CUBIC SPLINE ON SPLINE METHOD FOR THE SOLUTION OF ONE DIMENSIONAL DIFFUSION EQUATION

H.A.H. Abou Steit

Department of Engineering Mathematics and Physics, Faculty of Engineering,
Alexandria University, Alexandria, Egypt.

ABSTRACT

In this paper, the cubic spline on spline technique is used in conjunction with the finite difference method for the solution of a partial differential equation. Two different approaches of the proposed technique, for the solution of the one dimensional diffusion partial differential equation, are presented. The stability analysis of both resulting schemes are given. Numerical results for a test problem are also obtained.

1. INTRODUCTION

Consider the one dimensional diffusion parabolic partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad 0 < x < 1 \tag{1}$$

subject to the initial condition

$$u(x,0) = g(x) \qquad \text{for } 0 \le x \le 1 \tag{2}$$

and the boundary conditions

$$u(0,t) = f_1(t), \quad u(1,t) = f_2(t) \quad \text{for } t > 0 \tag{3}$$

where g (x), f_1 (t) and f_2 (t) are known functions which satisfy the standard requirements for the existence and uniqueness of the solution to the above problem.

The above model has several applications in many engineering problems. Sastry [1] has solved it by using a cubic spline S to approximate the function values u, the space derivative $\frac{\partial^2 u}{\partial x^2}$ was approximated by S″ and the time derivative $\frac{\partial u}{\partial t}$ by a finite difference approximation.

The first approach adopted in this paper to solve the given problem uses a forward difference approximation for the time derivative. Then the resulting second order ordinary differential equation is rewritten as a system of first order differential equations, and a cubic spline on spline [2] is used to reach the numerical solution of the original problem. This will be referred to as Method (1).

The second approach implemented in the present paper namely the spline on spline technique on u, uses as Sastry [1] a cubic spline S to approximate the function values u, and another cubic spline $\bar{S}$ to approximate the first derivative of S. In this technique, the space derivative $\frac{\partial^2 u}{\partial x^2}$ is approximated by $\bar{S}'$ and the time derivative by a finite difference approximation. This will be referred to as Method (2).

2- METHOD (1)

In this approach the time derivative $\frac{\partial u}{\partial t}$ at the arbitrary time level $t_j = jk$; where k denotes the time step and $j = 1,2,\ldots$; is replaced by its corresponding forward difference approximation $\frac{1}{k}(u_{j+1} - u_j)$. Subsequently the second order differential equation that results is written as

$$\frac{d^2 u_1(x)}{dx^2} = F(u_1, x) \tag{4}$$

where u_1 is now a function of x only and F represents the finite difference expression that results from the above procedure.

Equation (4) can be rewritten as a system of two first order differential equations as follows

$$\frac{du_1}{dx} = u_2 \tag{5.a}$$

$$\frac{du_2}{dx} = F(u_1, x) \tag{5.b}$$

This system of equations (5) can be formally written as

$$\frac{du_p}{dx} = F_p(u_1, u_2, x) \qquad \text{where } p = 1, 2 \qquad (6)$$

Subdividing the computational domain $x \in [0,1]$ into n equal subintervals of size h, we construct a set of computational nodes $x_i = ih$ ($i = 0,1,\ldots n$). Integrating equation (6) from x_{i-1} to x_i and denoting the resulting quantity by $\phi_{p,i}(u)$ we have

$$\phi_{p,i}(u) = \int_{x_{i-1}}^{x_i} \frac{du_p}{dx} dx - \int_{x_{i-1}}^{x_i} F_p(u_1, u_2, x) dx = 0$$

from which it follows that

$$\phi_{p,i}(u) = u_{p,i} - u_{p,i-1} - \int_{x_{i-1}}^{x_i} F_p(u_1, u_2, x) dx = 0 \quad p = 1,2 \qquad (7)$$

There are various numerical schemes to evaluate the above integral, among them is the following scheme that requires the numerical derivatives of F [3] leading to:

$$\phi_{p,i}(u) = u_{p,i} - u_{p,i-1} - \frac{h}{2}(F_{p,i} + F_{p,i-1}) + \frac{h^2}{10}(F'_{p,i} - F'_{p,i-1})$$

$$-\frac{h^3}{120}(F''_{p,i} - F''_{p,i-1}) + O(h^7) = 0 \qquad (8)$$

The subscript p will be dropped from now on.
To determine the derivatives F' and F'' from F we use a cubic spline S on F to obtain F', then we use another cubic spline $\bar{S}$ on S' to evaluate F''.

