CEAS #329

ON THE USE OF SPLINES FOR THE NUMERICAL SOLUTION OF NONLINEAR MULTIPOINT BOUNDARY VALUE PROBLEMS

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Abstract.

Cubic splines on splines and quintic spline interpolations are used to approximate the derivative terms in some highly accurate schemes for the numerical solution of multipoint boundary value problems. The storage requirements are the same as that for the usual trapezoidal rule schemes that do not use derivatives but the accuracy is improved from $O(h^3)$ to either $O(h^6)$ or $O(h^7)$, where h is the net size. The use of splines leads to solutions that reflect the smoothness of the slopes of the differential equations.

1. Introduction.

We consider the numerical solution of the system of differential equations

$$\frac{dy}{dx} - f(x,y(x)) = 0, \tag{1.1}$$

with the multipoint boundary conditions

$$g(y(0),\ y(1)) = 0, \tag{1.2}$$

where

$$y,\ f \text{ and } g \in R^m, \text{ and } 0 \leq x \leq 1.$$

Let us subdivide the x range $[0,1]$ into n equal parts, such that $h = 1/n$ and $x_i = ih$, $i = 0,1,\dots,n$. If we integrate the p^{th} equation of the system (1.1) in the interval $[x_{i-1},x_i]$ and denote the resulting quantity by $\phi_{pi}(y)$ then we have

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$$(1.3) \qquad \Phi_{pi}(y) = y_{pi} - y_{p,i-1} - \int_{x_{i-1}}^{x_i} f_p(x,y(x))dx = 0,$$

where $y_{pi} = y_p(x_i)$ and $p = 1,2,\ldots,m$; $i = 1,2,\ldots,n$. The integral in (1.3) can be evaluated by the various numerical schemes. In this paper we will discuss three such schemes that require the numerical derivatives of f_p [1,pp.284-285],

$$(1.4) \qquad \Phi_{pi}(y) = y_{pi}-y_{p,i-1}- \frac{h}{2}(f_{pi}+f_{p,i-1})+ \frac{h^2}{10}(f^1_{pi}-f^1_{p,i-1}) - \frac{h^3}{120}(f^2_{pi}+f^2_{p,i-1})+ \frac{h^7}{100,800} f^6_p(\xi_i),$$

$$(1.5) \qquad \Phi_{pi}(y) = y_{pi}-y_{p,i-1}- \frac{h}{2}(f_{pi}+f_{p,i-1})- \frac{h^2}{12}(f^1_{pi}-f^1_{p,i-1}) - \frac{h^4}{720}(f^3_{pi}-f^3_{p,i-1})+ \frac{h^7}{30,240} f^6_p(\xi_i)$$

and

$$(1.6) \qquad \Phi_{pi}(y) = y_{p,i+1}-y_{pi}+y_{p,i-1}- \frac{3h}{8}(f_{p,i+1}-f_{p,i-1}) + \frac{h^2}{24}(f^1_{p,i+1}-8f^1_{pi}+f^1_{p,i-1})- \frac{h^8}{60,480} f^7_p(\hat{\xi}_i),$$

where $x_{i-1} \leq \xi_i \leq x_i$, $x_{i-1} \leq \hat{\xi}_i \leq x_{i+1}$, $f_{pi} = f_p(x_i,y(x_i))$ and the superscripts on f denote its derivatives. Equation (1.4) is associated with the name of Obrechkoff, (1.5) is the Euler-Maclaurin sum formula and (1.6) is the highest precision three point formula which uses f and f^1.

Equations (1.4) or (1.5) along with (1.1) and (1.2) are sufficient to determine y_{pi}, where $p = 1,2,\ldots,m$, $i = 0,1,\ldots,n$. But in (1.6), since $i = 1,2,\ldots,n-1$, we need one additional equation with $O(h^8)$ accuracy to determine y_{pi}. This can be easily achieved by including one additional equation with (1.6) of the type (1.5) with its last term replaced by

$$(1.7) \qquad \frac{h^6}{30,240}(f_i^5 - f_{i-1}^5) + O(h^9).$$

From now on let us denote by y, ϕ and g the vectors with the components y_{pi}, ϕ_i and g_p respectively. Then equation (1.5), (1.6) or (1.7) can be written as

$$(1.8) \qquad \phi(y) = 0$$

and (1.2) as

$$(1.9) \qquad g(y) = 0.$$

Clearly, $\phi \in R^{mn}$, $y \in R^{m(n+1)}$ and $g \in R^m$. It is worth noting that in (1.8), m components of y can be eliminated directly by expressing them as linear functions of the rest of the components by using (1.9), provided that $g(y)$ is a linear function of y. We will assume that $g(y)$ is linear and the necessary elimination of y components has been done so that we only have (1.8) to solve.

