Higher-Order Numerical Solutions Using Cubic Splines

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A cubic spline collocation procedure has recently been developed for the numerical solution of partial differential equations. In the present paper, this spline procedure is reformulated, so that the accuracy of the second-derivative approximation is improved and parallels that previously obtained for lower derivative terms. The final result is a numerical procedure having overall third-order accuracy for a nonuniform mesh and overall fourth-order accuracy for a uniform mesh. Solutions using both spline procedures, as well as three-point finite difference methods, will be presented for several model problems.

I. Introduction

IN a recent study Rubin and Graves [1,2] present a cubic spline [3,4] collocation procedure for the numerical solution of partial differential equations. This technique exhibits the following desirable features: 1) the governing matrix system is always tridiagonal so that well-developed and highly efficient inversion algorithms are applicable; 2) cubic spline interpolation leads to second-order accuracy for second derivatives, e.g., diffusion terms in the Navier-Stokes equations; this order of accuracy is maintained even with rather large nonuniformities in mesh width; 3) first derivatives or convection effects are fourth-order accurate for a uniform mesh and third-order with mesh nonuniformity; 4) derivative boundary conditions can in many cases be applied more accurately and with less difficulty than with conventional finite-difference schemes; 5) a simple two-point relationship exists between the spline approximation for the first and second derivatives; and 6) unlike finite-element or other Galerkin (integral) methods, which are generally not tridiagonal, the evaluation of large numbers of quadratures is unnecessary.

Solutions have been obtained for a number of problems [1,2] with explicit, implicit, and spline-alternating direction-implicit (SADI) temporal or spatial marching procedures. Moreover, for the viscous and potential flow problems considered, it was found that with the spline procedure there was no particular advantage gained with the equations in divergence form. In some recent studies, it has been found that the divergence form may be desirable with flux boundary conditions.

Agreement of the spline solutions with exact analytic results and very accurate finite-difference solutions obtained with a very fine mesh has been quite good. [1,2] All comparisons [1,2] with conventional three-point finite difference formulations demonstrate the improved spline accuracy associated with i) the higher-order convection approximation, ii) the treatment of derivative boundary conditions, or iii) the higher-order accuracy of spline second derivatives (diffusion) when specifying a nonuniform mesh. Solutions for the Burgers equation, the two-dimensional diffusion equation, and the incompressible viscous flow in a driven cavity are found in Refs. 1 and 2.

In this paper, the cubic spline procedure is reformulated so that the accuracy of the second-derivative approximation is improved and parallels that obtained for the lower derivative terms. The final result is a combined spline-finite difference numerical procedure having overall third-order spatial accuracy for nonuniform meshes and overall fourth-order spatial accuracy with a uniform mesh. In order to differentiate the two spline procedures, we shall designate the original spline formulation [1,2] as spline 2 and the improved formulation presented here as spline 4.

As shown in Secs. II and III, the cubic spline collocation procedure involves a third-order interpolation polynomial with the function and the second (or first) derivative of the function as unknowns at each mesh point. Continuity of the first (or second) derivative leads to the tridiagonal system of equations to be considered.

Recently, several finite-difference schemes with similar properties have been proposed; i.e., the functions and derivatives have been considered unknown at each mesh point, or the functions collocated at three points instead of one. The methods, which have been termed Hermitian finite-difference, [5,6] Padé approximation [7] or compact differencing, [8] and Mehrstellung, [9] have been developed for a uniform mesh, and have somewhat lower truncation errors than the five-point pentadiagonal fourth-order finite difference procedure. As with the spline formulation, they remain of tridiagonal form.

In a recent study the authors [10] have examined these procedures, as well as a fourth-order spline-on-spline method, and found them to be, in fact, identical; i.e., any one can be derived from any of the others. Moreover, these procedures have been reformulated [10] so as to apply to nonuniform mesh systems as well. As with spline 4, these finite-difference or spline-on-spline methods are fourth-order with a uniform mesh and third-order with a nonuniform mesh. The relative advantage and/or disadvantages of these procedures, over spline 2 and spline 4, are discussed in Ref. 10. The main differences are the handling of boundary conditions, the relationship between the approximations for the convection and diffusion terms, and the truncation errors. The truncation errors for first derivatives are identical. The truncation error for the second-derivative to be discussed later for spline 4 is 50% smaller than that found with the finite-difference or spline-on-spline collocation formula.

In order to evaluate the spline procedures, the truncation errors, stability limitations, and effects of boundary conditions will be discussed. Spline 2 is reviewed in Sec. II, and spline 4 is introduced and discussed in Sec. III. The stability conditions for both methods are outlined in Sec. IV. Solutions using both spline procedures, as well as a three-point finite-difference method, are presented for several model problems in Sec. V. Both uniform and nonuniform meshes are considered. In each case the analytic solution or a very accurate numerical solution is available for comparison purposes. The problems to be considered include 1) potential flow over a circular cylinder with a spline successive approximation procedure, 2) the weak shock solution for the nonlinear Burgers equation by a two-step explicit or an implicit spline integration, and 3) the solution of the two-point boundary

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value problem describing similar boundary-layer behavior. The results will be summarized in Sec. VI.

II. Spline 2 – Review of Cubic Spline Theory

Consider a mesh with nodal points such that

$$a = x_0 < x_1 < x_2 \ldots < x_N < x_{N+1} = b$$

and with

$$h_i = x_i - x_{i-1} > 0.$$

Consider a function $u(x)$, such that at the mesh points x_i, $u(x_i) = u_i$. The cubic spline is a function $S_\Delta(u,x) = S_\Delta(x)$ which is continuous together with its first and second derivatives on the interval $[a,b]$, corresponds to a cubic polynomial in each subinterval $x_{i-1} \leq x \leq x_i$, and satisfies $S_\Delta(u_i; x_i) = u_i$.

If $u(x)$ and its derivatives are continuous, it has been shown that the spline function $S_\Delta(x)$ approximates $u(x)$ at all points in $[a,b]$ to fourth order in max h_i. First and second derivatives of $S_\Delta(x)$ approximate $u''(x)$ and $u'(x)$ to third and second order, respectively. See Ahlberg, Nilson, and Walsh[3] for detailed proofs of convergence.

