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A Finite Difference Formula of Implicit Type for IBVP of Heat Equation

Dhruti B. Joshi[1], Prof.(Dr.) A. K. Desai[2]

[1]Lecturer in Mathematics, Government Polytechnic,

Himmatnagar - 383001, India

E-mail: dkpatel1888@gmail.com

[2]Department of Mathematics, Gujarat University

Ahmedabad - 380009, India

E-mail: desai_ak@yahoo.com

Abstract

In this paper a different approach is adopted to develop a new finite difference formula of implicit type. To illustrate and explain the development of this formula for a given parabolic partial differential equation a simple Initial-Boundary Value Problem (IBVP) of Heat Equation is used. We have applied some known finite difference formulas in a specific way to get a new finite difference formula. In this process we get formulas, one of which proceeds from left boundary and moves to right boundary of the space variable and one another formula which proceeds from right boundary and moves to left boundary of the space variable. Using these formulas and grouping the grid points from both the boundaries a new finite difference formula is obtained and is compared in several different ways for its efficiency.

Keywords: Heat Equation; Finite Difference Formulas; Taylor Series Expansion
AMS Subject Classification: 35K05; 35K20; 58J35; 65M06

1 Introduction

As we know, numerical methods provide ways to tackle complex problems in mathematics, it is necessary to develop new numerical formulas to solve different types of problems. In explicit type methods the solution is determined at only one mesh point at a time. On the other hand implicit methods give solutions at more than one mesh points. Generally solutions at all the mesh points in one time row are determined at a time using matrices ([1] & [3]). To derive a New Finite Difference Formula of Implicit Type we use a different approach in this paper. To explain and illustrate the development of such formula for a given parabolic partial differential equation a simple Initial-Boundary Value Problem of Heat equation is used.

In section-2 we have applied some known finite difference formulas in a specific way to get a new finite difference formula of implicit type. In this process we get formulas, one of which proceeds from left boundary and moves to right boundary of the space variable and one another formula which proceeds from right boundary and moves to left boundary of the space variable [2]. We use these formulas and take groups of two mesh points in two different ways taking the Initial and Boundary Conditions in consideration. Further, we derive new Finite Difference Formula of Implicit Type by adding formulas obtained by grouping the mesh points in different ways.

In section-3 we solve an Initial-Boundary Value Problem of Heat equation using the formula obtained in section-2. We use Mathematica to compare the numerical solutions with the Mathematica Exact Values of the analytical solution.

2 A Finite Difference Formula of Implicit Type

We consider the Initial-Boundary Value Problem of Heat equation,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 \le x \le l,\ 0 \le t \le T \tag{2.1}$$

with initial condition,

$$u(x,0) = f(x), \quad 0 \le x \le l$$

and boundary conditions,

$$u(0,t) = g_0(t), \quad 0 \le t \le T$$

$$u(l,t) = g_l(t), \quad 0 \le t \le T$$

Here, to get finite difference formulas, we use Taylor Series Expansion and consider the scheme forward in time and centred in space.

Also we use the notations,

$$\begin{aligned} u(x,t) &= u(ih, jk) \\ &= u_{i,j} \\ u(x+h,t) &= u((i+1)h, jk) \\ &= u_{i+1,j} \\ u(x,t+k) &= u(ih,(j+1)k) \\ &= u_{i,j+1}. \end{aligned}$$

Where, $x = ih$ and $t = jk$, $i = 0, 1, 2, \ldots, m, \quad j = 0, 1, 2, \ldots, n$

Therefore, for $0 \le x \le l$,

$$l = mh \;\Rightarrow\; m = \frac{l}{h}$$

and for $0 \le t \le T$,

$$T = nk \;\Rightarrow\; n = \frac{T}{k}$$

Using Taylor Series expansion,

$$u_{i,j+1} = u_{i,j} + \frac{k}{1!}\frac{\partial u}{\partial t} + O(k^2)$$

we get,

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{k} + O(k). \tag{2.2}$$

Similarly,

$$\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j} = \frac{\partial u}{\partial x} + \frac{(\frac{h}{2})}{1!}\frac{\partial^2 u}{\partial x^2} + \frac{(\frac{h}{2})^2}{2!}\frac{\partial^3 u}{\partial x^3} + O(h^3)$$

and,

$$\left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j} = \frac{\partial u}{\partial x} - \frac{(\frac{h}{2})}{1!}\frac{\partial^2 u}{\partial x^2} + \frac{(\frac{h}{2})^2}{2!}\frac{\partial^3 u}{\partial x^3} + O(h^3).$$