In this paper we focus our attention primarily on the efficient computation of two items; the required derivatives of f and the roots of the nonlinear system (1.8). To this end, we will first utilize a cubic spline on spline technique or a quintic spline to determine some approximations to the derivatives, and then use a nonlinear iterative technique to solve the resulting system of equations (1.8).

It is possible to compute the derivatives of f directly by differentiating the differential equation ([1], p.246). For example

$$f^1 = f_x + f_y \frac{dy}{dx}$$

and since from (1.1) $\frac{dy}{dx} = f$, we get

$$f^1 = f_x + f_y f, \tag{1.10}$$

where the subscripts denote the partial derivatives. The computationa of higher derivatives of f is, in many cases, rather cumbersome. If the differentiation (1.10) is reasonably easy to perform then (1.6) can be used to give an $O(h^8)$ formula. Of course, as mentioned earlier, due to the use of one equation of the type (1.5) with the last term replaced according to (1.7), which is necessary to make (1.6) fully determined, we still need to compute the third and the fifth derivatives of f at the two points, say x_n and x_{n-1}. The general expressions for these are quite involved ([1], p.246). The evaluation of the partial derivatives can, in principle, be done analytically, but more often that not, f is a complicated computer program and these computations are not possible without the expenditure of a considerable amount of work. Alternatively, it is also possible to use numerical derivatives of f. This is done in [2] to solve equations of the type

$$\Phi_{pi} = y_{pi} - y_{p,i-1} - \frac{h}{2}(f_{pi} + f_{p,i-1}) + \frac{h^3}{12} f^2_{p,i-\frac{1}{2}} - \frac{h^5}{480} f^4_{p,i-\frac{1}{2}} + O(h^7) \tag{1.11}$$

in a defferred correction mode. The principal disadvantages of using numerical derivatives for $f^2_{p,i-\frac{1}{2}}$ and $f^4_{p,i-\frac{1}{2}}$ from the usual piecewise interpolating polynomials is that these polynomials not only overlap but also lack smoothness at the junctions (net points x_i). Furthmore, the defferred correction mode necessitates the repeated solution of equations of the type $u^1(y^{(k)})z^{(k)}=b$ for different right hand sides b. We shall have more to say about this aspect of the problem later on. The use of cubic spline on spline and the quintic spline, that we advocate in this paper, to compute the numerical derivatives imposes not only smoothness at the junctions but also requires only a very small amount of computational work as will be shown later.

To achieve $O(h^6)$ accuracy as the cubic spline on spline techniques considered in this paper, the Gap schemes of White [3] require the computation of $f^1 = f_x+f_yf$ and $f^2 = f_{xx}+2f_{xy}f+f_{yy}ff+f_xf_y+f_yf_yf$ at each of the m(n+1) points y_{pi}, $i = 0,1,\ldots,n$, $p = 1,2,\ldots,m$. The difficulties associated with the computation of partial derivatives have already been mentioned. Furthermore, a total of 8m(n+1) multiplications are necessary to compute f^1_{pi} and f^2_{pi} to achieve $O(h^6)$ accuracy even after the partial derivatives have been computed. For $O(h^8)$ accuracy Whites' gap schemes will require the computation of f^3. Of course, $O(h^7)$ is not realizable with these schemes.

The numerical results obtained with our technique cannot be easily compared with other techniques in view of the following reasons given in [3]:

"Due to the fact that most numerical tests in this area are published with little detail concerning implementation, computer times, and so on, it is hard to make any final judgements about the relative merits of different techniques. The ultimate comparison will be that given by the user which will require: ease of use, applicability or adaptibility to its particular problem, and overall ecconomy in computer cost and reliability."

It is possible to use Taylor's expansion to expand about $x_{i-\frac{1}{2}}$ and prove the following result

$$(1.12)\quad \phi_{pi} = y_{pi}-y_{p,i-1}-\frac{h}{2}(f_{pi}+f_{p,i-1})+\frac{h^3}{24}(f^2_{pi}+f^2_{p,i-1}) - \frac{h^5}{240}(f^4_{pi}+f^4_{p,i-1})+O(h^7).$$

But since the above requires the evaluation of the second and the fourth derivatives it is not competitive with (1.4), (1.5) and (1.6), unless f^2 and f^4 are readily computable.

In the next section, we first describe the cubic spline on spline and quintic spline, and then show how these can be used to determine f'_{pi}, f^2_{pi} and f^3_{pi}. Computational considerations are discussed in the last section.

2. <u>Use of Spline on Spline and Quintic Splines</u>.

For the sake of clarity of presentation we shall drop the subscript p from this point on. It is however understood that a seperate spline interpolant will be used for each value of p. Furthermore, for the cubic spline on spline $f \in C^5$ and for the quintic spline $f \in C^6$, the class of five or six times continuously differentiable functions. Seperate splines must be used in the x range if these conditions are not met in the whole interval $[0,1]$.

