1. Introduction

The objective of this assignment is to perform the numerical calculation of the heat equation in one spatial dimension, defined in Equation 1. This equation describes the diffusion of a passive scalar in a field for any number of spatial dimensions.

Equation 1. 1D Heat Equation.

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

The domain of this assignment is a simulated wall of a given thickness originally at a given temperature. The wall has a known diffusion of the heat transfer or temperature difference. In the transient simulation, the sides of the wall are suddenly increased to a given temperature, bringing the temperature of the wall up to some value. These values are summarized in Table 1.

Table 1. Conditions of Transient Analysis.

Parameter	Value
(L) Thickness of the simulated wall	0.3 [m]
(T_0) Initial uniform temperature of the wall	100 [K]
(α) Heat diffusivity	3e-6 [m^2/s]
(T_w) Sudden wall temperature	300 [K]
(dx) Spatial mesh spacing	0.015 [m]

2. Forward in Time, Central in Space Solution (FTCS)

FTCS Method

This method is a simple explicit formulation of a discretized heat equation. The step is a central second order derivative in space for a forward step in time, hence the name, described in Equation 2.

Equation 2. FTCS Discretization of 1D Heat Equation. n is the time step, and j is the spatial point.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \alpha \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}$$

This scheme's stability is determined by a parameter, S, although some references refer to it as r [1]. The FTCS scheme is stable for $S \in [0, 1/2]$.

Equation 3. S Parameter for FTCS.

$$S = \alpha \frac{\Delta t}{\Delta x^2}$$

The accuracy of the scheme can come from its Truncation Error (TE). This TE would suggest that the method is first (1^{st}) order accurate in time and second (2^{nd}) order accurate in space

Equation 4. Truncation Error for FTCS.

$$TE = \left(-\frac{1}{2}\alpha^2\Delta t + \alpha\frac{\Delta x^2}{12}\right)\frac{\partial^4 u}{\partial x^4} + \left\{\alpha^3\frac{\Delta t^2}{3} - \alpha^2\frac{\Delta t}{12}\Delta x^2 + \alpha\frac{1}{360}\Delta x^4\right\}\frac{\partial^6 u}{\partial x^6}\ldots$$

In Equation 4, there is a term in curved brackets. As the authors of [1] point out, there is a numerical phenomenon where if $S = 1/6$, then the 1st error term becomes zero, and thus the FTCS method becomes 2nd order in time and 4th order in space accurate.

Calculation Method

If one changes the FTCS formula with the stability parameter, S, the discretization of the heat equation becomes:

Equation 5. FTCS Discretization of 1D Heat Equation with Substituted Stability Factor.

$$u_j^{n+1} - u_j^n = S\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right)$$

Taking this a step further, the known values can all be moved to the right-hand side (RHS) of the equation, and the unknowns on the left-hand side (LHS) of the equation.

Equation 6. FTCS Discretization of 1D Heat Equation as Used in Linear Equation.

$$u_j^{n+1} = Su_{j+1}^n + (1-2S)u_j^n + Su_{j-1}^n$$

Thus, if this equation becomes a linear equation, it becomes:

Equation 7. FTCS Discretization Arranged in a Linear Equation.

$$\left[u_j^{n+1}\right] = [S, (1-2S), S]\begin{bmatrix} u_{j-1}^n \\ u_j^n \\ u_{j+1}^n \end{bmatrix}$$

Which can be re-arranged as:

Equation 8. FTCS Discretization Decomposed for Time and Spatial Gradient Components.

$$\left[u_j^{n+1}\right] = ([0,1,0] + S\cdot[1,-2,1])\begin{bmatrix} u_{j-1}^n \\ u_j^n \\ u_{j+1}^n \end{bmatrix}$$

