Unified Computational Analysis of Conventional Numerical Methods for Time Dependant Heat Equation

M. Naveed Akhtar, M. Hanif Durad and Anila Usman

Abstract—**The objective of this paper is to perform a unified error and computation time analysis of conventional numerical methods for solving heat equation. The numerical techniques employed include Forward Difference, Backward Difference, Crank Nicolson, Alternate Directions Scheme and DuFort-Frankel methods for time dependent heat equation. The heat equation has been implemented to 1-D, 2-D and 3-D problems, both for the Neumann and Dirichlet boundary conditions. On basis of experimental results theoretical justifications has been provided regarding the performance of each method..**

Index Terms—**Neuman Boundary Conditos, Dirichlet Boundary Conditions, Heat Equation, Forward Difference, Backward Difference, Crank Nicolson, Alternate Directions Method (ADI), DuFort-Frankel Scheme.**

I. Introduction

TIME dependant heat/diffusion equation is one the most important partial differential equations (PDEs), which is an example of a parabolic PDE [1]. Many numerical methods have been suggested in literature to solve heat equation. While selecting a numerical method the two important parameters are computation time and error. It is obvious that numerical method having lower error margin and fast to solve the problem will be preferred. In this paper we consider computation time and mean square error as a performance bench mark for computational analysis.

Error of numerical methods also depends upon the type of boundary conditions being used. Three common types of boundary conditions for the heat equation are Dirichlet, Neumann and mixed conditions [2]. In this paper we concentrate on first two types of boundary conditions for uniforms error analysis and expect a mix type behavior for the third type. Different authors have already presented error analysis for diffusion equation. In [3] the error analysis for convection diffusion equation has been presented for forward, center and backward difference methods. Three different PDE problems are considered in said paper to emphasize the results.

In [4] the FEM method has been applied to diffusion equation and for different conditions validity of this method for these conditions is discussed based on error analysis. In [5] Implicit-explicit (IMEX) schemes has been applied to time dependent diffusion equation and stability analysis for 1st, 2nd, 3rd, and 4th order multistep IMEX schemes is performed. Different authors have worked on individual methods and also for diffusion equation but we were not able to find a single paper implementing a number of classical methods form some uniform analysis.

In this paper we applied many of the conventional methods to solve different problems of heat equation in 1D, 2D and 3D space, using Neumann and Dirichlet types of boundary conditions. These methods include Forward Difference (FD), Backward Difference (BD), Crank Nicolson (CN), Alternate Directions Scheme (ADI) and DuFort-Frankel Scheme (DF). Purpose of this analysis is to obtain a unified picture for these numerical methods.

This paper organize as follows: Numerical methods used int this paper are presented in section II, the problems considered for solution are stated in section III. Section IV contains the results and analysis portion while section V summarizes the paper.

In the nutshell, we believe that the paper will provide some unified conceptual framework for the practical implementation of said numerical methods.

II. Numerical Methods

Several Finite Difference (FD) schemes have been suggested in text books [6], [7], [8] to solve PDEs. The basic heat equation is given by:

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

The methods investigated in this paper include Forward Difference (FD), Backward Difference (BD), Crank Nicolson (CN), Alternate Directions Scheme (ADI) and Dufort-Frankel Scheme (DF). Here we present a short description of all these methods used in this paper for performing computational analysis.

A. Forward Difference (FD)

The finite difference approximation to the above partial differential equation known as forward difference formula is given below [7].

$$\frac{w_i^{k+1} - w_i^k}{\Delta t} = c\frac{w_{i+1}^k - 2w_i^k + w_{i-1}^k}{\Delta x^2} \tag{2}$$

Or

$$w_i^{k+1} = w_i^k + \lambda\left(w_{i+1}^k - 2w_i^k + w_{i-1}^k\right)$$
$$where \quad \lambda = c\frac{\Delta t}{\Delta x^2}$$

The scheme can easily be extended to 2-D as:

$$\begin{aligned} w_{i,j}^{k+1} =& w_{i,j}^k + \lambda(w_{i+1,j}^k + w_{i-1,j}^k + \\ & w_{i,j+1}^k + w_{i,j-1}^k - 4w_{i,j}^k) \end{aligned} \tag{3}$$

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$$where \quad \lambda = c\frac{\Delta t}{h^2};\ h = \Delta x = \Delta y$$