If $S_\Delta(x)$ is cubic on $[x_{i-1}, x_i]$, then in general,

$$S''_\Delta(x) = M_{i-1}\left(\frac{x_i - x}{h_i}\right) + M_i\left(\frac{x - x_{i-1}}{h_i}\right)$$

where $M_i \equiv S''_\infty(x_i)$.

Integrating twice leads to the interpolation formula on $[x_{i-1}, x_i]$

$$S_\Delta(x) = M_{i-1}\frac{(x_i - x)^3}{6h_i} + M_i\frac{(x - x_{i-1})^3}{6h_i} + \left[u_{i-1} - \frac{M_{i-1}h_i^2}{6}\right]\frac{(x_i - x)}{h_i} + \left(u_i - \frac{M_i h_i^2}{6}\right)\frac{(x - x_{i-1})}{h_i} \tag{1a}$$

The constants of integration have been evaluated from $S_\Delta(x_i) = u_i$ and $S_\Delta(x_{i-1} = u_{i-1}$. $S_\Delta(x)$ on $[x_i, x_{i+1}]$ is obtained with $i+1$ replacing i in Eq. (1a).

The unknown derivatives M_l are related by enforcing the continuity condition on $S'_\Delta(x)$. With $S'_\Delta(x_i^-) = m_i^-$ on $[i-1, i]$ and $S'_\Delta(x_i^+) = m_i^+$ on $[x_i, x_{i+1}]$, we require $m_i^- = m_i^+ = m_i$. We find for $i = 1, \ldots, N$,

$$\frac{h_i}{6}M_{i-1} + \frac{h_i + h_{i+1}}{3}M_i \frac{h_{i+1}}{6}M_{i,1} = \frac{(u_{i+1} - u_i)}{h_{i+1}} - \frac{(u_i - u_{i-1}}{h_i} \tag{1b}$$

Additional spline relationships that are easily derived are listed below

$$\frac{1}{h_i}m_{i-1} + 2\left(\frac{1}{h_i} + \frac{1}{h_{i+1}}\right)m_i + \frac{1}{h_{i+1}}m_{i+1} = \frac{3(u_{i+1} - u_i)}{h_{i+1}^2} + \frac{3(u_i - u_{i-1})}{h_i^2} \tag{1c}$$

$$m_{i+1} - m_i = \frac{h_{i+1}}{2}(M_i + M_{i+1}) \tag{1d}$$

$$m_i = \frac{h_i}{3}M_i + \frac{h_i}{6}M_{i-1} + \frac{u_i - u_{i-1}}{h_i} \tag{1e}$$

$$m_i = -\frac{h_{i+1}}{3}M_i - \frac{h_{i+1}}{6}M_{i+1} + \frac{u_{i+1} - u_i}{h_{i+1}} \tag{1f}$$

$$M_i = \frac{2m_{i-1}}{h_i} + \frac{4m_i}{h_i} - 6\frac{u_i - u_{i-1}}{h_i^2} \tag{1g}$$

$$M_i = -\frac{4m_i}{h_{i+1}} - \frac{2m_{i+1}}{h_{i+1}} + 6\frac{u_{i+1} - u_i}{h_{i+1}^2} \tag{1h}$$

Equation (1b) or (1c) leads to a system of N equations for the $N+2$ unknowns M_i or m_i, respectively. The additional two equations are obtained from boundary conditions on m_0, m_{N+1} or M_0, M_{N+1}.[1,2] The resulting tridiagonal system for M_i or m_i is diagonally dominant and solved by an efficient inversion algorithm.[3]

Spline 2 for Solving Partial Differential Equations[1,2]

If the values u_i are not prescribed but represent the solution of a quasilinear second-order partial differential equation, $u_t = f(u, u_x, u_{xx})$, then an approximate solution for u_i can be obtained by considering the solution of

$$(u_t)_i = f(u_i, m_i, M_i).$$

This formulation is designated spline 2. If the time derivative is discretized in a simple finite-difference fashion, we have

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = (1-\theta)f^n + \theta f^{n+1} \tag{2a}$$

$\theta = 0$ is explicit; $\theta = 1$, implicit; $\theta = ½$, Crank-Nicolson. For the explicit integration the stability limitations are quite severe, see Refs. 1 and 2 and Sec. VI. Therefore a two-step procedure is considered and is given as

$$\text{Step 1:} \quad \frac{\bar{u}_i^{n+1} - u_i^n}{\Delta t} = f^n \, ‡$$

$$\text{Step 2:} \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} = \bar{f}^{n+1} \tag{2b}$$

For example, consider the linear Burgers equation

$$u_t + \bar{u}u_x = \nu u_{xx}; \quad \bar{u} = \bar{u}(x,t); \quad \nu = \nu(x,t) \tag{3a}$$

With Eqs. (lb) and (1c) we obtain a system of $3N$ equations for $3(N+2)$ unknowns (see Refs. 1 and 2 for further details on the derivations). The system in Eq. (2) can be written§ as

$$A_i V_{i-1}^{n+1} + B_i V_i^{n+1} + C_i V_{i+1}^{n+1} = D_i V_i^n + E_i[\sigma V_{i-1}^n + V_{i+1}^n] \tag{3b}$$

where

$$A_i = \begin{bmatrix} 0 & 0 & \gamma_1 \\ -1/h_i & 0 & h_i/6 \\ 3/h_i^2 & 1/h_i & 0 \end{bmatrix}$$

$$B_i = \begin{bmatrix} \alpha_0 & \alpha_1 & \alpha_2 \\ (1 + 1/\sigma)/h_i & 0 & (\sigma+1)h_i/3 \\ -3(1 - 1/\sigma^2)/h_i^2 & 2(1 + 1/\sigma)/h_i & 0 \end{bmatrix}$$

‡It is possible to treat the viscous terms (M_i) implicitly $(\theta = 1)$, and the convection terms explicitly. As shown in Refs. 1 and 2, the stability of the two-step procedure for viscous flows is improved.