Results

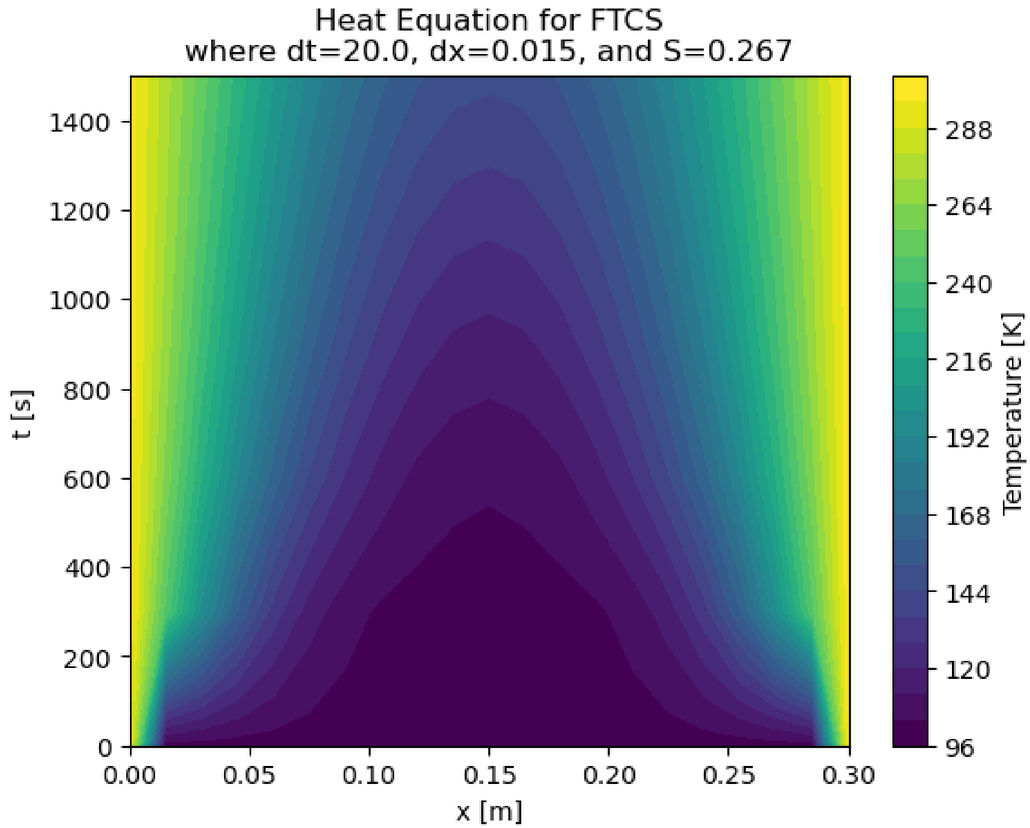

Figure 1.

For a relatively small time step with $S = 0.267$, the heat equation solution is what one would expect, seen in Figure 1. The temperature of the boundaries gradually spreads throughout the spatial domain.