Let S denotes a cubic spline interpolant so that

$$S(x_i) = F_i \qquad \text{for } i = 0,1,2,\ldots n$$

It is known that if

$$S'_0 = F'_0 \text{ and } S'_n = F'_n \text{ then S is unique [4].}$$

S'_i may be directly computed from F_i using the well known formula [4].

$$S'_{i+1} + 4S'_i + S'_{i-1} = \frac{3}{h}(F_{i+1} - F_{i-1}) \qquad (9)$$

At end points, approximations to first and second derivatives can be used in a manner similar to that implemented in [5], [6]

$$F'_0 = \frac{1}{12h}[-25F_0 + 48F_1 - 36F_2 + 16F_3 - 3F_4] + O(h^4)$$

$$F_0^2 = \frac{1}{h^2}[2F_0 - 5F_1 + 4F_2 - F_3] + O(h^2)$$

Corresponding formula for F'_n is skew symmetric to that of F'_0, and formula for F_n^2 is symmetric to that of F_0^2. The superscripts on S and F above denote the order of their derivatives.

Let $\bar{S}$ denotes a cubic interpolating spline on the S'_i values computed in (9). The first derivatives of $\bar{S}$ at x_i are computed from a formula similar to that mentioned above, hence:

$$\bar{S}'_{i+1} + 4\bar{S}'_i + \bar{S}'_{i-1} = \frac{3}{h}(S'_{i+1} - S'_{i-1}) \qquad (10)$$

with

$$\bar{S}'_0 = F_0^2 \text{ and } \bar{S}'_n = F_n^2$$

2.1 Error bounds

In this section we derive some error bounds related to the quantities involved in this method.

Error bounds for $|F'_i - S_i'|$ and $|F_i^2 - \bar{S}_i'|$ are to be determined. Let e_i denotes the difference given by $e_i = F'_i - S'_i$. Using the maximum norm definition we have

$$\|F(x)\| = \max_x |F(x)|$$

$$\|e\| = \max_{0 \le i \le n} |e_i|$$

We now prove some theoretical results related to these error bounds.

Theorem 1:

If S is a cubic interpolating spline on F such that

$$S'_{i+1} + 4S'_i + S'_{i-1} = \frac{3}{h}(F_{i+1} - F_{i-1})$$

with

$$S_0' = F_0' \text{ and } S_n' = F_n'$$

and $$S_0^2 = F_0^2 \text{ and } S_n^2 = F_n^2$$

then $$\| e \| = O(h^4)$$

Proof

By subtracting $F'_{i+1} + 4F'_i + F'_{i-1}$ from both sides of equation (11), we get

$$e_{i+1} + 4e_i + e_{i-1} = F'_{i+1} + 4F'_i + F'_{i-1} - \frac{3}{h}(F_{i+1} - F_{i-1})$$

Using Taylor's expansion this equation reduces to

$$e_{i+1} + 4e_i + e_{i-1} = \frac{h^4}{4}\left[\frac{1}{3}F^5(\eta i) - \frac{1}{5}F^5(\xi_i)\right]$$

where

$$x_{i-1} \le \eta_i, \xi_i \le x_{i+1} \quad i = 1, 2, .. n-1$$

For any function W and V defined at the knots such that

$$W_{i+1} + 4W_i + W_{i-1} = V_i$$

By the maximum principle argument for difference equation, it follows that

$$\| W \| < |W_0| + |W_n| + \frac{1}{2} \max_{0<i<n} |V_i|$$

Let $W = e$ and since by assumption $e_0 = e_n = 0$ therefore

$$\| e \| \le \frac{1}{2} \max_{0<i<n} \frac{h^4}{4} \left| \frac{1}{3}F^5(\eta_i) - \frac{1}{5}F^5(\xi_i) \right|$$

$$\| e \| \le \frac{1}{15} h^4 \| F^5 \| \qquad (12)$$

Error bounds on the cubic spline on spline used to interpolate the derivatives of S' are derived in the following theorem.