§A number of variations on this system can be derived with Eqs. (1).

$$C_i = \begin{bmatrix} 0 & 0 & \gamma_2 \\ -1/h_{i+1} & 0 & h_{i+1}/6 \\ -3/h_{i+1}^2 & 1/h_{i+1} & 0 \end{bmatrix}$$

$$D_i = \begin{bmatrix} \rho_0 & \rho_1 & \rho_2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$E_i = \begin{bmatrix} 0 & 0 & \delta_1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3c}$$

$$V_i = [u_i, m_i, M_i]^T,$$

and

$$\sigma = h_{i+1}/h_i; \quad \gamma_1 = \gamma_2 = \delta_1 = 0$$

$$\alpha_0 = 1; \quad \alpha_1 = \theta \bar{u}_i^{n+1}\Delta t; \quad \alpha_2 = -\theta v_i^{n+1}\Delta t;$$

$$\rho_0 = 1; \quad \rho_1 = -(1-\theta)\bar{u}_i^n \Delta t; \quad \rho_2 = (1-\theta) v_i^n \Delta t \tag{3d}$$

A significant advantage of the spline 2 formulation is that with Eqs. (1) it is possible to reduce the 3×3 matrix system (3) to a scalar set of equations for M_j alone. The details of this reduction process are found in Refs. 1 and 2.

For equations with two space dimensions such that $u_t = f(u, u_x, u_y, u_{xx}, u_{yy})$, a spline-alternating direction-implicit (SADI) procedure has been presented by Rubin and Graves[1,2]. A spline successive approximation method can also be simply formulated. Both techniques are discussed in Ref. 11, where several example problems are presented.

Truncation Error

For interior points, the spatial accuracy of the spline approximation can be directly estimated from Eqs. (1b and 1e, or 1f). Expanding m_i, M_i, and u_i in Taylor series, and assuming the necessary continuity of derivatives for $u(x,y)$, we obtain, with $\sigma = h_{i+1}/h_i$,

$$\begin{aligned}(u_{xx})_i &= M_i + (u^{iv})_i h_i^2(\sigma^3+1)/12(\sigma+1) \\ &- (u^v)_i h_i^3(\sigma-1)(2\sigma^2+5\sigma+2)/180 \\ &- (u^{vi})_i h_i^4[\sigma^2/360 + (\sigma-1)^2(7\sigma^2-2\sigma+7)/1080] \\ &+ 0(h_i^5)\end{aligned} \tag{4a}$$

and

$$\begin{aligned}(u_x)_i &= m_i + (u^{iv})_i h_i^3 \sigma(\sigma-1)/24 + \\ &+ (u^v)_i h_i^4 \sigma[1+\sigma(\sigma-1)]/180 + 0(h_i^5)^{\P}\end{aligned} \tag{4b}$$

Fyfe[12] and Daniel and Swartz[13] have presented similar relations, for constant h_i, in their collocation analysis of cubic splines for the solution of two-point boundary-value problems.

Therefore, the spline approximation with a nonuniform mesh is second-order accurate for M_i and third-order for m_i. For a uniform mesh m_i becomes fourth-order, with M_i remaining second-order accurate. In. Sec. III a finite-difference expression for $(u^{iv})_i$ is used to increase the accuracy of M_i, and hence the overall accuracy of the procedure. With this modification this formulation will be termed spline 4.

III. Spline 4 – Derivation and Discussion

In order to improve the overall accuracy of the spline 2 formulation, it is necessary to reduce the order of the truncation error for $(u_{xx})_i$ in Eq. (4a). Although a number of procedures are possible, we have chosen a very simple modification, whereby the error term in Eq. (4a) for $(u^{iv})_i$ is approximated by a three-point discretization for M_i. This approximation is first-order accurate with a nonuniform mesh and second-order with a uniform mesh. Therefore the spline approximation for $(u_{xx})_i$ is improved, and parallels that for $(u_x)_i$; i.e., third-order accuracy is achieved for a nonuniform grid and fourth-order accuracy for uniform mesh. This improvement leads to what is termed spline 4.

In a separate study[10] this procedure is described in somewhat greater detail and is also applied to the Hermitian or Padé[5-9] finite-difference and spline-on-spline methods, in order to develop these procedures for nonuniform grids.

The development of spline 4 is as follows: Eq. (4a) can be rewritten in the form

$$\begin{aligned}(u_{xx})_i &= M_i + h_i^2\sigma(\sigma+1)\Delta(M_{xx})_i/12 \\ &+ 0[(\sigma-1)h_i^3, h_i^4]\end{aligned} \tag{5a}$$

where $\Delta = (1+\sigma^3)/\sigma(1+\sigma)^2$.

The familiar three-point discretization formula[14] is

$$\begin{aligned}(M_{xx})_i &= \frac{2}{\sigma(\sigma+1)h_i^2}[M_{i+1} - (1+\sigma)M_i + \sigma M_{i-1}] \\ &- (\sigma-1)h_i(M_{xxx})_i/3 - h_i^2(1+\sigma^3)(M^{iv})_i/12(1+\sigma) + 0(h_i^3)\end{aligned} \tag{5b}$$

Therefore, Eq. (4a) or (5a) becomes

$$\begin{aligned}(u_{xx})_i &= M_i + (\Delta/6)(M_{i+1} - (1+\sigma)M_i + \sigma M_{i-1}) \\ &- 7h_i^3(1+\sigma^2)(\sigma-1)(u^v)_i/180 - h_i^4(u^{vi})_i[\sigma^2/360 \\ &+ (\sigma-1)^2(7\sigma^2-2\sigma+7)/1080] + 0(h_i^5)\end{aligned} \tag{5c}$$

With Eq. (4b)

$$(u_x)_i = m_i + O[(\sigma-1)h_i^3, h_i^4)^{**} \tag{5d}$$

and we obtain a uniform higher-order approximation termed spline 4. ‡‡When $\sigma = 1$, spline 4 is fourth-order accurate and the truncation error of Eq. (5b) is smaller than that obtained, with spline-on-spline,[10] Hermitian, or Padé methods [5-9] which are in turn smaller than the error obtained with five-point finite-different discretizations.

In the spline 4 procedure Eqs. (1b – 1h) still apply; however, the interpolation polynomial is not longer applicable as spline 4 respresents a higher-order interpolation. This point is discussed in greater detail in Ref. 10. The governing system remains tridiagonal. Unlike spline 2, where the system can be reduced to that for M_i alone, the appearance of off-diagonal terms in Eq. (5b) restricts the reduction process to a 2×2 system in (u_i, M_i).