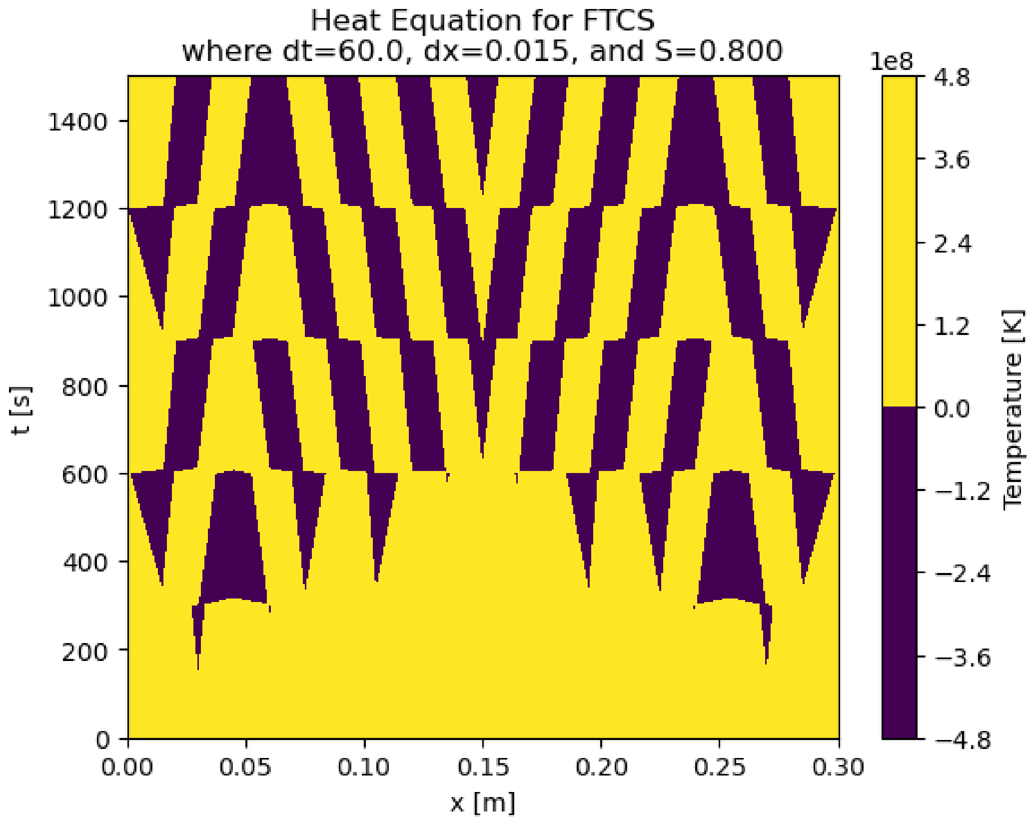

Figure 2.

However, when the time step is increased so $S = 0.80$, which should be unstable for FTCS, we see that the solve becomes immediately unstable. In this solution, none of the data makes sense.

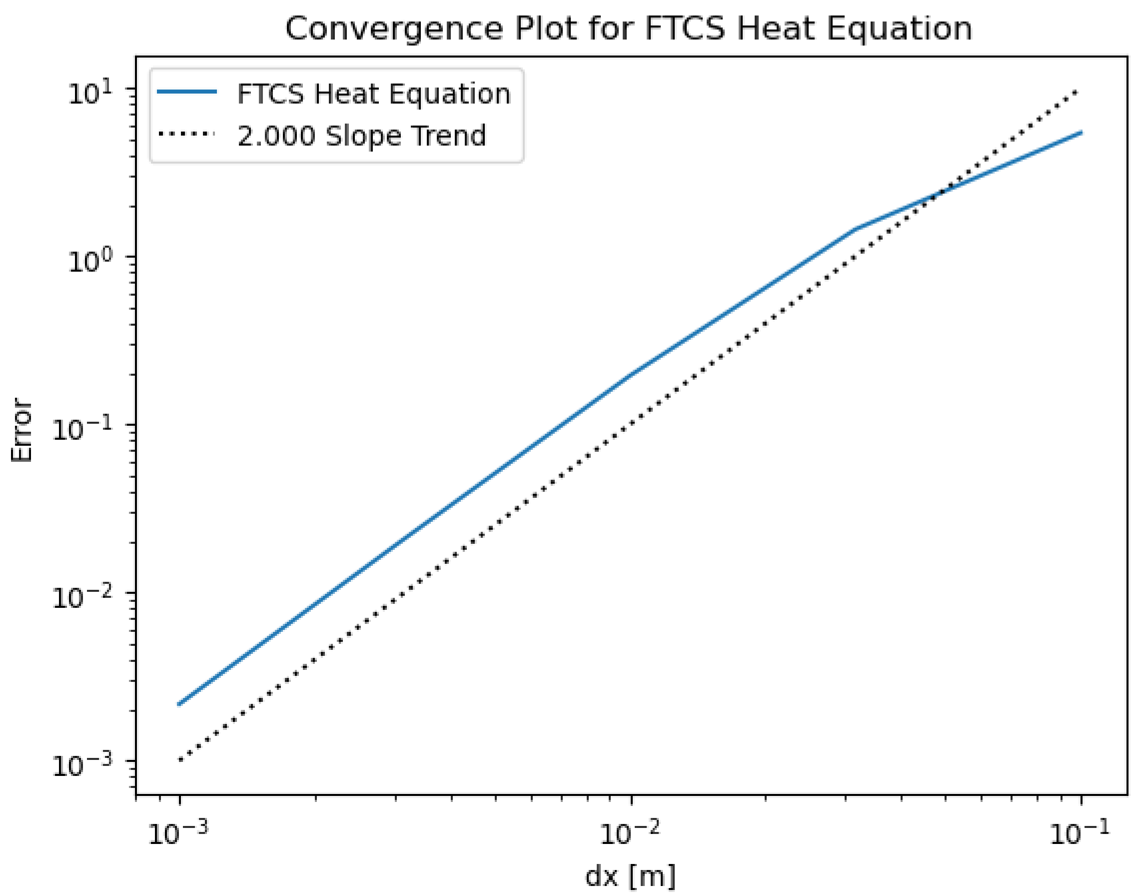

Figure 3.

When the same analysis is changed to vary the mesh spacing, it forms a clear trend, seen in Figure 3, that follows the expected order of accuracy according to the truncation error calculation.