Also this method can be extended to 3-D as given below:

$$\begin{aligned} w_{i,j,k}^{k+1} =& w_{i,j,k}^{k} + \lambda(w_{i+1,j,k}^{k} + w_{i-1,j,k}^{k} + w_{i,j+1,k}^{k} + \\ & w_{i,j-1,k}^{k} + w_{i,j,k+1}^{k} + w_{i,j,k-1}^{k} - 6w_{i,j,k}^{k}) \end{aligned} \quad (4)$$

$$where \quad \lambda = c\frac{\Delta t}{h^2};\ h = \Delta x = \Delta y = \Delta z$$

B. Backward Difference (BD)

The finite difference approximation to the above partial differential equation known as backward difference formula is given below [7].

$$\frac{w_i^{k+1} - w_i^k}{\Delta t} = c\frac{w_{i+1}^{k+1} - 2w_i^{k+1} + w_{i-1}^{k+1}}{\Delta x^2} \quad (5)$$

Or

$$w_i^{k+1} = w_i^k + \lambda\left(w_{i+1}^{k+1} - 2w_i^{k+1} + w_{i-1}^{k+1}\right)$$

$$where \quad \lambda = c\frac{\Delta t}{\Delta x^2}$$

The scheme can easily be extended to 2-D as:

$$\begin{aligned} w_{i,j}^{k+1} =& w_{i,j}^{k} + \lambda(w_{i+1,j}^{k+1} + w_{i-1,j}^{k+1} + \\ & w_{i,j+1}^{k+1} + w_{i,j-1}^{k+1} - 4w_{i,j}^{k+1}) \end{aligned} \quad (6)$$

$$where \quad \lambda = c\frac{\Delta t}{h^2};\ h = \Delta x = \Delta y$$

Also 3-D extension of Backward Difference Method is given below:

$$\begin{aligned} w_{i,j,k}^{k+1} =& w_{i,j,k}^{k} + \lambda(w_{i+1,j,k}^{k+1} + w_{i-1,j,k}^{k+1} + w_{i,j+1,k}^{k+1} + \\ & w_{i,j-1,k}^{k+1} + w_{i,j,k+1}^{k+1} + w_{i,j,k-1}^{k+1} - 6w_{i,j,k}^{k+1}) \end{aligned} \quad (7)$$

$$where \quad \lambda = c\frac{\Delta t}{h^2};\ h = \Delta x = \Delta y = \Delta z$$

C. Crank-Nicolson (CN)

Another methods known CrankNicolson method is centered in both space and time suggested in [7] is given below:

$$\begin{aligned} \frac{w_i^{k+1} - w_i^k}{\Delta t} =& \frac{c}{2}(\frac{w_{i+1}^{k+1} - 2w_i^{k+1} + w_{i-1}^{k+1}}{\Delta x^2} + \\ & \frac{w_{i+1}^{k} - 2w_i^{k} + w_{i-1}^{k}}{\Delta x^2}) \end{aligned} \quad (8)$$

Or

$$\begin{aligned} w_i^{k+1} =& w_i^k + \lambda(w_{i+1}^{k+1} - 2w_i^{k+1} + w_{i-1}^{k+1} + \\ & w_{i+1}^{k} - 2w_i^{k} + w_{i-1}^{k}) \end{aligned}$$

$$where \quad \lambda = c\frac{\Delta t}{2\Delta x^2}$$

The scheme can easily be extended to 2-D as:

$$\begin{aligned} w_{i,j}^{k+1} =& w_{i,j}^{k} + \lambda(w_{i+1,j}^{k+1} + w_{i-1,j}^{k+1} + w_{i,j+1}^{k+1} + \\ & w_{i,j-1}^{k+1} - 4w_{i,j}^{k+1} + w_{i+1,j}^{k} + w_{i-1,j}^{k} + \\ & w_{i,j+1}^{k} + w_{i,j-1}^{k} - 4w_{i,j}^{k}) \end{aligned} \quad (9)$$

$$where \quad \lambda = c\frac{\Delta t}{2h^2};\ h = \Delta x = \Delta y$$

Also this method can be extended to 3-D as given below:

$$\begin{aligned} w_{i,j,k}^{k+1} =& w_{i,j,k}^{k} + \lambda(w_{i+1,j,k}^{k+1} + w_{i-1,j,k}^{k+1} + w_{i,j+1,k}^{k+1} + \\ & w_{i,j-1,k}^{k+1} + w_{i,j,k+1}^{k+1} + w_{i,j,k-1}^{k+1} - 6w_{i,j,k}^{k+1} + \\ & w_{i+1,j,k}^{k} + w_{i-1,j,k}^{k} + w_{i,j+1,k}^{k} + w_{i,j-1,k}^{k} + \\ & w_{i,j,k+1}^{k} + w_{i,j,k-1}^{k} - 6w_{i,j,k}^{k}) \end{aligned} \quad (10)$$

$$where \quad \lambda = c\frac{\Delta t}{2h^2};\ h = \Delta x = \Delta y = \Delta z$$

D. Alternate Directions Scheme (ADI)

Another method to solve this heat equation is known as alternating direction (ADI) algorithm; which has only 2-D and 3-D extensions. The 2D formulation of this method is give as [9]:

$$\begin{aligned} \frac{w_{ij}^{n+1/2} - w_{ij}^{n}}{\Delta t/2} &= \left(\delta_x^2 w_{ij}^{n+1/2} + \delta_y^2 w_{ij}^{n}\right) \\ \frac{w_{ij}^{n+1} - w_{ij}^{n+1/2}}{\Delta t/2} &= \left(\delta_x^2 w_{ij}^{n+1/2} + \delta_y^2 w_{ij}^{n+1}\right) \end{aligned} \quad (11)$$

Also the 3D extension is give as [9]:

$$\begin{aligned} l\frac{w_{ijk}^{n+1/3} - w_{ijk}^{n}}{\Delta t/3} &= \left(\delta_x^2 w_{ijk}^{n+1/3} + \delta_y^2 w_{ijk}^{n} + \delta_z^2 w_{ijk}^{n}\right) \\ \frac{w_{ij}^{n+2/3} - w_{ij}^{n+1/3}}{\Delta t/3} &= (\delta_x^2 w_{ij}^{n+1/3} + \delta_y^2 w_{ij}^{n+2/3} + \\ & \quad \delta_z^2 w_{ijk}^{n+1/3}) \\ \frac{w_{ij}^{n+1} - w_{ij}^{n+2/3}}{\Delta t/3} &= (\delta_x^2 w_{ij}^{n+2/3} + \delta_y^2 w_{ij}^{n+2/3} + \\ & \quad \delta_z^2 w_{ijk}^{n+1}) \end{aligned} \quad (12)$$

E. DuFort- Frankel Scheme (DF)

Another method known as DufortFrankel scheme for the one-dimensional heat equation is give as in [8] :

$$\frac{w_i^{k+1} - w_i^{k-1}}{2\Delta t} = c\left(\frac{w_{i+1}^{k} + w_{i-1}^{k}}{\Delta x^2} - \frac{w_i^{k+1} + w_i^{k-1}}{\Delta x^2}\right) \quad (13)$$

Or

$$w_i^{k+1} = w_i^{k-1} + \lambda\left(w_{i+1}^{k+1} + w_{i-1}^{k} - w_i^{k+1} - w_i^{k-1}\right)$$

$$where \quad \lambda = c\frac{2\Delta t}{\Delta x^2}$$

This scheme is easily extended in 2D as follows:

$$\begin{aligned} w_{i,j}^{k+1} =& w_{i,j}^{k-1} + \lambda(w_{i+1,j}^{k} + w_{i-1,j}^{k} + w_{i,j+1}^{k} + \\ & w_{i,j-1}^{k} - 2(w_{i,j}^{k+1} + w_{i,j}^{k-1})) \end{aligned} \quad (14)$$

$$where \quad \lambda = c\frac{2\Delta t}{h^2};\ h = \Delta x = \Delta y$$

Also the 3D extension of method is as:

$$\begin{aligned} w_{i,j,k}^{k+1} =& w_{i,j,k}^{k-1} + \lambda(w_{i+1,j,k}^{k} + w_{i-1,j,k}^{k} + \\ & w_{i,j+1,k}^{k} + w_{i,j-1,k}^{k} + w_{i,j,k+1}^{k} + \\ & w_{i,j,k-1}^{k} - 3(w_{i,j,k}^{k+1} + w_{i,j,k}^{k-1})) \end{aligned} \quad (15)$$

$$where \quad \lambda = c\frac{2\Delta t}{h^2};\ h = \Delta x = \Delta y = \Delta z$$

III. PROBLEMS SOLVED

Different types of problems were considered to solve standard heat equation. These problems exploit various computational aspects of these methods to elaborate analysis.