For the linear Burgers equation the system is still of the

¶If, Eq. (1c) is used to evaluate the truncation error for m_i, the constant 24 in the second expression on the right-hand side becomes 72. For the uniform case, Eq. (4b) is recovered in all cases.

**It is possible to apply Eq. (5b) to Eq. (4b), to make $(u_x)_i$ fourth-order even with a nonuniform mesh.

††Higher-order procedures, e.g., spline 6, can be derived in a similar manner,[10] and spline 2 can be recovered from spline 4 with Δ set equal to zero.

form in Eq. (3b), with

$$\gamma_1 = -v_i^{n+1}\theta\Delta t\sigma\Delta/6; \quad \gamma_2 = -v_i^{n+1}\theta\Delta t\Delta/6$$

$$\alpha_2 = -v_i^{n+1}\theta\Delta t(1-(1+\sigma)\Delta/6)$$

$$\sigma_2 = (1-\theta)v_i^{n+1}\Delta t(1-(1+\sigma)\Delta/6)$$

$$\delta_1 = v_i^{n+1}(1-\theta)\Delta t\Delta/6 \tag{6}$$

All other entries in Eqs. (3c) and (3d) are unchanged.

IV. Stability

For the linear Burgers Eq. (3), with $\bar{u}$, v constant, the interior point stability can be assessed with the von Neumann Fourier decomposition of the system in Eq. (3) for $h_i = h = \text{constant}$.

With

$$V_{i+r}^n = \mathcal{V}_i^n \exp I\omega(x_i + rh), \; I = (-1)^{1/2},$$

Eq. (3) becomes

$$T_i \mathcal{V}_i^{n+1} = P_i \mathcal{V}_i^n \text{ or } \mathcal{V}_i^{n+1} = G_i \mathcal{V}_i^n,$$

where $G_i = T_i^{-1} P_i$ is the amplification matrix. The von Neumann condition necessary for the suppression of all error growth requires that the spectral radius $\rho(G_i) \leq 1$. The eigenvalues of G_i are λ_i.

For the one-dimensional Eq. (3), three numerical procedures were considered: i) convection m_i, and diffusion M_i explicit, ii) convection explicit, diffusion implicit (two steps required for inviscid stability), and iii) diffusion and convection implicit. With explicit convection, i) or ii), both divergence and nondivergence forms of the equations have been evaluated in Refs. 1 and 2.

The stability conditions imposed on these schemes is determined from $|\lambda_i| \leq 1$.

i) Explicit convection and diffusion: $\theta = 0$ in Eqs. (2a) and (3).

Spline 2[1,2]: $|\lambda_i|^2 = (1-6\beta(1-\cos\varphi)(2+\cos\varphi)^{-1})^2 + c^2\Phi^2 \leq 1$, where $\beta = v\Delta t/h^2$, $c = \bar{u}\Delta t/h$, $\Phi = 3\sin\varphi/(2+\cos\varphi)$, $\varphi = \omega h$.

Necessary stability limits are

$$\text{a)}\ \beta \leq 1/6$$

$$\text{b)}\ c \leq (3)^{-1/2}$$

$$\text{c)}\ R_c = c/\beta = \bar{u}h/v \leq 2(3)^{1/2} \tag{7a}$$

These results are more restrictive than the limits found for the forward time central space explicit finite-difference method[14] which are

$$\text{a)}\ \beta \leq 1/2; \quad \text{b)}\ c \leq 1; \quad \text{c)}\ R_c \leq 2$$

Spline 4: $|\lambda|^2 = (1-(5+\cos\varphi)\ (1-\cos\varphi)\ \beta/(2+\cos\varphi))^2 + [3c\sin\varphi/(2+\cos\varphi)]^2 << 1$, so that necessary stability limits are

$$\text{a)}\ \beta \leq 1/4, \qquad \text{b)}\ c \leq (10)^{1/2}/6, \ \text{c)}\ R_c \leq (40)^{1/2}/3. \tag{7b}$$

Once again these conditions are somewhat more restrictive than those obtained with second-order finite differences of Eq. (7b). The Pade finite-difference limitation $c \leq (6)^{1/2}/6$ is even more restrictive (see Appendix of Refs. 1 and 2). It is significant that in all cases the explicit method is unconditionally unstable for inviscid flow; i.e., $\beta = 0$.

ii) Two-step explicit integration in Eq. (2b):

This procedure, which alleviates the inviscid instability found in i), is a two-step predictor-corrector method (see Refs. 1 and 2) and is similar to the Brailovskaya two-step finite-difference technique. For $\beta = 0$, we obtain

$$c \leq \Phi_{\min}^{-1} = [(2+\cos\varphi)\ (3\sin\varphi)^{-1}]_{\min} = (3)^{-1/2} \tag{7c}$$

This result is more restrictive than the $c \leq 1$ CFL condition found for the Brailovskaya finite-difference method.

For $\beta \neq 0$, the effect of diffusion when treated implicitly is to improve the inviscid stability limitation. For $\bar{u} \to 0$, the method is unconditionally stable[1,2]. Since the convection terms are unchanged, spline 4 has the same stability condition.

iii) Implicit convection and diffusion:

The spline 2 and spline 4 procedures are unconditionally stable if $\theta \geq 1/2$ in Eqs. (2) and (3).

iv) SADI:

In Ref. 1, the interior point stability analysis is extended to the two-dimensional SADI procedure; unconditional stability is demonstrated.

Although the implicit procedures lead to unconditionally stable formulations, as with finite-difference methods, the tridiagonal system may not be diagonally dominant. In this case the inversion algorithm[3] may lead to large error growth. Diagonal dominance can be achieved by a spline adaptation of the finite-difference procedure given in Ref. 15. For all the problems treated here this modification is unnecessary. In other applications it may play a significant role if accurate solutions are to be obtained.