Theorem 2

Let $\bar{S}$ denotes a cubic interpolating spline on S'_i computed in (11), the first derivatives $\bar{S}'$ computed at x_i from

$$\bar{S}'_{i+1} + 4\bar{S}'_i + \bar{S}'_{i-1} = \frac{3}{h}(S'_{i+1} - S'_{i-1}) \qquad (13)$$

with

$$\bar{S}'_0 = F_0^2 \text{ and } \bar{S}'_n = F_n^2$$

Then

$$|F_i^2 - \bar{S}'_i| = O(h^3)$$

Proof:

Subtracting $F_{i+1}^2 + 4F_i^2 + F_{i-1}^2$ from both sides of equation (13) and let $F_i^2 - \bar{S}'_i = E_i$ then

$$E_{i+1} + 4E_i + E_{i-1} = \frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2$$

The R.H.S of the above equation can be rewritten as

$$-\frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2 = -\frac{3}{h}\left[(S'_{i+1} - F'_{i+1}) - (S'_{i-1} - F'_{i-1})\right]$$

$$+ \left[-\frac{3}{h}(F'_{i+1} - F'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2\right]$$

Expanding the terms in the second bracket in Taylor series about the point x_i up to order h^4 and using the result given by equation (12) in theorem 1 above, it is found that

$$\left\| \frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2 \right\| \le \frac{1}{5} h^3 \| F^5 \|$$

Applying the maximum principle for difference equation, we get

$$|F_i^2 - \bar{S}'_i| \le \frac{1}{10} h^3 \| F^5 \|$$

Replacing F'_i and F_i^2 in equation (8) by S'_i and $\bar{S}'_i$

respectively we obtain

$$\phi_i(u) = u_i - u_{i-1} - \frac{h}{2}(F_i + F_{i-1}) + \frac{h^2}{10}(S'_i - S'_{i-1}) - \frac{h^3}{120}(\bar{S}'_i + \bar{S}'_{i-1}) + O(h^6) \quad (14)$$

In order to solve the system of equations (14), let

$$\phi_i\,(u) = V_i\,(u) + W_i\,(u) \quad (15)$$

where

$$V_i = u_i - u_{i-1} - \frac{h}{2}\,(F_i + F_{i-1}) \quad (16)$$

$$W_i = \frac{h^2}{10}\left[(S'_i - S'_{i-1}) - \frac{h}{12}(\bar{S}'_i + \bar{S}'_{i-1})\right] \quad (17)$$

Using the modified Newton's non-linear iterative technique, then

$$u^{(k+1)} = u^{(k)} - J^{-1}\,(V)\;\phi\,(u^k) \qquad k = 0,1,2,\ldots \quad (18)$$

where J (V) is the Jacobian of the values of V given by equation (16). The convergence of the modified Newton technique is proved in [7]. It is evident that J (V) has a sparse structure and has only few elements per row. Various sparse matrix techniques can be used for the solution of equation (18), for details of such techniques we refer to the work given in [8].

2.2 Stability of the numerical scheme in Method (1)

Since all computations involved are done using a finite number of decimal places, then round off errors are unavoidably introduced.

Following Von Neuman argument the difference between the exact numerical solutions and those that are computed, can be expressed as a linear combination of exponential function in time multiplied by harmonic ones in space. Let us denote these differences by $E_{u_p}, E_{s_p'}$ and $E_{\bar{s}_p'}$ for the function u_p, the cubic spline S_p' and the spline $\bar{S}_p'$, p=1,2. Due to the linearity of the problem in hand, we can consider one term of such combination, hence we have

$$E_{u_p} = a_p\; e^{\hat{i}i\beta h}\; e^{\alpha jk}$$

$$E_{s_p'} = b_p\; e^{\hat{i}i\beta h}\; e^{\alpha jk}$$

$$E_{\bar{s}_p'} = c_p\; e^{\hat{i}i\beta h}\; e^{\alpha jk} \qquad p = 1,2$$

where a_p, b_p, c_p, α and β are arbitrary constants and $\hat{i} = \sqrt{-1}$.