Let s denote a cubic spline interpolant [4] so that $s(x_i) = f_i$ for $i = 0,1,\dots,n$. Let the r^{th} derivatives of s at x_i be denoted by s_i^r. It is well known that if we have either

(2.1) $$s_0^1 = f_0^1 \text{ and } s_n^1 = f_n^1,$$

or

(2.2) $$s_0^2 = f_0^2 \text{ and } s_n^2 = f_n^2,$$

then s is unique [4].

It is customary to compute s_i^1 and s_i^2 directly from the f_i values by the following well known formulas

(2.3) $$s_{i+1}^1+4s_i^1+s_{i-1}^1 = \frac{3}{h}(f_{i+1}- f_{i-1})$$

and

(2.4) $$s_{i+1}^2+4s_i^2+s_{i-1}^2 = \frac{6}{h^2}(f_{i+1}-2f_i+f_{i-1}),$$

with (2.1) and (2.2) respectively for the boundary values at $i = 0$ and n.

To compute a bound on the error between s_i^r and f_i^r, we define

(2.5) $$e_i^r = f_i^r - s_i^r,$$

$\|f(x)\| = \max_x |f(x)|$, $\|e^r\| = \max_i |e_i^r|$, and then prove the following theorem.

Theorem 1. If $f \in C^5$ then

$$\|e^1\| \leq \frac{h^4}{15} \|f^5\| \tag{2.6}$$

and

$$\|e^2\| \leq \frac{3h^2}{4} \|f^4\|. \tag{2.7}$$

Proof. Subtracting $f^1_{i+1}+4f^1_i+f^1_{i-1}$ from both sides of (2.3), using (2.5) with $r = 1$, and then Taylor's expansion we get

$$\begin{aligned} e^1_{i+1}+4e^1_i+e^1_{i-1} &= -\frac{3}{h}(f_{i+1}-f_{i-1}) + (f^1_{i+1}+4f^1_i+f^1_{i-1}), \\ &= \frac{2h^4}{15} f^5(\mu_i),\ x_{i-1} \leq \mu_i \leq x_{i+1}, \end{aligned} \tag{2.8}$$

where $i = 1,2,\ldots,n-1$. Now due to (2.1) $e^1_0 = e^1_n = 0$, and if we let e and f^5 denote the vectors

$(e^1_1, e^1_2, \ldots, e^1_{n-1})^T$ and $(f^5(\mu_1), \ldots, f^5(\mu_{n-1}))^T$ respectively, then (2.8) can be written as

$$Ae^1 = \frac{2h^4}{15} f^5 \text{ or } e^1 = \frac{2h^4}{15} A^{-1} f^5.$$

If B is a matrix such that $(B)_{ij} = 1$ if $i = j+1$ or $i+1 = j$ and zero otherwise, then

$$\|A^{-1}\| = \|(4I+B)^{-1}\| = \frac{1}{4} \|(I+\tfrac{1}{4}B)^{-1}\| \leq \frac{1}{4} \frac{1}{\|I\| - \frac{1}{4}\|B\|}$$

$$\leq \frac{1}{4} \frac{1}{1-\frac{1}{2}} = \frac{1}{2}$$

and therefore

$$\|e^1\| \leq \frac{2}{15} h^4 \|A^{-1}\| . \|f^5\| \leq \frac{h^4}{15} \|f^5\| .$$

(It has come to our attention that an alternative proof of (2.6) is given in a book just published [10].)

This proves (2.6). To prove (2.7) we subtract $f^2_{i+1}+4f^2_i+f^2_{i-1}$ from both sides of (2.4) and use (2.5) with $r = 2$ and then use Taylor's theorem to get

$$(2.9)\quad e^2_{i+1}+4e^2_i+e^2_{i-1} = -\frac{6}{h^2}(f_{i+1}-2f_i+f_{i-1})+f^2_{i+1}+4f^2_i+f^2_{i-1}$$

$$= h^2(f^4(\eta_i)-\tfrac{1}{2}f^4(\xi_i)),\ x_{i-1}\leq\eta_i,\ \xi_i\leq x_{i+1},$$

$$i=1,2,\ldots,n-1.$$

Arguments similar to those used in proving (2.6) yeild

$$\|e^2\| \leqslant h^2\ \|A^{-1}\|\ \frac{3}{2}\ \|f^4\| \leqslant \frac{3}{4}\ h^2\ \|f^4\| .$$ ∎

We will need the following.