Using above two equations, we get,

$$\frac{\partial^2 u}{\partial x^2} = \frac{\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j} - \left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j}}{h} + O(h^2) \tag{2.3}$$

Also by taking central difference,

$$\begin{aligned} & u\left[\left(x+\tfrac{h}{2}\right)+\tfrac{h}{2},t\right] - u\left[\left(x+\tfrac{h}{2}\right)-\tfrac{h}{2},t\right] \\ &= \left[u\left(x+\tfrac{h}{2},t\right)+\tfrac{h}{2}u_x\left(x+\tfrac{h}{2},t\right)\right] - \left[u\left(x+\tfrac{h}{2},t\right)-\tfrac{h}{2}u_x\left(x+\tfrac{h}{2},t\right)\right] + O(h^2) \\ &= hu_x\left(x+\tfrac{h}{2},t\right) + O(h^2) \end{aligned}$$

Therefore,

$$u_x\left(x+\frac{h}{2},t\right) = \frac{u\left[\left(x+\frac{h}{2}\right)+\frac{h}{2},t\right] - u\left[\left(x+\frac{h}{2}\right)-\frac{h}{2},t\right]}{h} + O(h)$$

Similarly,

$$u_x\left(x-\frac{h}{2},t\right) = \frac{u\left[\left(x-\frac{h}{2}\right)+\frac{h}{2},t\right] - u\left[\left(x-\frac{h}{2}\right)-\frac{h}{2},t\right]}{h} + O(h)$$

Hence,

$$u_x\left(x+\frac{h}{2},t\right) = \frac{u\left[x+1,t\right] - u\left[x,t\right]}{h} + O(h)$$

and

$$u_x\left(x-\frac{h}{2},t\right) = \frac{u\left[x,t\right] - u\left[x-1,t\right]}{h} + O(h)$$

This implies,

$$\begin{aligned} \left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j} &= \frac{u_{i+1,j} - u_{i,j}}{h} + O(h) \\ \left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j} &= \frac{u_{i,j} - u_{i-1,j}}{h} + O(h) \end{aligned}$$

In formula (2.3), on replacing $\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j}$ by $\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j+1}$ we get,

$$\frac{\partial^2 u}{\partial x^2} = \frac{\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j+1} - \left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j}}{h} + O(h^2) \tag{2.4}$$

Therefore,

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j+1} - u_{i,j+1} - u_{i,j} + u_{i-1,j}}{h^2} + O(h^2) \tag{2.5}$$

Using (2.5) and (2.2) in (2.1) (i.e. Heat equation), we get,

$$\frac{u_{i,j+1}-u_{i,j}}{k} = \frac{\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j+1} - \left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j}}{h} + O(k+h^2)$$

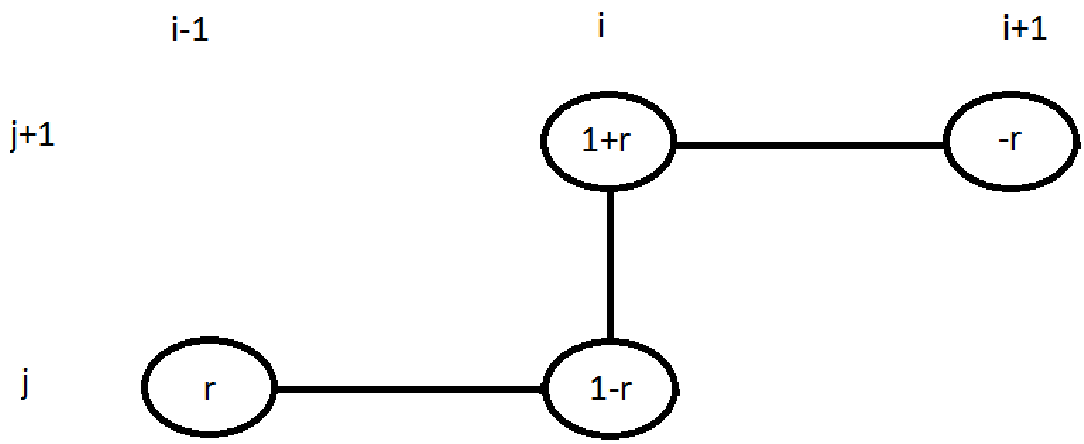
$$\Rightarrow \quad u_{i,j+1}-u_{i,j} = \left(\frac{k}{h^2}\right)(u_{i+1,j+1}-u_{i,j+1}-u_{i,j}+u_{i-1,j}) + O(k+h^2)$$