V. Results

Several model problems have been considered in order to evaluate the cubic spline collocation methods presented here. For each of these problems an analytic solution or reliable numerical solution is available for comparison purposes. Spline interpolation (spline 2 and spline 4) is used to approximate the spatial gradients. For the one-dimensional Burgers equation the integration procedure outlined in Sec. II is adopted. Implicit or two-step explicit methods are used. For the two-dimensional diffusion equation, solutions are obtained with the SADI formulation. The Laplace equation in Cartesian[11] and polar coordinates is evaluated with a spline successive approximation procedure. Finally, the similarity equations for the flat plate boundary-layer and the two-dimensional stagnation point are solved by direct integration of the resulting two-point boundary value problems.

Solutions are obtained with both uniform and nonuniform meshes. Three-point finite-difference calculations are included in order to assess the relative increase in accuracy associated with the higher-order procedures. The results are presented in tabular form so that meaningful comparisons are possible.

Burgers Equation

The nonlinear Burgers Eq. (3a), with $x = \bar{x}$, $\bar{u} = u\ (\bar{x}, t)$ and $x = \bar{x} - (1/2)t$, becomes

$$u_t + (u - 1/2)u_x = vu_{xx} \tag{8a}$$

with v constant and the boundary conditions

$$u \to 1 \text{ as } x \to -\infty \text{ and } u \to 0 \text{ as } x \to \infty \tag{8b}$$

The steady-state solution of Eq. (8a) is

$$u = [1 - \tanh(x/4v)]/2 \tag{8c}$$

Spline 2 and the finite-difference solutions of Eqs. (8) have been discussed in Refs. 1 and 2. Both implicit‡‡ and two-step explicit integration techniques, as outlined in Sec. II, have been applied successfully[1,2]. Spline 4 solutions have now been obtained with the implicit‡‡ and/or two-step procedures in

‡‡The nonlinear coefficient u is treated iteratively or with quasilinearization.[1,2]

Eq. (2a), (2b). The system Eqs. (3) with the coefficients Eqs. (6), are considered. In the actual calculations the 3×3 system of Eq. (3) is reduced to a 2×2 system. m_i in V_i is eliminated with Eqs. (1e) or (1f). The boundary conditions in Eq. (8b) on u_1, u_{N+1} are specified at $x=x_{\max}$, with $x_{\max}\geq 3$. The boundary conditions on M_i are obtained from the third-order accurate relation

$$(u_{xx})_{i+1}-(u_{xx})_i=M_{i+1}-M_i \tag{9a}$$

where $i=1$ or N.

a) The boundary condition of Eq. (9a) can be applied in two forms. These are outlined for the boundary $i=1$

$$(u_{xx})_1=(u_{xx})_2-(M_2-M_1)$$

With $(u_{xx})_2$ evaluated from Eq. (5c), we obtain

$$(u_{xx})_1=M_1+(\Delta/6)\,(M_3-(1+\sigma)M_2+\sigma M_1) \tag{9b}$$

where $\sigma=h_3/h_2$. From the governing Eq. (8a)

$$(u_{xx})_1=(u_x)_1/2v=m_1/2v$$

so that with Eq. (1f)

$$m_1=-h_2M_1/3-h_2M_2/6+(u_2-1)/h_2$$

and Eq. (9b) becomes

$$M_1(2v+\sigma v\Delta/3+h_2/3)+M_2(h_2/6-v(1+\sigma)\Delta/3)$$

$$+(v\Delta/3)M_3-u_2/h_2=-1/h_2 \tag{9c}$$

b) An alternate form of Eq. (9a), relating only the two points, $i=1$ and $i=2$, can be derived by evaluating $(u_{xx})_2$ from Eq. (8a). The temporal discretization is given by Eq. (2a). We obtain

$$a_1M_1^{n+1}+a_2M_2^{n+1}+a_3u_2^{n+1}=a_4 \tag{9d}$$

where

$$a_1=\Delta t(v+(u_2^n+0.5)h_2/6)$$

$$a_2=-\Delta t(v-(u_2^n-0.25)h_2/3)$$

$$a_3=(1+\Delta t(u_2^n-1)/h_2)$$

$$a_4=(u_2^n+(u_2^n-1)\Delta t/h_2)$$

For spline 4, $\Delta=(1+\sigma^2)/\sigma(1+\sigma)^2$. For spline 2, set $\Delta=0$ so that Eq. (9c) is second-order accurate. Equation (9b) is third-order accurate for both spline 2 and spline 4. Similar relations are obtained for the other boundary, where $u_{N+1}=0$. Results with fourth-order boundary conditions are given in Ref. 10.

The condition in Eq. (9c) is independent of the time step Δt, and somewhat less cumbersome. It was found that the accuracy of the solutions and the time to attain a converged steady-state solution were virtually uninfluenced by the choice of the boundary condition, (9c) or (9d). This conclusion remains unchanged if the higher-order effects in Eq. (9b), i.e., those terms multiplied by Δ, are treated explicity in Eq. (9c). In this way, (9c) reduces to a two-point implicit formula.

Typical results are shown, for $v=1/8$, on Tables 1–3. The increase in accuracy as one progresses from the finite-difference results to those of spline 2, and finally to spline 4, is apparent. This is particularly true with the nonuniform meshes of Tables 2 and 3. For the conditions of Table 3, the finite-difference calculations with the two-step explicit procedure did not converge. Oscillatory behavior was observed after 3,200 iterations. In certain cases, where h_i is relatively large, the nature of the truncation errors in Eqs. (4a) and (4b) of spline 2 and spline 4 is such that a local value obtained with spline 2 may be as accurate or more accurate than that obtained with spline 4. These are exceptional cases, however, and never occur for $h_i<<1$.

Solutions for other v values are of a similar nature and therefore have not been included here.