A. 1-D Applications

Three 1-D problems considered as exponential, sinusoidal and linear with sinusoidal initial conditions. These three problems have been solved for both Neuman and Dirichlet boundary conditions.

1) Exponential initial conditions: General 1-D Heat Equation (1) is Considered with exponential initial conditions as first case. The Dirichlet boundary conditions for problem are $[A1(D)]$ given as:

$$u(x,0)=e^{-x},\ u(0,t)=e^{t},\ u(1,t)=e^{t-1},\\ 0\le x\le 1,\ 0\le t\le 1$$

Also the Neuman boundary conditions for problem are $[A1(N)]$ given as:

$$u(x,0)=e^{-x},\ u_x(0,t)=-e^{t},\ u_x(1,t)=-e^{t-1},\\ 0\le x\le 1,\ 0\le t\le 1$$

This problem has Analytical solution as:

$$u(x,t)=e^{t-x} \tag{16}$$

2) Sinusoidal initial conditions: General 1-D Heat Equation (1) is Considered with sinusoidal initial conditions as second case. The Dirichlet boundary conditions for problem $[A2(D)]$ are given as [10]:

$$u(x,0)=\sin(\pi x),\ u(0,t)=u(1,t)=0,\\ 0\le x\le 1,\ 0\le t\le 1$$

Also the Neuman boundary conditions for this problem $[A2(N)]$ are given as:

$$u(x,0)=\sin(\pi x),\ u_x(0,t)=\pi e^{-\pi t},\\ u_x(1,t)=-\pi e^{-\pi t},\ 0\le x\le 1,\ 0\le t\le 1$$

This problem has the analytical solution as:

$$u(x,t)=e^{-\pi t}\sin(\pi x) \tag{17}$$

3) Linear combined with Sinusoidal initial conditions: General 1-D Heat Equation (1) is Considered with sinusoidal initial conditions as third case [11]. The Dirichlet boundary conditions for problem $[A3(D)]$ are given as:

$$u(x,0)=x+\sin(\pi x),\ u(0,t)=u(1,t)=0,\\ 0\le x\le 1,\ 0\le t\le 1$$

Also the Neuman boundary conditions for this problem $[A3(N)]$ are given as:

$$u(x,0)=x+\sin(\pi x),\ u_x(0,t)=\pi e^{-\pi t},\\ u_x(1,t)=-\pi e^{-\pi t},\ 0\le x\le 1,\ 0\le t\le 1$$

B. 2-D Applications

General 2-D Heat Equation (18) Considered with exponential initial conditions

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2} \tag{18}$$

Subject to Drichlet boundary conditions $[B(D)]$ as:

$$u(x,y,0)=e^{-x}+e^{-y},\ u(x,0,t)=e^{t-x}+e^{t},\\ u(x,1,t)=e^{t-x}+e^{t-1},\ u(0,y,t)=e^{t-y}+e^{t},\\ u(1,y,t)=e^{t-y}+e^{t-1},\ 0\le x,y\le 1,\ 0\le t\le 1$$

The problem also solved for the Neuman Boundary conditions $[B(N)]$ as:

$$u(x,y,0)=e^{-x}+e^{-y},\\ u_x(x,0,t)=u_y(0,y,t)=-e^{t},\\ u_x(x,1,t)=u_y(1,y,t)=-e^{t-1},\\ 0\le x,y\le 1,\ 0\le t\le 1$$

This problem has following Analytical solution,

$$u(x,y,t)=e^{t}\left(e^{-x}+e^{-y}\right) \tag{19}$$

C. 3-D Applications

General 3-D Heat Equation (20) Considered with exponential initial conditions

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2} \tag{20}$$

Subject to Drichlet boundary conditions $[C(D)]$ as:

$$u(x,y,z,0)=e^{-x}+e^{-y}+e^{-z},\\ u(x,y,0,t)=e^{t-x}+e^{t-y}+e^{t},\\ u(x,y,1,t)=e^{t-x}+e^{t-y}+e^{t-1},\\ u(x,0,z,t)=e^{t-x}+e^{t-z}+e^{t},\\ u(x,1,z,t)=e^{t-x}+e^{t-z}+e^{t-1},\\ u(0,y,z,t)=e^{t-y}+e^{t-z}+e^{t},\\ u(1,y,z,t)=e^{t-y}+e^{t-z}+e^{t-1},\\ 0\le x,y,z\le 1,\ 0\le t\le 1$$