Hence, taking $r=\frac{k}{h^2}$,

$$(1+r)u_{i,j+1} - ru_{i+1,j+1} = (1-r)u_{i,j} + ru_{i-1,j} + O(k+h^2) \tag{2.6}$$

This is a right to left type equation as it proceeds from a left boundary point and ends at a right boundary point.

The computational molecule representation of formula (2.6) is,



Now, in formula (2.3), on replacing $\left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j}$ by $\left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j+1}$ we get,

$$\frac{\partial^2 u}{\partial x^2} = \frac{\left(\frac{\partial u}{\partial x}\right)_{i+\frac{1}{2},j} - \left(\frac{\partial u}{\partial x}\right)_{i-\frac{1}{2},j+1}}{h} + O(h^2) \tag{2.7}$$

Therefore,

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j}-u_{i,j}-u_{i,j+1}+u_{i-1,j+1}}{h^2} + O(h^2) \tag{2.8}$$

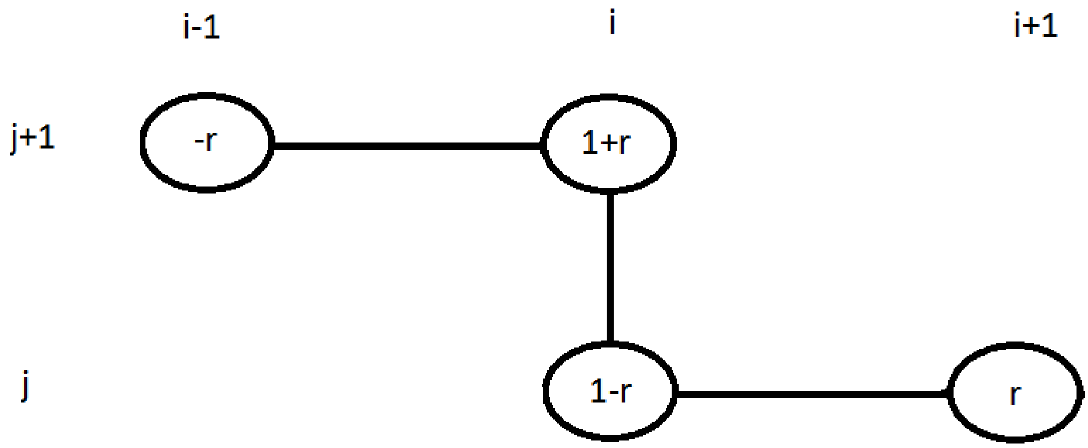
Applying (2.2) and (2.8) in Heat Equation (2.1) and taking $\frac{k}{h^2}=r$, we get,

$$(1+r)u_{i,j+1} - ru_{i-1,j+1} = (1-r)u_{i,j} + ru_{i+1,j} + O(k+h^2) \tag{2.9}$$

This is a left to right type equation as it proceeds from a right boundary point and ends at a left boundary point.

The computational molecule representation of formula (2.9) is,

We have taken, $i=0,1,2,\ldots,m$ and $j=0,1,2,\ldots,n$. Hence, $u_{0,j}$ & $u_{m,j}$ for all j are known as these values are obtained from the initial and boundary conditions.