Table 1 Solution of Burgers equation – $v=1/8$, $\sigma=1.0$, 31 equally spaced points

$X \setminus u$	F.D.	Spline 2	Spline 4	Exact
0	0.5000	0.5000	0.5000	0.5000
−0.2	0.6999	0.6860	0.6900	0.6900
−0.4	0.8447	0.8290	0.8322	0.8320
−0.6	0.9269	0.9160	0.9170	0.9170
−0.8	0.9673	0.9620	0.9609	0.9610
−1.0	0.9857	0.9830	0.9820	0.9820
−1.2	0.9938	0.9930	0.9918	0.9920
−1.4	0.9973	0.9970	0.9963	0.9960
−1.6	0.9988	0.9990	0.9983	0.9980
−1.8	0.9995	0.9990	0.9993	0.9990

Table 2 Solution of Burgers equation – $v=1/8$, $\sigma=1.2$, 15 points

$x \setminus u$	F.D.	Spline 2	Spline 4	Exact
0	0.5000	0.5000	0.5000	0.5000
−0.3859	0.9510	0.8214	0.8297	0.8240
−0.8494	1.0030	0.9778	0.9654	0.9676
−1.4060	0.9990	1.0004	0.9951	0.9964
−2.0750	1.0	1.0	0.9989	0.9997
−2.8770	1.0	1.0	0.9999	1.0
−3.8420	1.0	1.0	0.9996	1.0
−5.000	1.0	1.0	1.0	1.0

Table 3 Solution of Burgers equation – $v1/8$, $\sigma=1.8$, 15 points

$x \setminus u$	Spline 2	Spline 4	Exact
0	0.5000	0.5000	0.5000
−0.0662	0.5740	0.5691	0.5659
−0.1855	0.6986	0.6858	0.6774
−0.4001	0.8695	0.8452	0.8321
−0.7864	1.0012	0.9689	0.9587
−1.4818	1.0165	1.0083	0.9973
−2.7334	1.0267	1.0257	1.0
−4.9864	1.0	1.0	1.0

Potential Flow over a Circular Cylinder

The governing equation in cylindrical coordinates for the potential flow over a circular cylinder is given by

$$u_{rr}+\frac{1}{r}u_r\frac{1}{r^2}u_{\theta\theta}=0 \tag{10}$$

The boundary conditions are $u_r(1,\theta)=0$, and

$$\lim_{r\to\infty} u(r,\theta)\to r\cos\theta$$

The exact solution of Eq. (10), with these boundary conditions is $u=(r+1/r\cos\theta$.

The resulting 3×3 system for u_{ij}, L_{ij}, and M_{ij} is of the form

$$V_{ij}^{(k+1)}=B_{ij}^{-1}[A_{ij}V_{i,j-1}^{(k+1)}+C_{ij}V_{i,j+1}^{(k)}+D_{ij}V_{i-1,j}^{(k+1)}+E_{ij}V_{i+1,j}^{(k)}] \tag{11}$$

where k is the iteration parameter.

The results of the iterative solution are presented in Tables 4 and 5. As in the previous examples, the finite-difference solutions are obtained by using three-point central difference

Table 4 Potential flow over a circular cylinder

Method	r \ θ	0	$\pi/10$	$2\pi/10$	$3\pi/10$	$4\pi/10$
Exact Solution	1.0500	2.0024	1.9044	1.6200	1.1770	0.6188
$\Delta\theta=\pi/10$	1.2795	2.0611	1.9602	1.6674	1.2115	0.6369
$h_2=0.05$	1.9428	2.4575	2.3372	1.9881	1.4445	0.7594
$\sigma=1.7$	3.8596	4.1187	3.9171	3.3321	2.4209	1.2727
$r_{max}=15.3285$	9.3991	9.5055	0.0403	7.6901	5.5872	2.9374
Finite difference	1.0500	1.8626	1.7714	1.5069	1.0948	0.5757
	1.2795	1.9365	1.8417	1.5667	1.1383	0.5985
	1.9428	2.3597	2.2442	1.9091	1.3871	0.7293
	3.8596	4.0573	3.8587	3.2824	2.3848	1.2538
	9.3991	9.4618	8.9987	7.6547	5.5615	2.9239
Spline 2	1.0500	1.9249	1.8307	1.5573	1.1314	0.5948
	1.2795	1.9821	1.8851	1.6035	1.1650	0.6125
	1.9428	2.3726	2.2565	1.9195	1.3946	0.7332
	3.8596	4.0285	3.8314	3.2591	2.3679	1.2449
	9.3991	9.4254	8.9641	7.6253	5.5401	2.9126
Spline 4	1.0500	2.0089	1.9106	1.6253	1.1808	0.6208
	1.2795	2.0677	1.9665	1.6728	1.2154	0.6390
	1.9428	2.4639	2.3433	1.9934	1.4483	0.7614
	3.8596	4.1185	3.9169	3.3319	2.4208	1.2727
	9.3991	9.4760	9.0122	7.6663	5.5699	2.9283

Table 5 Slip velocity on the front of a circular cylinder $\Delta\theta=\pi/10$

θ	F.D.	Spline 2	Spline 4	Exact
$\pi/10$	-0.564	-0.594	-0.620	-0.628
$2\pi/10$	-1.073	-1.130	-1.179	-1.176
$3\pi/10$	-1.477	-1.555	-1.623	-1.618
$4\pi/10$	-1.736	-1.828	-1.908	-1.902
$5\pi/10$	-1.825	-1.922	-2.006	-2.000

formula. In Table 5, the slip velocity on the fore surface of the cylinder is presented. The superiority of the spline solutions over those resulting from finite-difference discretization is evident. It should be noted that the slip velocity in the finite-difference case is obtained by using a three-point central difference formula, while the spline solutions require only the two-point formula (1e). The higher accuracy of the two-point spline formula over the three-point finite-difference relations can be of considerable importance for problems with derivative boundary conditions.

In Ref. 11 additional solutions using successive approximation for the Laplace equation and the SADI procedure for the diffusion equation are discussed.

Similarity Boundary Layers

The boundary-layer equations for the flow over a flat plate ($\beta=0$) and the two-dimensional stagnation point ($\beta=1$) can be reduced to the following ordinary differential system by using appropriate similarity transformations[16]:

$$u''+fu'+\beta(1-u^2)=0 \tag{12a}$$

$$f'=u \tag{12b}$$

The boundary conditions are

$$f(0)=0, \quad u(0)=0, \quad \lim_{x\to\infty} u(x)=1.0 \tag{12c}$$

Accurate numerical solutions have been reported in the literature.[16]