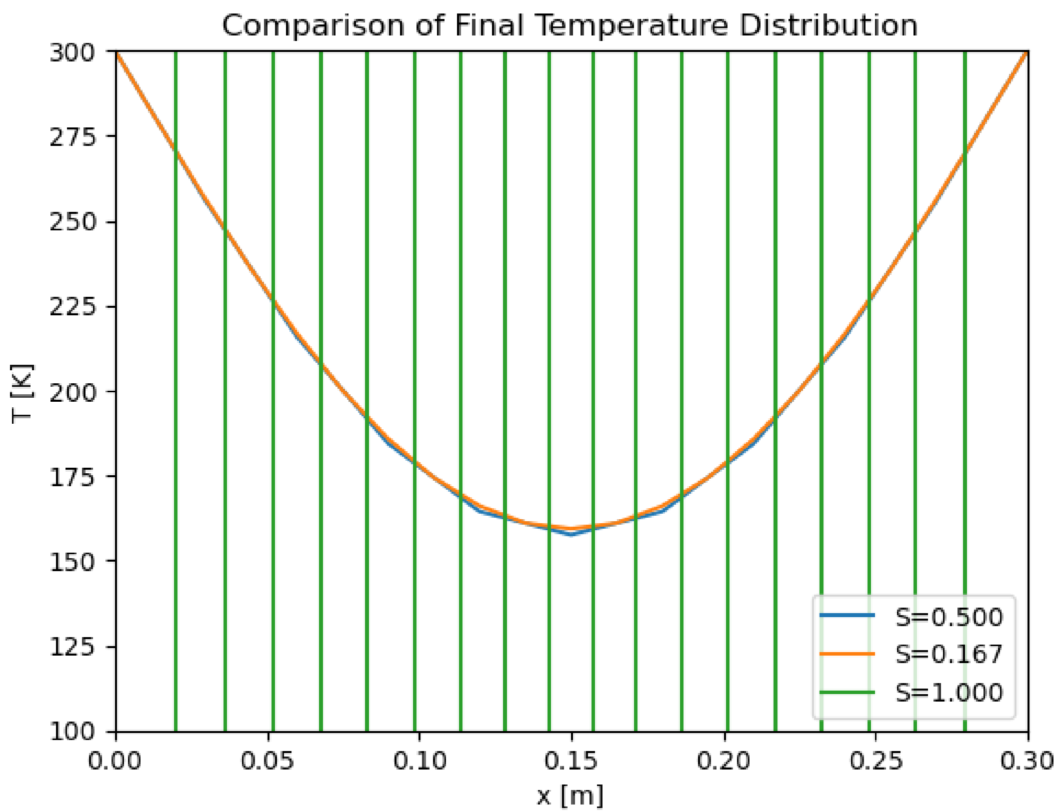

Figure 4.

When we compare the results for the final time, $t = 30[min]$, there is a similar trend with stability. When $S \leq 1/2$, the results are in good agreement and form the expected sine or parabolic trend. However, when the solve is unstable, like with $S = 1.0$, the solve is unstable and produces unrealistic results.

Comparing the two conditions of $S = 1/2$ and $S = 1/6$, there is not a significant difference in truncation error between them, seen Table 2. The higher value of S does have a slightly higher error, but it is only a 4.09% difference.

Table 2. Truncation Error Sweep for FTCS.

S	Error
1/6	1002.04
½	1043.92

3. Crank-Nicolson (CN) Solution

CN Method

The Crank-Nicolson method is effectively central in time while being central in space. The discretization of the heat equation is outlined in Equation 9.

Equation 9. CN Discretization of 1D Heat Equation. n is the time step, and j is the spatial point.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \alpha \frac{\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \left(u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^n\right)}{2\Delta x^2}$$

The stability parameter, defined in Equation 10, is the same, although the discretization is unconditionally stable.

Equation 10. S Parameter for CN.

$$S = \alpha \frac{\Delta t}{\Delta x^2}$$

The truncation error of this method is a little more complicated than for FTCS. CN truncation error will be second (2^{nd}) order in space and second (2^{nd}) order in time, but the second order in time comes from a higher derivative in the Taylor series. Also, unlike FTCS, there is no value of *S* where the truncation error discretely drops.