Also as in each of (2.6) and (2.9), exactly two mesh points from unknown time row $j+1$ are involved, for the pairs $(u_{0,j+1},\ u_{1,j+1})$ and $(u_{m,j+1},\ u_{m-1,j+1})$ exactly one of them (i.e. $u_{0,j+1}$ & $u_{m,j+1}$) is known and therefore $u_{1,j+1}$ and $u_{m-1,j+1}$ are obtained using (2.6) and (2.9).
Now, we take pairs of two mesh points $u_{m-2,j+1}$ and $u_{m-3,j+1}$ and rewrite formulas (2.9) and (2.6). Here we will use (2.6) to get value of $u_{m-1,j+1}$ taking the value of $u_{m,j+1}$ from the given boundary condition.

$$-ru_{m-2,j+1} + (1+r)u_{m-3,j+1} = (1-r)u_{m-3,j} + ru_{m-4,j} \tag{2.10}$$

$$-ru_{m-3,j+1} + (1+r)u_{m-2,j+1} = (1-r)u_{m-2,j} + ru_{m-1,j} \tag{2.11}$$

We solve above two equations for $u_{m-2,j+1}$ and $u_{m-3,j+1}$ using matrices.

$$\begin{pmatrix} 1+r & -r \\ -r & 1+r \end{pmatrix} \begin{pmatrix} u_{m-3,j+1} \\ u_{m-2,j+1} \end{pmatrix} = \begin{pmatrix} 1-r & 0 \\ 0 & 1-r \end{pmatrix} \begin{pmatrix} u_{m-3,j} \\ u_{m-2,j} \end{pmatrix} + r \begin{pmatrix} u_{m-4,j} \\ u_{m-1,j} \end{pmatrix} \tag{2.12}$$

Similarly, we may write matrix equations for other pairs (i.e. $(u_{m-4,j+1}, u_{m-5,j+1})$, $(u_{m-6,j+1}, u_{m-7,j+1}), \ldots,\ (u_{2,j+1}, u_{1,j+1})$) and combining all the equations, we get,

$$A[u_{j+1}] = B[u_j] + b_1. \tag{2.13}$$

Here,

$$A = [a_{ij}],\ B = [b_{ij}],\ b_1 = r[b^1_{ij}],\ u_{j+1} = [U^{j+1}_{i1}] \text{ and } u_j = [U^j_{i1}].$$

where,

$$a_{ij} = \begin{cases} 1+r & \text{if } \ i=j \\ -r & \text{if } \ i=2q, j=2q-1 \\ -r & \text{if } \ i=2q-1, j=2q \end{cases}$$

$$b_{ij} = \begin{cases} 1-r & \text{if } \ i=j \\ r & \text{if } \ i=2q+1,\ j=2q \\ r & \text{if } \ i=2q,\ j=2q+1 \end{cases}$$

$$b^1_{ij} = \begin{cases} u_{0,j} & \text{if } i = 1,\ j = 1 \\ u_{m,j+1} & \text{if } i = m-1,\ j = 1 \\ 0 & \text{otherwise.} \end{cases}$$

$$U^{j+1}_{i1} = u_{i,j+1}$$

and

$$U^{j}_{i1} = u_{i,j}$$

$$i = 1, 2, \ldots, m-1, q = 1, 2, \ldots, \tfrac{m-2}{2}$$

We note that,

A & B are tridiagonal matrices of order $(m-1)$.

The matrices $u_j, u_{j+1},$ & b_1 are column matrices of order $(m-1) \times 1$.

Further, it is also clear that m must be even.

The matrices A and B can be rewritten as,

$$A = I + rM_1$$

and

$$B = I - rM_2$$

Here, I is Identity Matrix, $M_1 = [M^1_{ij}]$ and $M_2 = [M^2_{ij}]$.