In the spline 2 and spline 4 formulation, Eq. (12a) is reduced to a 2×2 system for u_i and M_i and the two-point boundary value problem is solved subject to Eq. (12c). For the first-order Eq. (12b), we obtain the following spline approximation from Eq. (1f):

$$f_{i+1}=f_i+h_{i+1}u_i+\frac{h_{i+1}^2}{3}(MF_i+.5MF_{i+1}) \tag{13}$$

where $MF_i=(u')_i$ for spline 2. For spline 4, the following relation to evaluate MF_i is easily derived from Eqs. (1e) and (1f):

$$MF_{i+1}+MF_i=2[(u')_{i+1}-(u')_i]/h_{i+1}$$

$$MF_o=(u')_o \tag{14}$$

Equations (13) and (14) give rise to an initial value problem for f_i and MF_i which is solved by a marching procedure. Equation (13) leads to third-order accurate expression for f_i; therefore, for nonuniform meshes and third-order accurate solutions, this approximation is adequate even for spline 4. For the finite-difference solutions, a second-order accurate two-point formula for f_i, which is consistent with the accuracy of the overall scheme, is obtained with the trapezoidal rule. For $\beta=1$, the nonlinear term u^2 is treated by quasilinearization so that

$$(u^{k+1})^2=u^{(k)}(2u^{(k+1)}-u^{(k)})$$

where k is the iteration parameter.

The results of these computations for both uniform as well as nonuniform meshes are tabulated in Tables 6–10. The shear at the wall is proportional to $f''(0)$ and this term has been evaluated for a variety of meshes. The results are given in Tables 9 and 10 for $\beta=0$ and $\beta=1$, respectively. Finite-difference solutions for u_i are obtained by using the three-point central difference approximation.

As noted previously, the notation $\sigma=1.8/1$ means that $\sigma=1.8$ until h_i reaches 1.0, at which point $\sigma=1.0$ h_2 is the first mesh width off the wall $x=0$; N is the total number of mesh points. N_6 is the number of mesh points in the boundary layer defined by $x\le6$. At $x=6$. $|u-1\text{m}0|<10^{-5}$.

$\beta=0$ Blasius Solution

The spline 4 solution for $N=61$, $h_2=0.1$ and $\sigma=1.0$ is almost identical with the "exact" solution of $f''(0)=0.469600$[16]. With $\sigma=1.8/2$, $h_2=0.5$, $N=21$ and only 5 points in the boundary layer ($N_6=5$), the spline 2 value of $f''(0)$ is in error by only 2%. For the larger h_2 values the spline 2 solutions are even more accurate than those found with spline 4. Similar behavior was observed with Burgers equation in the section entitled "Burgers Equation".

$\beta=1$ Stagnation Point Flow

For $\beta=0$, the exact solution for $u'''(0)=u^{iv}(0)=0$ and therefore the inherent lower-order accuracy of the finite-

Table 6 Blasius profile: $\sigma = 1.0$, $h_2 = 0.1$, $N = 61$

	f				f'			
x	F.D.	Spline 2	Spline 4	Exact	F.D.	Spline 2	Spline 4	Exact
0.1	0.002348	0.002348	0.002348	0.002348	0.046967	0.046962	0.046959	0.046959
0.2	0.009392	0.009392	0.009391	0.009391	0.093923	0.093908	0.093905	0.093905
0.4	0.037555	0.037551	0.037549	0.037549	0.187648	0.187604	0.187605	0.187605
0.6	0.084399	0.084387	0.084386	0.084386	0.280651	0.280563	0.280576	0.280575
0.8	0.149697	0.149673	0.149675	0.149675	0.372076	0.371934	0.371964	0.371963
1.0	0.233026	0.232982	0.232990	0.232990	0.460788	0.460583	0.460633	0.460632
1.5	0.515111	0.514990	0.515032	0.515031	0.661735	0.661379	0.661474	0.661473
2.0	0.886938	0.886707	0.886798	0.886796	0.817023	0.816600	0.816695	0.816694
4.0	2.784256	2.783770	2.783890	2.783885	0.997824	0.997790	0.997771	0.997770
6.0	4.783607	4.783110	4.783220	4.783217	1.0	1.0	1.0	1.0

Table 7 Blasius profile: $\sigma = 1.0$, $h_2 = 1.0$, $N = 21$

	f				f'			
x	F.D.	Spline 2	Spline 4	Exact	F.D.	Spline 2	Spline 4	Exact
1.0	0.23859	0.23768	0.23490	0.23299	0.47718	0.45853	0.46175	0.46063
2.0	0.90351	0.89181	0.88831	0.88679	0.85265	0.81125	0.81795	0.81669
3.0	1.82705	1.79403	1.80274	1.79557	0.99444	0.97059	0.96996	0.96905
4.0	2.82470	2.77982	2.78658	2.78389	1.00085	0.99948	0.99701	0.99777
5.0	3.82500	3.77942	3.78874	3.78323	0.99975	0.99999	1.00001	0.99994
6.0	4.82492	4.77947	4.78555	4.78322	1.00010	1.00002	0.99989	1.0
20.0	18.8249	18.7795	18.7857	18.78322	1.0	1.0	1.0	1.0

Table 8 Blasius profile: $\sigma = 1.8/1$, $h_2 = 0.5$, $N = 21$

	f				f'			
x	F.D.	Spline 2	Spline 4	Exact	F.D.	Spline 2	Spline 4	Exact
0.5	0.05910	0.05835	0.05888	0.05864	0.23642	0.23230	0.23477	0.23423
1.4	0.45557	0.45051	0.45722	0.45072	0.64461	0.61651	0.62568	0.62439
2.4	1.24551	1.22531	1.24067	1.23153	0.93527	0.89654	0.90300	0.90107
3.4	2.21456	2.17478	2.19064	2.18747	1.00284	0.99037	0.98802	0.98797
4.4	3.21568	3.16972	3.18422	3.18338	0.99940	1.00010	0.99898	0.99940
5.4	4.21548	4.16985	4.18386	4.18322	1.00020	1.00001	1.00003	0.99999
19.4	18.2155	18.1698	18.18380	18.18322	1.0	1.0	1.0	1.0

Table 9 $f''(0)$ for blasius equation[a]

x_{MAX}	h_2	σ	Finite Difference	Spline 2	Spline 4	N_6/N
6.0	0.1	1.0	0.469726	0.469634	0.469601	61/61
20.0	1.0	1.0	0.528041	0.475357	0.476359	7/21
5.6665	0.05	1.5	0.516646	0.470718	0.466048	11/11
11.3330	0.1	1.5	0.604955	–	0.493598	9/11
6.4344	0.2	1.5	0.498214	–	0.455623	7/8
13.365	0.01	1.8/1	0.474643	–	0.469188	13/21
16.063	0.05	1.8/1	0.473974	–	0.469438	10/21
19.400	0.5	1.8/1	0.479715	0.466839	0.469509	7/21
37.020	0.5	1.8/2	0.551803	0.460823	0.477930	5/21
53.936	0.5	1.8/3	0.827648	0.506798	0.523256	5/21

[a] $f'(0) = 0.469600$ (Rosenhead[16]).