Equation 11. Truncation Error for CN.

$$TE = \alpha \frac{\Delta x^2}{12} \frac{\partial^4 u}{\partial x^4} + \left\{\alpha^3 \frac{\Delta t^2}{12} + \alpha \frac{\Delta x^4}{360}\right\} \frac{\partial^6 u}{\partial x^6}$$

Calculation Method

If one changes the CN formula with the stability parameter, S, the discretization of the heat equation becomes:

Equation 12. CN Discretization of 1D Heat Equation with Substituted Stability Factor.

$$u_j^{n+1} - u_j^n = S \frac{\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \left(u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^n\right)}{2}$$

Taking this a step further, the known values can all be moved to the right-hand side (RHS) of the equation, and the unknowns on the left-hand side (LHS) of the equation.

Equation 13. CN Discretization of 1D Heat Equation as Used in Linear Equation.

$$-\frac{S}{2} u_{j-1}^{n+1} + (1+S) u_j^{n+1} - \frac{S}{2} u_{j+1}^{n+1} = \frac{S}{2} u_{j-1}^n + (1-S) u_j^n + \frac{S}{2} u_{j+1}^n$$

Becoming a linear equation, it becomes:

Equation 14. CN Discretization Arranged in a Linear Equation.

$$\left[-\frac{S}{2}, (1+S), -\frac{S}{2}\right] \begin{bmatrix} u_{j-1}^{n+1} \\ u_j^{n+1} \\ u_{j+1}^{n+1} \end{bmatrix} = \left[\frac{S}{2}, (1-S), \frac{S}{2}\right] \begin{bmatrix} u_{j-1}^n \\ u_j^n \\ u_{j+1}^n \end{bmatrix}$$

Which can be re-arranged as:

Equation 15. CN Discretization Decomposed for Time and Spatial Gradient Components.

$$\left([0,1,0]-\frac{S}{2}[1,-2,1]\right)\begin{bmatrix}u_{j-1}^{n+1}\\ u_j^{n+1}\\ u_{j+1}^{n+1}\end{bmatrix}=\left(-[0,1,0]+\frac{S}{2}[1,-2,1]\right)\begin{bmatrix}u_{j-1}^{n}\\ u_j^{n}\\ u_{j+1}^{n}\end{bmatrix}$$

Comparison to FTCS

Some differences between the FTCS and CN method were discussed, but to summarize and add to them:

- CN is a central in time gradient, whereas FTCS is forward in time only
- CN is unconditionally stable for all real values of stability factor, whereas FTCS is only stable for $S \in (0, 1/2]$.
- CN requires a system of linear equations on both sides, whereas FTCS only has linear equations on the knowns side.
- CN has a higher order of accuracy in time than FTCS (2nd order vs 1st order). This order terms comes from the higher order Taylor series terms.

Recommendations for the Heat Equation

The heat equation can be simply solved using this discretization method. On the RHS, the system of linear equations can form a vector of known values determined by the previous time steps. On the LHS, this system of linear equations is solved to find the next step of conditions. This can take the form of Equation 16 and Equation 17.

Equation 16. Known Values SLE for Explicit Solving.

$$b = Cu^n$$

Equation 17. Unknown Values SLE for Explicit Solving.