Corollary 1. If f_i have errors of $O(h^{t+1})$ and/or f^1_0 and f^1_n have errors of $O(h^t)$, then

$$\|e^1\| = O(h^{\min(4,t)}).$$

Proof. In (2.8), an $O(h^t)$ term will result on the right hand side due to these errors. Hence the minimum of t and 4 will be the power of h in the overall resulting error order estimate. ∎

Corollary 2. If f_i have errors of $O(h^{t+2})$ and/or f^2_0 and f^2_n have errors of $O(h^t)$, then

$$\|e^2\| = O(h^{\min(2,t)}).$$

Proof. In (2.9) the right hand side will have an $O(h^t)$ term due to these errors and the minimum of 2 and t will be the resulting power of h in the overall error. ∎

These two corollaries have two important consequences. First, at the end points, instead of (2.1) and (2.2), $O(h^4)$

and $O(h^2)$ approximations to the first and second derivatives can be used. Therefore, we can use the following [5].

(2.10a) $f_0^1 = \frac{1}{12h}(-25f_0+48f_1-36f_2+16f_3-3f_4)+ \frac{1}{5}h^4 f^5,$

(2.10b) $f_n^1 = \frac{1}{12h}(25f_n-48f_{n-1}+36f_{n-2}-16f_{n-3}+3f_{n-4})+ \frac{1}{5}h^4 f^5,$

(2.11a) $f_0^2 = \frac{1}{h^2}(2f_0-5f_1+4f_2-f_3)+ \frac{11}{12}h^2 f^4,$

(2.11b) $f_n^2 = \frac{1}{h^2}(2f_n-5f_{n-1}+4f_{n-2}-f_{n-3})+ \frac{11}{12} h^2 f^4,$

For later use we will also need the following formulas:

(2.12a) $f_0^2 = \frac{1}{12h^2}(35f_0-104f_1+114f_2-56f_3+11f_4)- \frac{5h^3}{6} f^5,$

(2.12b) $f_n^2 = \frac{1}{12h^2}(35f_n-104f_{n-1}+114f_{n-2}-56f_{n-3}+11f_{n-4})+ \frac{5h^3}{6} f^5,$

(2.13a) $f_0^3 = \frac{1}{2h^3}(-5f_0+18f_1-24f_2+14f_3-3f_4)+ \frac{7}{4}h^2 f^5,$

(2.13b) $f_n^3 = \frac{1}{2h^3}(5f_n-18f_{n-1}+24f_{n-2}-14f_{n-3}+3f_{n-4})+ \frac{7h^2}{4} f^5,$

(2.14a) $f_0^2 = \frac{1}{12h^2}(45f_0-154f_1+214f_2-156f_3+61f_4-10f_5)+ \frac{137}{180} h^4 f^6,$

(2.14b) $f_n^2 = \frac{1}{12h^2}(45f_n-154f_{n-1}+214f_{n-2}-156f_{n-3}+61f_{n-4}-10f_{n-5}) + \frac{137}{180}h^4 f^6,$

(2.15a) $f_0^4 = \frac{1}{h^4}(3f_0-14f_1+26f_2-24f_3+11f_4-2f_5)+ \frac{17}{6}h^2 f^6,$

(2.15b) $f_n^4 = \frac{1}{h^4}(3f_n-14f_{n-1}+26f_{n-2}-24f_{n-3}+11f_{n-4}-2f_{n-5})+ \frac{17}{6}h^2 f^6,$

(2.15c) $f_1^4 = \frac{1}{h^4}(2f_0-9f_1+16f_2-14f_3+6f_4-f_5)+ \frac{5}{6}h^2 f^6,$

(2.15d) $f^4_{n-1} = \frac{1}{h^4}(2f_n - 9f_{n-1} + 16f_{n-2} - 14f_{n-3} + 6f_{n-4} - f_{n-5}) + \frac{5}{6}h^2 f^6$,

(2.15e) $f^4_0 = \frac{1}{h^4}(f_0 - 4f_1 + 6f_2 - 4f_3 + f_4) - 2hf^5$,

and

(2.15f) $f^4_n = \frac{1}{h^4}(f_n - 4f_{n-1} + 6f_{n-2} - 4f_{n-3} + f_{n-4}) + 2hf^5$.

The derivatives of f in the error terms of the above formulas are evaluated at some point x in the interval defined by the x_i's corresponding to the extreme f_i values used in that particular formula.