The problem also solved for the Neuman Boundary conditions $[C(N)]$ as:

$$u(x,y,z,0)=e^{-x}+e^{-y}+e^{-z},\\ u_z(x,y,0,t)=u(x,0,z,t)=u(0,y,z,t)=-e^{t},\\ u_z(x,y,1,t)=u(x,1,z,t)=u(1,y,z,t)=-e^{t-1},\\ 0\le x,y,z\le 1,\ 0\le t\le 1$$

This problem has following Analytical solution.

$$u(x,y,z,t)=e^{t}\left(e^{-x}+e^{-y}+e^{-z}\right) \tag{21}$$

IV. RESULTS AND ANALYSIS

A unified computation error and timing analysis for said conventional numerical methods has been performed for five heat equation problems stated earlier. Results have been obtained by incrementing the time and space steps for each case. These results are analyzed for both accuracy and computation time, are summarized in this section. Figure 1 presents a uniform error analysis for small time step i.e.

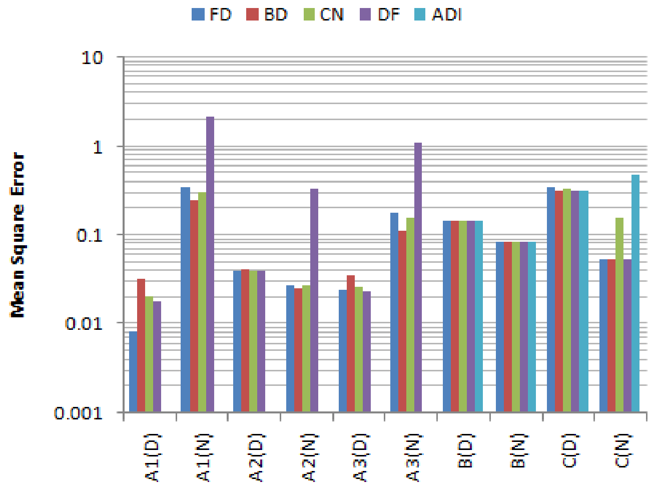

Fig. 1. Uniform error analysis for small time step

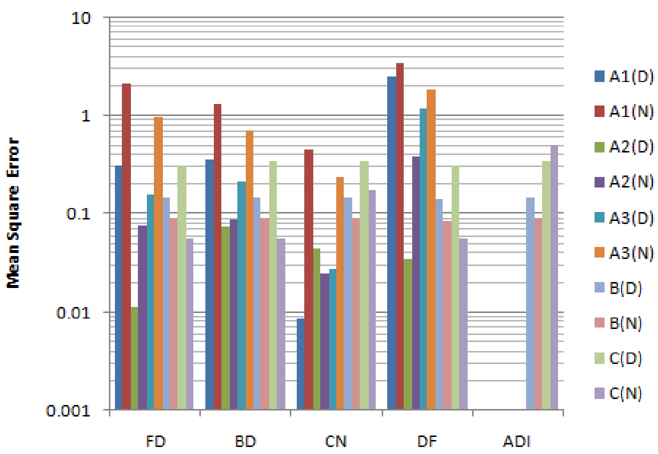

Fig. 2. Uniform error analysis for large time step

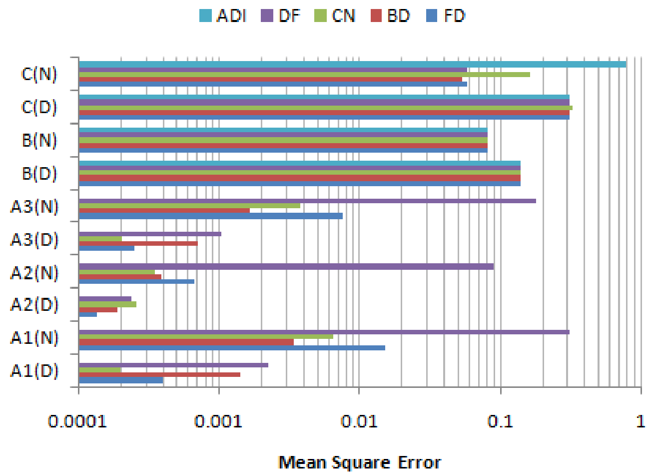

Fig. 3. Uniform error analysis for fine grid

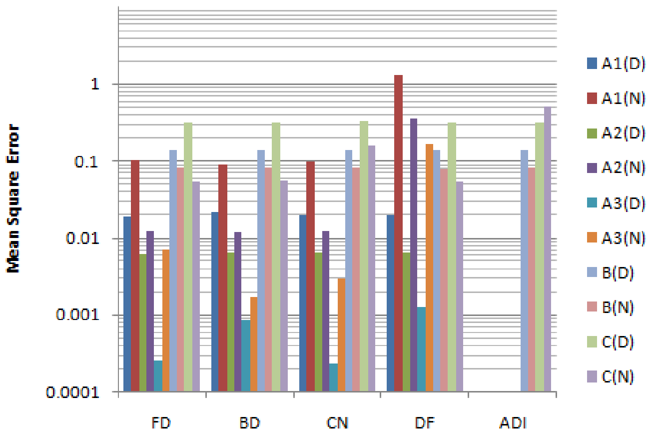

Fig. 4. Uniform error analysis for coarse grid

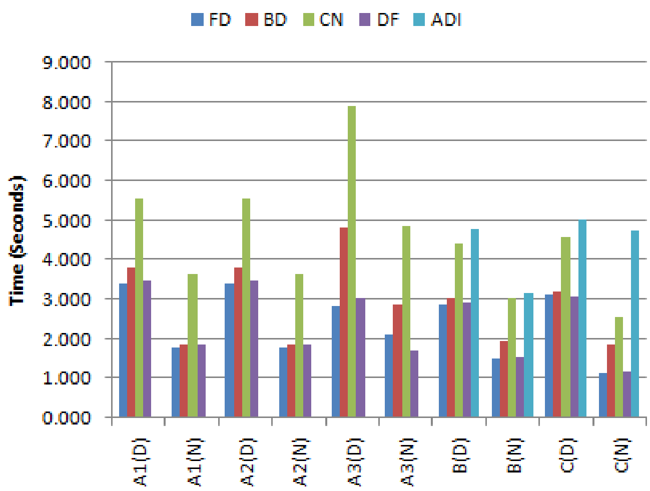

Fig. 5. Uniform computation time analysis

$\Delta t = 1/1000$ whereas space step is fixed at 1/4 in this case. It can be observed that problems with Dirichlet boundary conditions have reduced error than their Neuman counterpart. We deem this is due to derivative estimation on boundary points.

Uniform error analysis for large time step is presented in Figure 2. In this case the time step is taken as 1/40 while still the space step is fixed at 1/4. This is evident that CN performs best in case of exponential 1D problems while FD and DF performs best for 1D sinusoidal problem. Similarly BD is best for 3D Neuman problem and ADI performs worse in case of 3D problems.