Where,

$$M^1_{ij} = \begin{cases} 1 & \text{if } i = j \\ -1 & \text{if } i = 2q,\ j = 2q-1 \\ -1 & \text{if } i = 2q-1,\ j = 2q \end{cases}$$

and

$$M^2_{ij} = \begin{cases} 1 & \text{if } i = j \\ -1 & \text{if } i = 2q+1,\ j = 2q \\ -1 & \text{if } i = 2q,\ j = 2q+1 \end{cases}$$

$$q = 1, 2, \ldots, \tfrac{m-2}{2}$$

Hence, (2.13) is rewritten as,

$$[I - rM_1][u_{j+1}] = [I - rM_2][u_j] + b_1 \tag{2.14}$$

Now, we take pairs of two mesh points $u_{m-1,j+1}$ and $u_{m-2,j+1}$ and rewrite formulas (2.9) and (2.6). Here we will use (2.9) to get value of $u_{1,j+1}$ taking the value of $u_{0,j+1}$ from the boundary condition.

$$-ru_{m-1,j+1} + (1+r)u_{m-2,j+1} = (1-r)u_{m-2,j} + ru_{m-3,j}$$

$$-ru_{m-2,j+1} + (1+r)u_{m-1,j+1} = (1-r)u_{m-1,j} + ru_{m,j}$$

We solve these equations for $u_{m-1,j+1}$ and $u_{m-2,j+1}$ using matrix method.

$$\begin{pmatrix} 1+r & -r \\ -r & 1+r \end{pmatrix} \begin{pmatrix} u_{m-2,j+1} \\ u_{m-1,j+1} \end{pmatrix} = \begin{pmatrix} 1-r & 0 \\ 0 & 1-r \end{pmatrix} \begin{pmatrix} u_{m-2,j} \\ u_{m-1,j} \end{pmatrix} + r \begin{pmatrix} u_{m-3,j} \\ u_{m,j} \end{pmatrix}$$

In a similar way we may write matrix equations for other pairs (i.e. $(u_{m-3,j+1}, u_{m-4,j+1})$, $(u_{m-5,j+1}, u_{m-6,j+1})$, . . ., $(u_{3,j+1}, u_{2,j+1})$) and combining all the matrix equations we get,

$$A^{'}[u_{j+1}] = B^{'}[u_j] + b_2. \tag{2.15}$$

Here,

$$A^{'} = [a^{'}_{ij}],\ B^{'} = [b^{'}_{ij}] \text{ and } b_2 = [b^2_{ij}].$$

Where,

$$a^{'}_{ij} = \begin{cases} 1+r & \text{if } i = j \\ -r & \text{if } i = 2q+1,\ j = 2q \\ -r & \text{if } i = 2q,\ j = 2q+1 \end{cases}$$

$$b^{'}_{ij} = \begin{cases} 1-r & \text{if } i = j \\ r & \text{if } i = 2q,\ j = 2q-1 \\ r & \quad i = 2q-1,\ j = 2q \end{cases}$$

and

$$b^2_{ij} = \begin{cases} u_{0,j+1} & \text{if } i = 1,\ j = 1 \\ u_{m,j} & \text{if } i = m-1,\ j = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$q = 1, 2, \ldots, \tfrac{m-2}{2}$$

We note that $A^{'}$ & $B^{'}$ are tridiagonal matrices of order $(m-1)$ and b_2 is a column matrix of order $(m-1) \times 1$.

Now, using the matrices M_1 & M_2 which we have defined earlier, (2.15) is rewritten as,

$$[I + rM_2][u_{j+1}] = [I - rM_1][u_j] + b_2 \tag{2.16}$$

We add (2.14) and (2.16) to get our desired implicit type finite difference formula for the numerical solution of Heat Equation (2.1).

$$[2I + r(M_1 + M_2)][u_{j+1}] = [2I - r(M_1 + M_2)][u_j] + (b_1 + b_2) \tag{2.17}$$

3 Example

Here we discuss an example using (2.17) for different values of r and we also compare it with Mathematica Exact Values of Analytical Solution.

Solve the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

with initial condition

$$u(x, 0) = 4x(1-x), \qquad 0 \le x \le 1$$

and boundary conditions

$$u(0,t) = u(1,t) = 0, \qquad t \geq 0$$

Solution:

First of all we note that the analytical solution of this IBVP of Heat Equation is,

$$u(x,t) = \frac{32}{\pi^3} \sum_{p=0}^{\infty} \frac{1}{(2p+1)^3} e^{-(2p+1)^2\pi^2 t} \sin((2p+1)\pi x). \tag{3.1}$$

which is derived using known methods [4].