The second consequence of the Corollaries 1 and 2 is in the use of spline on spline computation as follows:

Theorem 2. Let $\tilde{s}$ denote a cubic interpolating spline on the s^1_i values computed in (2.3), and the first and second derivatives of $\tilde{s}$ at x_i are computed from the formulas

(2.16) $$\tilde{s}^1_{i+1} + 4\tilde{s}^1_i + \tilde{s}^1_{i-1} = \frac{3}{h}(s^1_{i+1} - s^1_{i-1})$$

with

(2.17) $$\tilde{s}^1_0 = f^2_0 \quad \text{and} \quad \tilde{s}^1_n = f^2_n$$

and

(2.18) $$\tilde{s}^2_{i+1} + 4\tilde{s}^2_i + \tilde{s}^2_{i-1} = \frac{6}{h^2}(s^1_{i+1} - 2s^1_i + s^1_{i-1})$$

with

(2.19) $$\tilde{s}^2_0 = \tilde{f}^3_0 \quad \text{and} \quad \tilde{s}^2_n = f^3_n,$$

then

(2.20) $$|f^2_i - \tilde{s}^1_i| = O(h^3) \quad \text{and} \quad |f^3_i - \tilde{s}^2_i| = O(h^2).$$

Proof. From (2.5) and (2.6) we have $s^1_i = f^1_i + O(h^4)$

and therefore from Corollary 1 and (2.16) we get the first equation in (2.20). Similarly, (2.5), (2.7), Corollary 2 and (2.18) lead to the second equation in (2.20). ∎

Thus we have seen that spline on spline computation gives an additional power of h improvement in the order of accuracy in the second and third derivatives. Rigorous theoretical error bounds for spline on spline computations for any point in the interval [0,1] will be published elsewhere [6]. It should be noted that instead of (2.17) and (2.19) we can use (2.12) and (2.13) respectively.

Now, we can replace f_i^1, f_i^2 and f_i^3 in (1.4), (1.5) and (1.6) by s_i^1, $\underset{\sim}{s}_i^1$ and $\underset{\sim}{s}_i^2$ respectively. We recall that the subscript p had been dropped earlier. Therefore, in view of (2.6) and (2.20) we get

$$(2.21)\quad \phi_i(y)=y_i-y_{i-1}-\frac{h}{2}(f_i+f_{i-1})+\frac{h^2}{10}(s_i^1-s_{i-1}^1)-\frac{h^3}{120}(\underset{\sim}{s}_i^1+\underset{\sim}{s}_{i-1}^1)+O(h^6),$$

$$(2.22)\quad \phi_i(y)=y_i-y_{i-1}-\frac{h}{2}(f_i+f_{i-1})+\frac{h^2}{12}(s_i^1-s_{i-1}^1)-\frac{h^4}{720}(\underset{\sim}{s}_i^2-\underset{\sim}{s}_{i-1}^2)+O(h^6),$$

$$(2.23)\quad \phi_i(y)=y_{i+1}-2y_i+y_{i-1}-\frac{3h}{8}(f_{i+1}-f_{i-1})+\frac{h^2}{24}(s_{i+1}^1-8s_i^1+s_{i-1}^1)+O(h^6).$$

We recall that (2.23) requires the use of one equation of the type (2.21) or (2.22), since in (2.23), $i = 1,2,\ldots,n-1$.

It is possible to use a quintic spline to improve the accuracy in (2.21), (2.22) and (2.23) from $O(h^6)$ to $O(h^7)$. Since the formulas for the quintic spline are not readily available for equally spaced knots and the various derivatives of the spline, we give a short derivation of some of the results that we will use later on. Let us define the quintic polynomial in the i^{th} interval $[x_{i-1}, x_i]$ by

$$(2.24)\quad s(x)=f_i w+f_{i-1}\bar{w}+\frac{h^2}{6}((w^3-w)M_i+(\bar{w}^3-\bar{w})M_{i-1})$$
$$+\frac{h^4}{360}((3w^5-10w^3+7w)F_i+(3\bar{w}^5-10\bar{w}^3+7\bar{w})F_{i-1}),$$

where $i = 1,2,\ldots,n$, $w = (x-x_{i-1})/h$ and $\bar{w} = 1-w$. It is easy to verify that $w^1 = 1/h = -\bar{w}^1$, and when $x = x_{i-1}$, $w = 0$ and $\bar{w} = 1$, when $x = x_i$, $w = 1$ and $\bar{w} = 0$. As before, let s_i^r denote the r^{th} derivative of $s(x)$ evaluated at x_i. Now, matching the $s^1(x_i)$ for the i^{th} and $(i+1)^{th}$ interval we have

$$(2.25)\quad M_{i+1}+4M_i+M_{i-1}=\frac{h^2}{60}(7F_{i+1}+16F_i+7F_{i-1})+\frac{6}{h^2}(f_{i+1}-2f_i+f_{i-1}).$$

Similarly, matching $s^3(x_i)$ for the same two intervals, we get

$$(2.26)\quad M_{i+1}-2M_i+M_{i-1}=\frac{h^2}{6}(F_{i+1}+4F_i+F_{i-1}).$$

Subtracting (2.26) from (2.25) and dividing by six, we get

$$(2.27)\quad M_i=-\frac{h^2}{120}(F_{i+1}+8F_i+F_{i-1})+\frac{1}{h^2}(f_{i+1}-2f_i+f_{i-1}).$$

Substituting for M_{i-1}, M_i and M_{i+1} from (2.27) in (2.26) we have on simplification

$$(2.28)\quad F_{i+2}+26F_{i+1}+66F_i+26F_{i-1}+F_{i-2}=\frac{120}{h^4}(f_{i+2}-4f_{i+1}+6f_i-4f_{i-1}+f_{i-2})$$

It is easy to verify that

$$(2.29)\qquad s_i^2 = M_i \quad\text{and}\quad s_i^4 = F_i$$

and these automatically match for the i^{th} and $(i+1)^{th}$ intervals at x_i.