These expressions are known to satisfy similar equations as (9), (10) and (14) respectively. Hence it follows that equation (9) leads to

$$b_1\,(2 + \cos\beta h) = \frac{3}{h} a_2\,\hat{i}\,\sin\beta h \quad (19)$$

and

$$b_2\, e^{\alpha k}(2 + \cos\beta h) = \frac{3}{hk} a_1 \hat{i}\,\sin\beta h\;(e^{\alpha k} - 1) \quad (20)$$

Equation (10) gives

$$c_1\,(2 + \cos\beta h) = \frac{3}{h}\, b_1 \hat{i}\,\sin\beta h \quad (21)$$

and

$$c_2\,(2 + \cos\beta h) = \frac{3}{h}\, b_2 \hat{i}\,\sin\beta h \quad (22)$$

Using equation (14) we can arrive at

$$2a_1\hat{i}\;\sin\beta h - ha_2\,(1 + \cos\beta h)$$

$$+\;\frac{h^2}{5} b_1 \hat{i}\,\sin\beta h - \frac{h^3}{60} c_1 (1 + \cos\beta h) = 0 \quad (23)$$

and

$$2a_2 e^{\alpha k}\hat{i}\sin\beta h - \frac{h}{k} a_1 (e^{\alpha k} - 1)(1 + \cos\beta h) + \frac{h^2}{5} b_2 e^{\alpha k}\hat{i}\sin\beta h$$

$$-\frac{h^3}{60} c_2 e^{\alpha k}(1 + \cos\beta h) = 0 \quad (24)$$

The Von Neuman stability condition requires that

$$|e^{\alpha k}| \leq 1$$

The above system of equations (19-24) leads to

$$e^{\alpha k} = \frac{Q(\theta)}{Q(\theta) + rT(\theta)} \quad (25)$$

where $r = \frac{k}{h^2}$, $\theta = \beta h$,

$$Q(\theta) = 121\,Cos^5\theta + 1617\,Cos^5\theta + 8342\,Cos^3\theta + 20582\,Cos^2\theta + 23937\,Cos\theta + 10201$$

and

$$T(\theta) = r[-1600\cos^5\theta - 11200\,Cos^4\theta - 25600\,Cos^3\theta - 12800\,Cos^2\theta + 25600\cos\theta + 25600]$$

By plotting the values of $| e^{\alpha k} |$ as θ varies from 0 to 2π and using different values for r ($r = \frac{k}{h^2}$), it was found that all the orbits remain within the unit circle for all choices of h and k. Hence it follows that the scheme is unconditionally stable.

3- METHOD (2)

In this alternative method we use a different approach namely cubic spline on spline on u.

Let S denotes a cubic spline approximation on u, and $\bar{S}$ a cubic spline approximation on $\bar{S}'$ (which is the first derivative of S w.r.t.x). Then a suitable approximation of equation (1) is given by

$$\frac{1}{k}[u_{i,j+1} - u_{i,j}] = (1-\mu)\bar{S}'_{i,j+1} + \mu\,\bar{S}'_{i,j} \qquad (26)$$

where μ is a weighing parameter, if $\mu = 1$ the method is explicit, if $\mu = 0$ it is fully implicit; in general $0 < \mu < 1$.

The cubic spline on u and that on S' satisfy

$$S'_{i+1} + 4\,S'_i + S'_{i-1} = \frac{3}{h}\,(u_{i+1} - u_{i-1}) \qquad (27)$$

$$\bar{S}'_{i+1} + 44\bar{S}'_i + \bar{S}'_{i-1} = \frac{3}{h}((S'_{i+1} - S'_{i-1})) \qquad (28)$$

It is clear that the above system leads to a triadiagonal one. Upon solving this system, together with the supplementary conditions

$$\bar{S}'_o = f'_1\,(t) \quad \text{and} \quad \bar{S}'_n = f'_n\,(t)$$

resulting from

$$\frac{\partial}{\partial t}S(x_i, t) = \frac{\partial}{\partial x}\bar{S}(x_i\,t) = \bar{S}'_i\,(t)$$

and the requirements

$$S\,(x_0,\, t) = f_1\,(t) \text{ and } S\,(x_n, t) = f_2\,(t)$$

the values of $\bar{S}'$ at each point of time can be obtained.