Note:

In following tables,

- For The Analytical Solution (3.1),

$$u(1-x,t) = \frac{32}{\pi^3} \sum_{p=0}^{\infty} \frac{1}{(2p+1)^3} e^{-(2p+1)^2\pi^2 t} \sin((2p+1)\pi(1-x))$$

  Also,

$$\begin{aligned} \sin((2p+1)\pi(1-x)) &= \sin((2p+1)\pi - (2p+1)\pi x)) \\ &= \sin((2p+1)\pi x), \qquad p = 0,1,2,\ldots,\infty. \end{aligned}$$

  Therefore,

$$\begin{aligned} u(1-x,t) &= \frac{32}{\pi^3} \sum_{p=0}^{\infty} \frac{1}{(2p+1)^3} e^{-(2p+1)^2\pi^2 t} \sin((2p+1)\pi(1-x)) \\ &= \frac{32}{\pi^3} \sum_{p=0}^{\infty} \frac{1}{(2p+1)^3} e^{-(2p+1)^2\pi^2 t} \sin((2p+1)\pi x) \\ &= u(x,t) \end{aligned}$$

  Hence,

$$\begin{aligned} u(0.1,t) &= u(0.9,t) \\ u(0.2,t) &= u(0.8,t) \\ u(0.3,t) &= u(0.7,t) \\ u(0.4,t) &= u(0.6,t) \end{aligned}$$

- We shall calculate the first time row (i.e. $j = 1$) from the initial condition (i.e. $j = 0$).
- Numerical Solutions obtained by (2.17) implementing on Mathematica are denoted by NS.
- Mathematica Exact Values of The Analytical Solution are denoted by AS.
- Absolute Difference between numerical solution and mathematica exact value of analytical solution is denoted by AD.

1) We consider $r = 0.1$, with $h = 0.1$ and $k = 0.001$. As $j = 1$, $t = jk = 0.001$.

Table 1: $u[x,0.001]$, & $r = 0.1$

	x=0.1 & x=0.9	x=0.2 & x=0.8	x=0.3 & x=0.7	x=0.4 & x=0.6	x=0.5
NS	0.352364	0.632017	0.832001	0.952000	0.992000
AS	0.352045	0.632000	0.832000	0.952000	0.992000
AD	0.000319	0.000016	0.000000	0.000000	0.000000

2) We consider $r = 0.2$, with $h = 0.1$ and $k = 0.002$. As $j = 1$, $t = jk = 0.002$.

Table 2: $u[x,0.002]$, & $r = 0.2$

	x=0.1 & x=0.9	x=0.2 & x=0.8	x=0.3 & x=0.7	x=0.4 & x=0.6	x=0.5
NS	0.345343	0.624113	0.824009	0.944001	0.984000
AS	0.344592	0.624003	0.824000	0.944000	0.984000
AD	0.000750	0.000109	0.000000	0.000000	0.000000

3) We consider $r = 0.5$, with $h = 0.1$ and $k = 0.005$. As $j = 1$, $t = jk = 0.005$.

Table 3: $u[x,0.005]$, & $r = 0.5$

	x=0.1 & x=0.9	x=0.2 & x=0.8	x=0.3 & x=0.7	x=0.4 & x=0.6	x=0.5
NS	0.326862	0.601177	0.80020	0.920035	0.960011
AS	0.326027	0.600461	0.800016	0.920000	0.960000
AD	0.000836	0.000716	0.000185	0.000035	0.000012

Conclusion

We have derived (in section-2) a finite difference formula of implicit type for Initial-Boundary Value Problem of Heat Equation and (in section-3) we have computed numerical solutions taking different values of r by implementing the new finite difference formula in Mathematica. Also we have compared the numerical solutions obtained by our finite difference formula with the Mathematica exact values of analytical solution. The above tables indicate that the numerical solutions obtained using the new finite difference formula are very close to the analytical solutions.

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