$$Au^{n+1} = b$$

Results

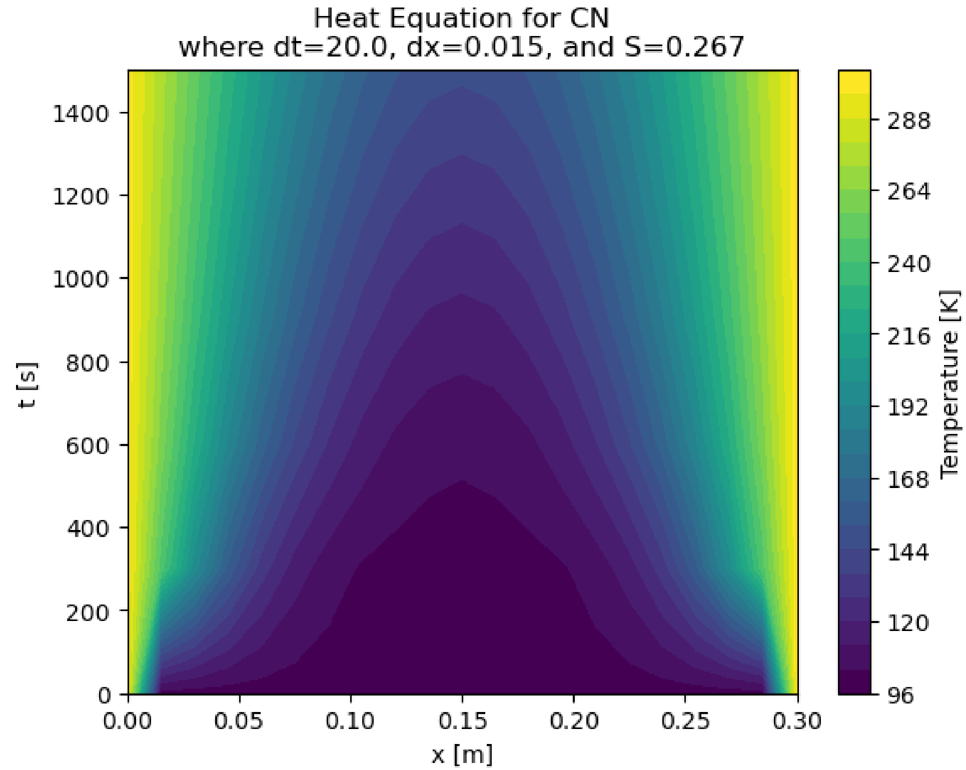

Figure 5.

The results for the CN method, shown in Figure 5 & Figure 6, look identical to the FTCS method with a particular exception of the value for *S* that was unstable for FTCS, the CN results shown in Figure 6.

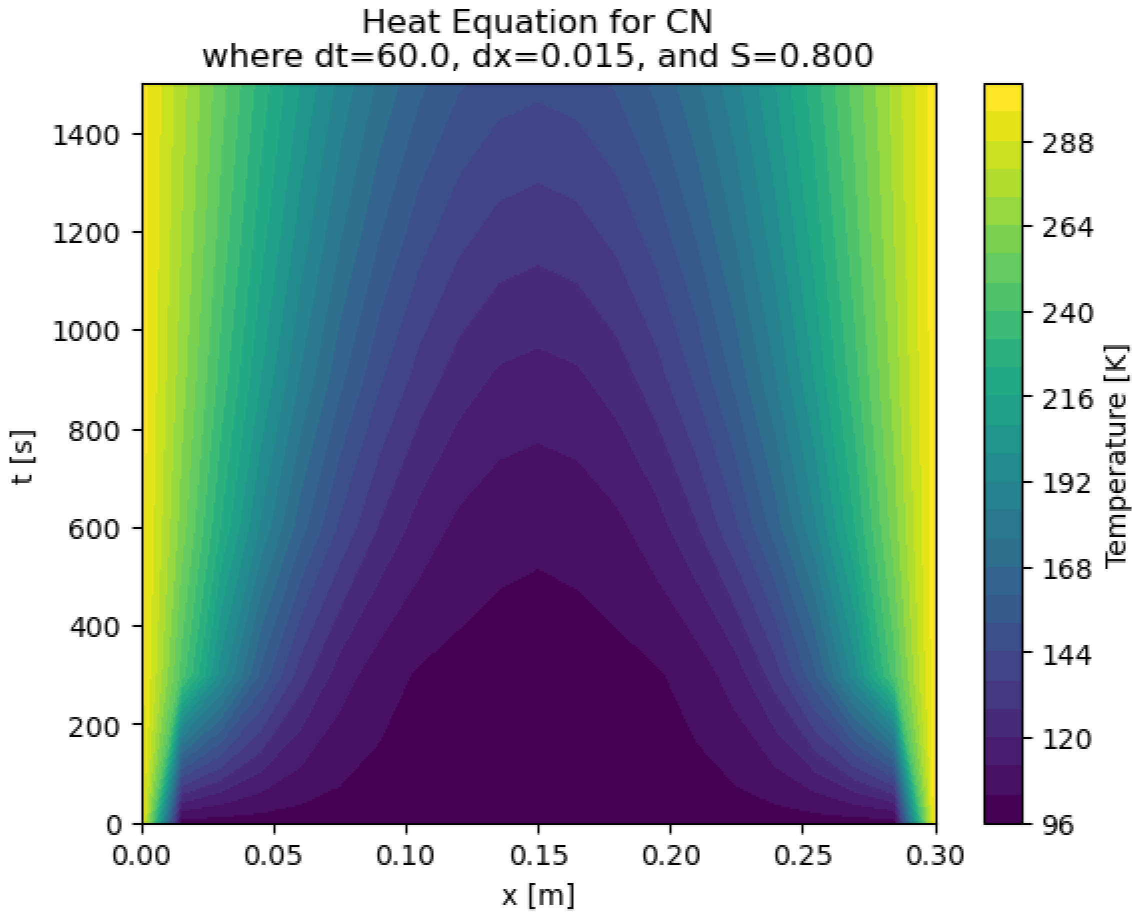
Heat Equation for CN
where dt=60.0, dx=0.015, and S=0.800
t [s]
x [m]
Temperature [K]
0
200
400
600
800
1000
1200
1400
0.00
0.05
0.10
0.15
0.20
0.25
0.30
96
120
144
168
192
216
240
264
288