3.1 Stability analysis of Method (2)

Following the Von Neuman argument and in a similar manner as that discussed earlier we arrive at:

$$\frac{a}{k}(e^{\alpha k} - 1) = c[(1-\mu) + \mu\,e^{\alpha k}] \qquad (29)$$

$$b(2 + \cos\beta h) = \frac{3a}{h}\hat{i}\,\sin\beta h \qquad (30)$$

$$c(2 + \cos\beta h) = \frac{3b}{h}\hat{i}\,\sin\beta h \qquad (31)$$

which are obtained using equations (26), (27), (28) respectively. This leads to the following expression for $e^{\alpha k}$.

$$e^{\alpha k} = 1 - \frac{9 r \sin^2\beta h}{(2 + \cos\beta h)^2 + 9\,r\mu\,\sin^2\beta h} \qquad (32)$$

For stability we must impose the condition

$$| e^{\alpha k} | \le 1$$

which leads to

$$r\,(1-2\,\mu) \le \frac{2}{3}$$

Therefore the numerical scheme based on the cubic spline on spline on u is conditionally stable. However, the proposed scheme mentioned above is less restrictive than that obtained by Sastry [1], where the stability condition for his scheme leads to $r\,(1-2\,\mu) \le \frac{1}{6}$.

4- NUMERICAL RESULTS

This paper does not intend to solve a difficult problem, but rather to present the numerical methods discussed above and to illustrate their computational performance.

Equation (1) was solved with the initial condition $u = \sin \pi x$ $(0 \leq x \leq 1)$ at $t = 0$, and the boundary conditions $u = 0$ at $x = 0$ and $x = 1$ $(t \geq 0)$, h was chosen $= \frac{1}{20}$ and $r = \frac{1}{\sqrt{20}}$

.

The results were in very good agreement with the exact solution which is $u = \sin \pi x \; e^{-\pi^2 t}$.

These results are shown in the following table.

x	Method 1	Method 2	Exact solution
0.25	0.7001961	0.7001613	0.7001622
0.5	0.9902269	0.9901791	0.9901789
0.75	0.7001961	0.7001630	0.7001619

CONCLUSION

Two different approaches for the application of cubic spline on spline technique are presented. Both methods give a good approximation of the one dimensional parabolic diffusion equation. The first method, as shown, is unconditionally stable. In the second method, although the stability analysis leads to a restrictive condition on the choice of h (the space step) and k (the time step), it is noticed that it is less restrictive than that when a cubic spline is used on the value of u directly.

REFERENCES

[1] S.S Sastry, "Finite difference approximations to one-dimensional parabolic equations using a cubic spline technique", *Journal of computational and Applied Mathematics*, vol. 2, no.1, 1976, pp. 23-26.

[2] R.P. Tewarson, "On the use of splines for numerical solution of non-linear two point boundary value problems", *BIT*, vol. 20, 1980, pp. 223-232.

[3] F.B. Hildebrand, *Introduction to Numerical Analysis*, McGraw-Hill, New York, 1974.

[4] J.H. Ahlberg, E.N. Wilson and J.H. Walsh, *The Theory of Splines and their Applications*, Academic Press, New York, 1967.

[5] Z. Kopal, *Numerical Analysis*, John Wiley, New York, 1961.

[6] H.A.H. Abou Steit, "A cubic spline on spline method for non-linear boundary value problems", Proceedings of the 4th *Conference on Theoretical and Applied Mechanics*, Academy of Scientific Research and Technology, Cairo-Egypt, 1991, pp. 21-29.

[7] J.M. Ortega and W.C. Rheinboldt, *Iterative Solution of Non-linear Equations in Several Variables*, Academic Press, New York, 1970.

[8] R.P. Tewarson, *Sparse Matrices*, Academic Press, New York, 1973.