In order to use (2.28) to compute F_i from f_i we prescribe that $F_0 = s_0^4 = f_0^4$, $F_n = s_n^4 = f_n^4$, $F_1 = s_1^4 = f_1^4$ and $F_{n-1}=s_{n-1}^4=f_{n-1}^4$. It can be shown by arguments similar to those used for the cubic splines that for the quintic spline

(2.30) $$|s_i^r - f_i^r| = 0(h^{6-r}),\ r = 1,2,3 \text{ and } 4.$$

Now, since $F_i = s_i^4$ we have

$$|F_i - f_i^4| = 0(h^2),$$

so equation (2.15) can be used to compute f_0^4, f_1^4, f_n^4 and f_{n-1}^4 without sacrificing the order estimate for the errors. The use of (2.26) requires that $M_0 = s_0^2 = f_0^2$ and $M_n = s_n^2 = f_n^2$ and (2.14) can be used to compute f_0^2 and f_n^2.

Now from (2.24) routine computation gives

(2.31) $$s_i^1-s_{i-1}^1 = \frac{h}{2}(M_i+M_{i-1})- \frac{h^3}{24}(F_i+F_{i-1})$$

and

(2.32) $$s_i^3 - s_{i-1}^3 = \frac{h}{2}(F_i+F_{i-1}).$$

Replacing the derivatives of f in (1.4) by the corresponding spline derivatives and in view of (2.30) we have

$$\phi_i(y)=y_i-y_{i-1}- \frac{h}{2}(f_i+f_{i-1})+ \frac{h^2}{10}(s_1^1-s_{i-1}^1)- \frac{h^3}{120}(s_i^2+s_{i-1}^2)+0(h^7),$$

which by using (2.31) and (2.32) becomes

(2.33) $$\phi_i(y)=y_i-y_{i-1}- \frac{h}{2}(f_i+f_{i-1})+ \frac{h^3}{24}(M_i+M_{i-1})- \frac{h^5}{240}(F_i+F_{i-1})+0(h^7).$$

It can be verified that even from (1.5) when we use (2.30), (2.31) and (2.32) we get also the same equation as (2.33) ! Furthermore, replacing the second and fourth derivatives in (1.12) by M_i and F_i, respectively, again gives (2.33) ! Thus we have seen that in the case of quintic spline (1.4), (1.5) and (1.12) all lead to the same formula (2.33). The third equation (1.6), in view of (2.30), (2.31) and (2.32), after routine simplification leads to

$$(2.34)\quad \phi_i(y)=y_{i+1}-2y_i+y_{i-1}-\frac{h}{2}(f_{i+1}-f_{i-1})+\frac{h^3}{24}(M_{i+1}-M_{i-1})$$
$$-\frac{h^5}{240}(F_{i+1}-F_{i-1})+O(h^7).$$

It is interesting to not that the right hand side of (2.34) can be obtained from (2.33) by subtracting ϕ_i from ϕ_{i+1}. Instead of the quintic spline the f_i^4 values in (1.12) can be computed by three applications of cubic splines as follows. Use (2.3) to compute s_i^1, then (2.16) to evaluate $\underset{\sim}{s}_i^1$ and then

$$(2.35)\qquad \hat{s}_{i+1}^2+4\hat{s}_i^2+\hat{s}_{i-1}^2=\frac{6}{h^2}(\underset{\sim}{s}_{i+1}^1-2\underset{\sim}{s}_i^1+\underset{\sim}{s}_{i-1}^1)$$

with $f\in C^6$,

$$(2.36)\qquad \hat{s}_0^2=f_0^4 \quad\text{and}\quad \hat{s}_n^2=f_n^4$$

to compute $\hat{s}_i^2$ as the approximations to f_i^4 values. Now, in view of (2.20) and Corollary 2,

$$|\hat{s}_i^2-f_i^4|=O(h),$$

and therefore $O(h)$ approximations can be used in (2.36) for f_0^4 and f_n^4. From the above facts and (1.12) it follows that

$$(2.37)\quad \phi_i(y)=y_i-y_{i-1}-\frac{h}{2}(f_i+f_{i-1})+\frac{h^3}{24}(\underset{\sim}{s}_i^1+\underset{\sim}{s}_{i-1}^1)-\frac{h^5}{240}(\hat{s}_i^2+\hat{s}_{i-1}^2)+O(h^6).$$

In the following section, we describe a method for solving the system (1.8) for y.

