = ,4000

X	U(X)	U'(X)	U"(X)	D		POLE	
,30000	,30933625	1,09568892	,67787260	1,00718652	10	1,29286476	1,73425808
,70000	,83842994	1,70296476	3,18384164	1,11133558	7	1,59981822	1,55643192
1,10000	1,97816315	4,91312945	18,57717022	2,11546559	6	1,57270918	1,57571861
1,50000	13,60557766	186,11174333	5104,97899781	13,75342189	6		1,57317207

H = ,2000

X	U(X)	U'(X)	U"(X)	D		POLE	
,30000	,30933625	1,09563892	,67787260	1,15192158	7	1,16811465	1,73425808
,50000	,54608991	1,29821418	1,48705267	,95892388	5	1,54283564	1,60382751
,70000	,84253117	1,70985878	2,81673433	1,25144173	4	1,49907836	1,59213020
,90000	1,25964463	2,58670459	6,68440084	1,46006956	5	1,58488949	1,56884041
1,10000	1,96581521	4,85442943	18,83630338	2,14737706	4	1,56568440	1,57352703
1,30000	3,59901631	13,95291841	101,43143720	3,69333058	4	1,57075832	1,57015881
1,50000	14,15219362	201,28458437	5683,10146002	14,13261274	4		1,57060165

H = ,1000

X	U(X)	U'(X)	U"(X)	D		POLE	
,30000	,30933625	1,09560892	,67787260	1,25339274	6	1,09783452	1,73425808
,40000	,42278420	1,17874310	1,01304608	1,04426510	4	1,35761124	1,65448921
,50000	,54631036	1,29845501	1,41034548	1,14485631	4	1,37347206	1,62348728
,62000	,68411929	1,40801920	2,03113446	1,07924788	4	1,52657120	1,59486413
,70000	,84230553	1,70947861	2,86110805	1,25456889	4	1,49708656	1,58749363
,80000	1,02961112	2,06009906	4,27750562	1,29552463	4	1,57188806	1,57615144
,90000	1,26019176	2,58808326	6,48578857	1,54564472	4	1,54697921	1,57559911
1,00000	1,55735776	3,42536319	10,73300431	1,73609425	4	1,57600559	1,57117549
1,10000	1,96463313	4,86055923	19,01801726	2,15062492	4	1,56498113	1,57201404
1,27000	2,57203357	7,61535666	39,32420856	2,68428186	3	1,57253912	1,57050153
1,30000	3,60233443	13,97601334	100,43592813	3,70162622	* 4	1,57015153	1,57104847
1,40000	5,79733212	34,60905966	401,97940718	5,85303421	3	1,57085156	1,57071646
1,50000	14,10490703	199,94840241	5636,53808763	14,11401612	3		1,57079553

GIVEN THE FOLLOWING INITIAL VALUE PROBLEM:

X	U(X)	U[1](X)	U"(X)	0			POLE
H = ,4000							
,30000	,30000000	1,18000000	1,30800000	1,03979096	11	1,26173177	1,45205731
,70000	,95115243	2,39469095	6,56421315	1,35866718	7	1,43601543	1,37289780
1,10000	3,05930032	11,56931846	68,98676496	2,97605385	7		1,40720014
H = ,2000							
,30000	,30000000	1,18000000	1,30800000	1,17921760	7	1,14801991	1,45205731
,50000	,57023383	1,57516662	2,93130389	1,03194186	5	1,46904684	1,38035206
,70000	,95913965	2,40004887	5,86457813	1,43771415	5	1,39554856	1,39865763
,90000	1,60575906	4,38846216	16,21662564	1,91042320	4	1,42344423	1,39776364
1,10000	3,00833327	11,26006907	68,73430075	3,25297245	5	1,40741115	1,40757580
1,30000	9,19472408	87,23258319	1611,32917076	9,31002045	5		1,40746868
H = ,1000							
,30000	,30003400	1,18000000	1,30800000	1,28148813	6	1,08034277	1,45205731
,40000	,42552128	1,34105134	1,97369779	1,07873639	4	1,32701053	1,40442253
,50000	,57065818	1,57566217	2,77972311	1,20892640	3	1,32718022	1,39607182
,60000	,74404431	1,91360194	4,09143625	1,18490466	4	1,44394976	1,38774333
,70000	,95861149	2,40093599	5,97303071	1,42660779	4	1,40096351	1,39440326
,80000	1,23433979	3,16359472	9,47843576	1,56763624	4	1,43790309	1,39533915
,90000	1,60692198	4,39213398	15,60842748	1,96145624	4	1,40982529	1,40201163
1,00000	2,14444431	6,59864139	30,43382436	2,40229444	4	1,41626871	1,40354424
1,10000	3,00459144	11,23756972	69,39195980	3,24947578	4	1,40774195	1,40660103
1,20000	4,64232301	23,99116296	225,57795463	4,81028584	3	1,40788785	1,40697177
1,30000	9,21475703	87,60174705	1613,86178973	9,31018050	4	1,40740930	1,40741243
1,40000	134,95203914	18215,01286718	**************	134,96545882	4		1,40740952