Error analysis in case of fine and course grid is presented in Figure 3 and Figure 4. The time step is fixed at 1/1000 for both the cases while space step is 1/100 for fine grid and it is set at 1/10 for course grid solution. A close observation indicates that almost every method performs its best for linear and sinusoidal combined problem. It is also evident is DF is not a good choice in coarse grid for any type of 1D problem.

Uniform computational time analysis is given in Figure 5. FD takes the minimum time to solve a problem and DF is second most efficient to solve the problem. At the same time ADI is the most time taking scheme and the 2nd worse is CN for the same problem. The latter two method take more time as they are the most computationally intensive than all methods.

V. Summary

In this paper we have presented a uniform analysis of some conventional numerical method to solve five different problems of heat equation. All these problems and methods have been analyzed for accuracy and computation time. The summary of obtained results is furnished below.

a) For Drichlet boundary conditions
   - FD method provides better accuracy for 1D problems.
   - DF is more accurate for both 2D and 3D problems, but is not good is 1D case.
   - BD is least accurate to solve 1D and 2D problems.
   - CN should be avoided for 3D problem as this is also least accurate for the case.

b) For Neuman boundary conditions
   - BD method provides better accuracy for 1D problem.
   - DF provides more accuracy for 2D problems but at the same time it is least accurate for 1D problem.
   - FD is most accurate for 3D problems but meanwhile it is least accurate for 2D problems.

c) ADI should be avoided for 3D problem as this is also least accurate for the case.

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