3. Solution of the Nonlinear Algebraic Equations.

Let

(3.1a) $\phi(y) = u(y) + \frac{h}{10}v(y)$ for (2.21), (2.22) and (2.23),

and

(3.1b) $\phi(y) = u(y) + \frac{h^2}{24}\, v(y)$ for (2.33), (2.34) and (2.37),

where

(3.2) $u_i(y) = y_i - y_{i-1} - \frac{h}{2}(f_i + f_{i-1})$ for (2.21), (2.22), (2.33) and (2.37),

$= y_{i+1} - 2y_i + y_{i-1} - \frac{3h}{8}(f_{i+1} - f_{i-1})$ for (2.23),

$= y_{i+1} - 2y_i + y_{i-1} - \frac{h}{2}(f_{i+1} - f_{i-1})$ for (2.34),

and

(3.3a) $v_i(y) = h(s_i^1 - s_{i-1}^1) - \frac{h^2}{12}(\tilde{s}_i^1 + \tilde{s}_{i-1}^1)$ for (2.21),

(3.3b) $= \frac{5h}{6}(s_i^1 - s_{i-1}^1) - \frac{h^3}{72}(\tilde{s}_i^2 - \tilde{s}_{i-1}^2)$ for (2.22),

(3.3c) $= \frac{5h}{12}(s_{i+1}^1 - 8s_i^1 + s_{i-1}^1)$ for (2.23),

(3.3d) $= h(M_i + M_{i-1}) - \frac{h^3}{10}(F_i + F_{i-1})$ for (2.33),

(3.3e) $= h(M_{i+1} - M_{i-1}) - \frac{h^3}{10}(F_{i+1} - F_{i-1})$ for (2.34),

(3.3f) $= h(\tilde{s}_i^1 + \tilde{s}_{i-1}^1) - \frac{h^3}{10}(\hat{s}_i^2 + \hat{s}_{i-1}^2)$ for (2.37).

It is necessary to leave the first power of h in the leading term of $v_i(y)$ so that it is of the same order as $u_i(y)$. (If

y_i and y_{i-1} are very close then the dominating part in $u_i(y)$ has the first power of h).

An iterative method is used to solve the system (3.1). It best described in the following algorithmic form.

<u>Algorithm 1.</u>

Given an initial approximation $y^{(0)}$ for y, do the following steps for k = 0, 1, 2, ... until

(3.4) $\|\phi(y^{(k)})\| < \epsilon$ for some prechosen tolerance ϵ.

1. Compute $z^{(k)}$ by solving the linear system

(3.5) $$u^1(y^{(k)})z^{(k)} = \phi(y^{(k)}),$$

where u^1 is the Jacobian of u with respect to y.

2. Update the value of $y^{(k)}$ as follows:

(3.6) $$y^{(k+1)} = y^{(k)} - z^{(k)}.$$

It is worth observing that the Jacobian u^1 in (3.5), which is computed from the value of u given by (3.2) has a sparse structure because u^1 is of order mn and, in view of (1.1) and (3.2), it has only O(m) elements per row. In many problems (e.g., flow networks [7]) every f_i is a function of only a few components of y and for such problems u^1 has a few elements per row. Various sparse matrix techniques can be used in solving (3.5) [8].

The convergence of the sequence $\{y^{(k)}\}$ determined by (3.5) and (3.6) is guaranteed by the following theorem ([9], Theorem 12.6.4).

Theorem 3. (Ortega and Rheinboldt).

Suppose $\phi : D \subset R^n \to R^n$ is F-differentiable on the convex set $D_0 \subset D$ and

$$\|\phi^1(y) - \phi^1(z)\| \leq \gamma \|y-z\|, \quad y,z \in D_0.$$

Let $y^{(0)} \in D_0$ be such that with $\delta_0, \delta_1 \geq 0$

$$\left.\begin{array}{l} \|u^1(y)-u^1(y^{(0)})\| \leq \mu \|y-y^{(0)}\| \\ \|v^1(y)\| \leq \Lambda(\delta_0 + \delta_1 \|y-y^{(0)}\|) \end{array}\right\} \quad \forall\, y \in D_0$$

where $\Lambda = 10/h$ for (3.1a) and $24/h^2$ for (3.1b). Assume, moreover, that $u^1(y^{(0)})$ is nonsingular and

$\left\| \left[u^1(y^{(0)})\right]^{-1} \phi(y^{(0)}) \right\| \leq \eta$, $\|u^1(y^{(0)})\| \leq \beta$, and that $\beta\delta_0 < 1$ and $\alpha = \sigma\beta\gamma\eta/(1-\beta\delta_0)^2 \leq \frac{1}{2}$, where $\sigma = \max\left[1, \frac{\mu+\delta_1}{\gamma}\right]$.