Table 10 Stagnation point flow[a]

			$f''(0)$			
x_{MAX}	h_2	σ	Finite difference	Spline 2	Spline 4	N_5/N
6.0	0.1	1.0	1.23257	1.23227	1.23258	51/61
20.0	1.0	1.0	1.07167	1.20612	1.20882	6/21
9.4448	0.001	1.8/1	1.26353	1.23604	1.23299	16/21
19.40	0.5	1.8/1	1.24031	1.22764	1.23617	6/21

			$f(h_2)$			
x_{MAX}	h_2	σ	Finite difference	Spline 2	Spline 4	Rosenhead[16]
6.0	0.1	1.0	0.005915	0.005995	0.005996	0.005996
20.0	1.0	1.0	0.390440	0.436393	0.450482	0.459227
19.40	0.5	1.8/1	0.128780	0.132622	0.135410	0.133585

[a] $f'(0) = 1.232588$ (Rosenhead[16])

difference calculation is somewhat obscured near the wall $x = 0$. For the stagnation point solution where $f''(0) = 1.232588$, the improvement associated with the spline formulation is clearly demonstrated. Therefore, it would appear that spline integration should be extremely useful for boundary-layer problems.

VI. Summary

It has been demonstrated that higher-order calculation procedures using cubic spline collocation provide accurate solutions to a number of model problems. The spline methods termed spline 2 and spline 4 can be used for two-point boundary-value problems, as well as implicit, explicit, two-step, ADI, and iterative integration procedures.

Spline 4 is fourth-order accurate with a uniform mesh and third-order with a moderate nonuniform mesh. Spline 2 is second-order accurate for diffusion terms and fourth-order (third-order) for convection with a uniform (nonuniform) mesh. Derivative boundary values are obtained directly without the need for end differencing. For implicit linear systems, the spline methods remain unconditionally stable.

The results confirm the higher-order accuracy of the spline methods and lead to the hopeful conclusion that accurate solutions for more practical flow problems can be obtained with relatively coarse nonuniform meshes. The relationship between the spline methods and similar Hermitian finite-difference procedures must be explored.

There has been no attempt to optimize the temporal integration procedure so as to minimize computer times or increase temporal accuracy. The finite-difference calculations run 50% to 75% faster than the spline integrations. When spline fitting is used to evaluate finite-difference derivatives, the computer times are comparable. It is anticipated that the reduced mesh requirements with these spline methods will result in a net improvement in computer storage and time.

References

[1] Rubin, S.G. and Graves, R.A., "Cubic Spline Approximation for Problems in Fluid Mechanics," NASA TR R-436, 1975.

[2] Rubin, S.G. and Graves, R.A., "Viscous Flow Solutions with a Cubic Spline Approximation," *Computers and Fluids,* Vol. 3, March 1975, pp. 1-36.

[3] Ahlberg, J., Nilson, E., and Walsh, J., *The Theory of Splines and Their Applications*, Academic Press, New York, 1967.

[4] Papamichael, N. and Whiteman, J., "A Cubic Spline Technique for the One-Dimensional Heat Conduction Equation," J. Inst. Math. Appl., Vol. 11, 1973, pp. 111 – 113.

[5] Peters, N., "Boundary – layer Calculations by a Hermitian Finite Difference Method" *Fourth International Conference on Numerical Methods in Fluid Mechanics,* Boulder, Colo. 1974.

[6] Collatz, L., *The Numerical Treatment of Differential Equations.* Springer-Verlag, Berlin, 3rd edition, 1960.

[7] Orszag, S. and Israeli, M., " Numerical Simulation of Viscous Incompressible Flows." *Annual Review of Fluid Mechanics,* Vol. 6, 1974, pp. 281-318.

[8] Hirsh, R., "Higher-Order Accurate Difference Solutions of Fluid Mechanics Problems by a Compact Differencing Technique.". J. Comp. Phys. Vol. 19, Sept. 1975, pp. 90-109.

[9] Krauss, E., Hirschel, E.H. and Kordulla, W., "Fourth Order 'Mehrstellen'-Integration for Three-Dimensional Turbulent Boundary Layers," *Proceedings of AIAA Computational Fluid Dynamics Conference*, Palm Springs, Calif., pp. 92-102, 1973.

[10] Rubin, S.G. and Khosla, P.K., "Higher Order Numerical Methods Derived From Three-Point Polynomial Interpolation," General Applied Science Labs., GASL TR 228, 1976.

[11] Rubin, S.G. and Khosla, P.K., "Higher-Order Numberical Solutions Using Cubic Splines," Proceedings AIAA 2nd Computational Fluid Dynamics Conference, Hartford, Conn., pp. 55-66, see also NASA CR2653, Feb. 1976.

[12] Fyfe, D.J., "The Use of Cubic Splines in the Solutions of Two-Point Boundary Value Problems," Comput. J., Vol. 12, 1969, pp. 188-192.

[13] Daniel, J.W. and Swartz, B., "Extrapolated Collocation for Two-Point Boundary Value Problems Using Cubic Splines," Los Alamos Scientific Lab. Rept. La-DC-72-1520,1972.
Gas," *Soviet Physics-Doklady,* Vol. 10, 1965, pp. 107-110.

[14] Roache, P., *Computational Fluid Dynamics,* Hermosa Publishers, Albuquerque, N.M., 1972.

[15] Khosla, P.K. and Rubin, S.G., "A Diagonally Dominant Second-Order Accurate Implicit Scheme," *Computers and Fluids,* Vol. 2, June 1974, pp. 207-209.

[16] Rosenhead, L., *Laminar Boundary Layers,* Oxford at the Clarendon Press, England, 1963.