VEN THE **FOLLOWING INITIAL** VALUE *PROBLEM:*

X	u'(X)	U'(X)	U"(X)	D			POLE
.30000	.30000000	1.00810000	.10843740	2.72562711	8	.66688804	1.90696985
.40000	.40155534	1.02579947	.26173361	1.80665898	5	.95350789	1.71329630
.50000	.50585439	1.06397217	.51216432	2.02636705	5	.99349401	1.62655110
.60000	.61546322	1.13636619	1.01027732	1.45748336	4	1.28611418	1.53982163
.70000	.73501306	1.26471966	1.62762712	1.84677392	5	1.24148479	1.51299313
.80000	.87142359	1.48600261	2.99416152	1.54897029	4	1.44559018	1.47491252
.90000	1.03771496	1.87225040	4.95411134	2.06581185	5	1.38407119	1.47129673
1.00000	1.25616003	2.57793802	9.91878046	2.13099558	4	1.46926423	1.45639338
1.10000	1.57607820	4.00910089	20.35630315	2.92735792	5	1.44160497	1.45874815
1.20000	2.12179705	7.48291270	57.53788145	3.87588766	4	1.45800541	1.45425265
1.30000	3.33985339	19.85130892	250.50962733	6.45327112	5	1.45496017	1.45561034
1.40000	8.85654302	154.73917445	5614.87960220	18.19499417	5		1.45520096

H = .0500

.30000	.30000000	1.00810000	.10843740	3.02097247	6	.63101924	1.90346355
.35000	.35056465	1.01505471	.17722731	2.38953457	5	.76849154	1.80204983
.40000	.40156899	1.02580122	.25960206	2.42888989	4	.81171072	1.73086163
.45000	.45322841	1.04159674	.38282520	1.95881641	5	.96051237	1.66560286
.50000	.50583874	1.06396821	.52154937	2.08868907	4	.97876920	1.62174788
.55000	.55976511	1.09478444	.72611146	1.72189341	4	1.13075604	1.57863372
.60000	.61549748	1.13638137	.95126094	1.90552103	4	1.12479085	1.55218441
.65000	.67363084	1.19172142	1.28455116	1.61907848	4	1.26763529	1.52396348
.70000	.73496404	1.26468435	1.65477728	1.84076275	4	1.24325306	1.50886342
.75000	.80047640	1.36042889	2.21073521	1.62824934	4	1.36415655	1.49085825
.80000	.87150618	1.48609474	2.85216789	1.88314901	4	1.33102542	1.48298805
.85000	.94974671	1.65170860	3.83722210	1.74942810	4	1.42161538	1.47190959
.90000	1.03758845	1.87203773	5.04983851	2.04207278	4	1.38969851	1.46841110
.95000	1.13822043	2.16923004	6.97587766	2.00473590	4	1.44881882	1.46191074
1.00000	1.25637320	2.57847362	9.57666219	2.35428652	4	1.42475714	1.46082514
1.05000	1.39886485	3.15739723	13.94397147	2.45380061	4	1.45753107	1.45724793
1.10000	1.57660223	4.00766624	20.65034406	2.91317763	4	1.44326777	1.45727751
1.15000	1.80719938	5.31924480	33.11565616	3.24804338	4	1.45787766	1.45548738
1.20000	2.12258220	7.48771149	56.35425758	3.97361234	4	1.45166018	1.45583483
1.25000	2.58487632	11.43997750	109.52412407	4.84933307	4	1.45621392	1.45507662
1.30000	3.33760012	19.82588101	251.94429158	6.46696118	4	1.45463213	1.45533406
1.35000	4.79431863	42.89105759	813.22089197	9.50062860	4	1.45525619	1.45511752
1.40000	8.87522765	155.38854513	5620.93572262	18.12326301	4	1.45517770	1.45518177
1.45000	91.52109921	17611.77464071	**************	193.13588483	4		1.45517809