Set

$$t^* = \frac{1-(1-2\alpha)^{\frac{1}{2}}}{\alpha} \frac{\eta}{1-\beta\delta_0}, \quad t^{**} = \frac{1+(1-2\alpha/\sigma)^{\frac{1}{2}}}{\alpha} \frac{\sigma\eta}{1-\beta\delta_0}.$$

If $\bar{S}(y^{(0)},t^*) \subset D_0$, then the sequence $\{y^{(k)}\}$ defined by

$$y^{(k+1)} = y^{(k)} - \left[u^1(y^{(k)})\right]^{-1} \phi(y^{(k)}), \quad k=0,1,2,\ldots$$

remains in $S(y^{(0)},t^*)$ and converges to a solution y^* of $\phi(y) = 0$ which is unique in $D_0 \cap S(y^{(0)},t^{**})$.

4. Computational Considerations.

We will now give some estimates of the computational work involved in the determination of spline derivatives s_i^1, $\tilde{s}_i^1$, $\tilde{s}_i^2$, F_i, M_i and $\hat{s}_i^2$. The derivatives are necessary when computing $v(y)$ according to (3.3). We recall that in (3.3c) one additional equation of the type (3.3a) or (3.3b) is necessary to make it fully determined because $i = 1, 2, \ldots, n-1$. Therefore, we shall not consider (3.3c) as the work involved will be the same as in (3.3a) or (3.3b). In order to make relative comparisons of the computational work, we have considered the total number of multiplications and divisions in various computations. It must be kept in mind that this is only a rough measure of the computational work; data transfers, additions, subtractions and other overhead can often add substantially to the estimates.

In Table 1 we have given the approximate number of multiplications and divisions required to compute the spline derivatives. In constructing this table we have used the fact that (2.3), (2.16), (2.18), (2.25) and (2.35) all entail the solution of a tridiagonal system of linear equations, but in (2.28) it is necessary to solve a pentadiagonal system. We have assumed that the quantities $h^2/60$, $3/h$, $1/12h$, $1/h^2$, $6/h^2$, $1/12h^2$, $1/2h^3$ and $120/h^4$ are computed only once at the begining of the computer implmentation and are, therefore, not included in Table 1.

In Table 2, we give the total number of operation counts for the spline derivatives used in (3.3). Note that for (3.3f) in this table, the value of s_i^1 is included because it is necessary to compute $\underset{\sim}{s}_i^1$.

It follows from Table 2 that (3.3f) is a poor choice for computing $v(y)$ since (3.3a), (3.3b) and (3.3f) all have $O(h^6)$ accuracy. On the other hand, the accuracy acheived by (3.3d) or (3.3e) is $O(h^7)$ and, therefore, in many cases, the additional work is justified. For example, when $n = 10$,

$(23n-32)/8n = 2.48$ and this increase in work will lead to an improvement in accuracy by an additional decimal digit.

Spline derivative Equation used	s_i^1 (2.3)	$\underset{\sim}{s}_i^1$ (2.16)	$\underset{\sim}{s}_i^2$ (2.18)	F_i (2.28)	M_i (2.25)	$\hat{s}_i^2$ (2.35)
Numerical derivative at the end points Equation used	12 (2.10)	12 (2.12)	12 (2.13)	26 (2.15 a-d)	14 (2.14)	8 (2.15e,f)
Right hand side	n-1	n-1	n-1	4n-12	6n-6	n-1
Solution of band type equations: Forward course Back substitution	 2n-8 n-3	 2n-8 n-3	 2n-8 n-3	 8n-36 2n-7	 2n-8 n-3	 2n-8 n-3
Total	4n	4n	4n	14n-29	9n-3	4n-4

Table 1. Number of multiplications and divisions necessary to compute the derivatives of splines from the function values.

Equation	Derivatives needed	Total number of operations
(3.3a)	s_i^1, $\underset{\sim}{s}_i^1$	8n
(3.3b)	s_i^1, $\underset{\sim}{s}_i^2$	8n
(3.3d) or (3.3e)	F_i, M_i	23n - 32
(3.3f)	s_i^1, $\underset{\sim}{s}_i^1$, $\hat{s}_i^2$	12n - 4

Table 2. Spline derivatives used in computing v(y) according to (3.3).

5. Acknowledgements.

The continued interest and support of Dr. J. L. Stephenson is greatfully acknowledged. The author is also indebted to Prof. V. Dolezal, Mr. R. Mejia, Prof. R. Kellogg, Mr. C. Song and D. Salane for their valuable advice and critical comments.

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