H = .0250

.30000	.30000000	1.00810000	.10843740	3.18655991	5	.61381804	1.90171527
.32500	.32523932	1.01117308	.13910408	2.81016033	4	.68085158	1.85005907
.35000	.35056540	1.01505477	.17306001	2.79202498	4	.70816298	1.80532287
.37500	.37599992	1.01988099	.21503977	2.47760963	4	.77861483	1.76457244
.40000	.40156858	1.02580117	.26051172	2.49937828	4	.80009950	1.72939563
.42500	.42730444	1.03297954	.31614902	2.22982441	4	.87346581	1.69672052
.45000	.45322956	1.04159695	.37551285	2.27929652	4	.88873186	1.66886676
.47500	.47939392	1.05185281	.44778076	2.04425249	4	.96417636	1.64248158
.50000	.50583771	1.06396795	.52409830	2.11395790	3	.97304632	1.62043096
.52500	.53262983	1.07818743	.61681512	1.90693649	4	1.04940131	1.59910291
.55000	.55976692	1.09478585	.71416290	1.99212828	3	1.05197571	1.58173285
.57500	.58737142	1.11406734	.83244702	1.80901510	4	1.12778698	1.56454306
.60000	.61549557	1.13638052	.95643179	1.90661858	3	1.12448875	1.55097416
.62500	.64421892	1.16211641	1.10735125	1.74486247	4	1.19811107	1.53719787
.65000	.67363366	1.19172303	1.26589030	1.85290195	3	1.18969397	1.52671613
.67500	.70384155	1.22571340	1.45945775	1.71106322	4	1.25943194	1.51576017
.70000	.73496084	1.26468205	1.66399333	1.82834887	3	1.24694157	1.50777502
.72500	.76712280	1.30931843	1.91473519	1.70585299	4	1.31121699	1.49914355
.75000	.80046077	1.36043282	2.18218463	1.83182491	3	1.29590370	1.49316277
.77500	.83520625	1.41897767	2.51169718	1.72884899	4	1.35341952	1.48643707
.80000	.87150105	1.48608902	2.86769316	1.86353164	3	1.33661552	1.48204973
.82500	.90959322	1.56312179	3.30895786	1.78099375	4	1.38648428	1.47687504
.85000	.94975350	1.65171792	3.79343843	1.92504734	3	1.36946775	1.47373872
.87500	.99229184	1.75386737	4.39840177	1.86469703	4	1.41128015	1.46981482
.90000	1.03758023	1.87202391	5.07566871	2.01957832	3	1.39515287	1.46764521
.92500	1.08605132	2.00921607	5.92916990	1.98421502	4	1.42897764	1.46471911
.95000	1.13823129	2.16925236	6.90608112	2.15249282	3	1.41457762	1.46328146
.97500	1.19474376	2.35693415	8.15361339	2.14637921	4	1.44090090	1.46114128
1.00000	1.25635959	2.57843942	9.62072515	2.33230329	3	1.42876070	1.46024327
1.02500	1.32401321	2.84175716	11.52274560	2.36191651	4	1.44838499	1.45871303
1.05000	1.39888330	3.15745411	13.82859498	2.57244822	3	1.43873474	1.45819884
1.07500	1.48243810	3.53962777	16.88044035	2.64787405	4	1.45266147	1.45713392
1.10000	1.57657789	4.00757338	20.73008151	2.89463364	3	1.44546686	1.45687932
1.12500	1.68375101	4.58806898	25.97093418	3.03229508	3	1.45478321	1.45616232
1.15000	1.80723436	5.31941203	32.90031672	3.33550153	3	1.44980499	1.45607059
1.17500	1.95143635	6.25756333	42.72113739	3.56393901	3	1.45558842	1.45560765
1.20000	2.12253163	7.48740235	56.52343148	3.96117017	3	1.45245065	1.45560611
1.22500	2.32932173	9.14200069	77.28522048	4.33469888	3	1.45569653	1.45532345
1.25000	2.58495873	11.44064318	109.02817410	4.90305992	3	1.45395427	1.45536041
1.27500	2.90987589	14.76411864	161.40275753	5.53936806	3	1.45552601	1.45520119
1.30000	3.33745492	19.82424308	252.41851782	6.46300208	3	1.45472686	1.45524319
1.32500	3.92714311	28.07604406	428.28282869	7.67316731	3	1.45532428	1.45516445
1.35000	4.79464999	42.80684843	811.37036597	9.51818975	3	1.45506199	1.45519370
1.37500	6.19979848	73.67090058	1833.48284036	12.46843701	3	1.45520251	1.45516347
1.40000	8.87401684	155.34642293	5622.94999630	18.12816287	3	1.45516279	1.45517534
1.42500	15.97125535	518.97391518	34394.45291138	33.14515421	3	1.45517032	1.45516973
1.45000	91.66483591	17667.13460333	**************	193.41152353	3		1.45517022

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