Figure 6.

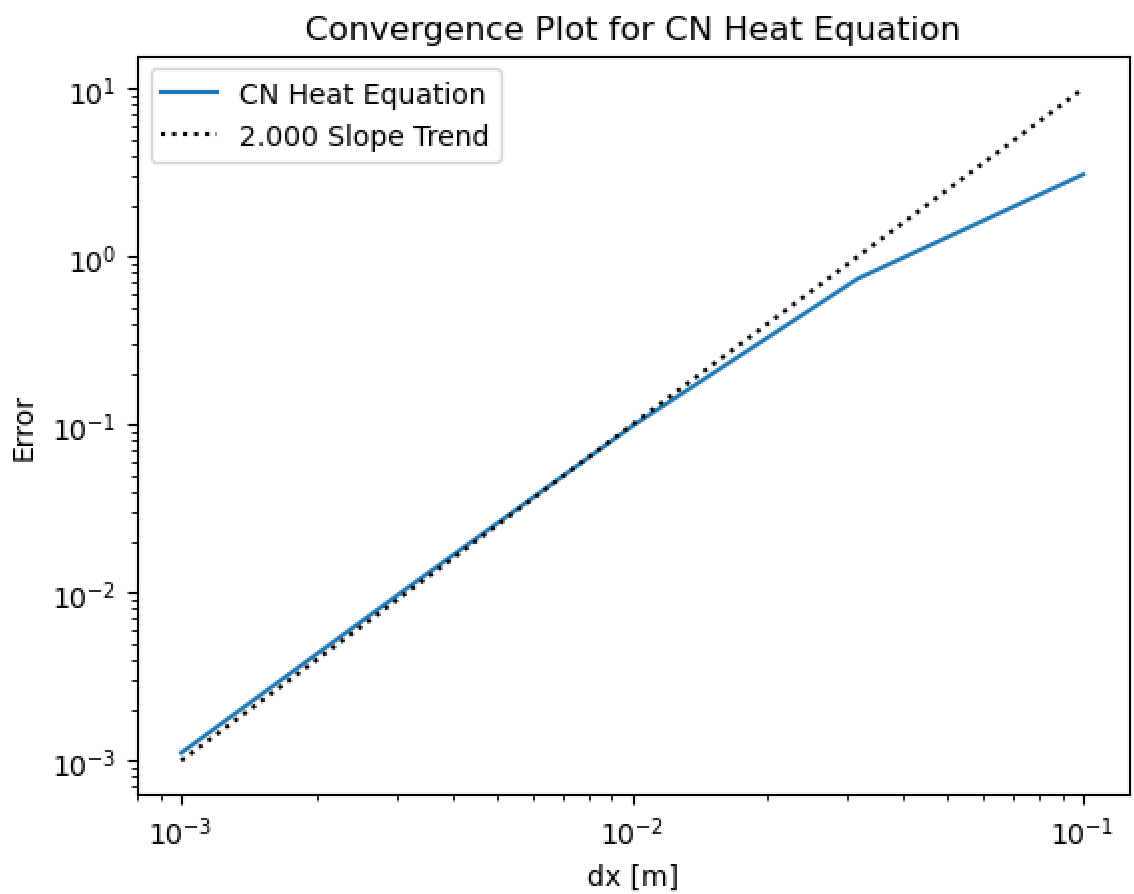

Figure 7.

The convergence plot for the CN method, see Figure 7, like with FTCS, confirms the 2nd order accuracy of the numerical heat equation solve.

The same trend is present when looking at the final temperature values, seen in Figure 8. The high values for S are now stable and in good agreement with the lower values. However, in this comparison, there is a trend forming. The larger S values, which result in larger time steps, have lower values in the middle than the smaller S values and time steps.

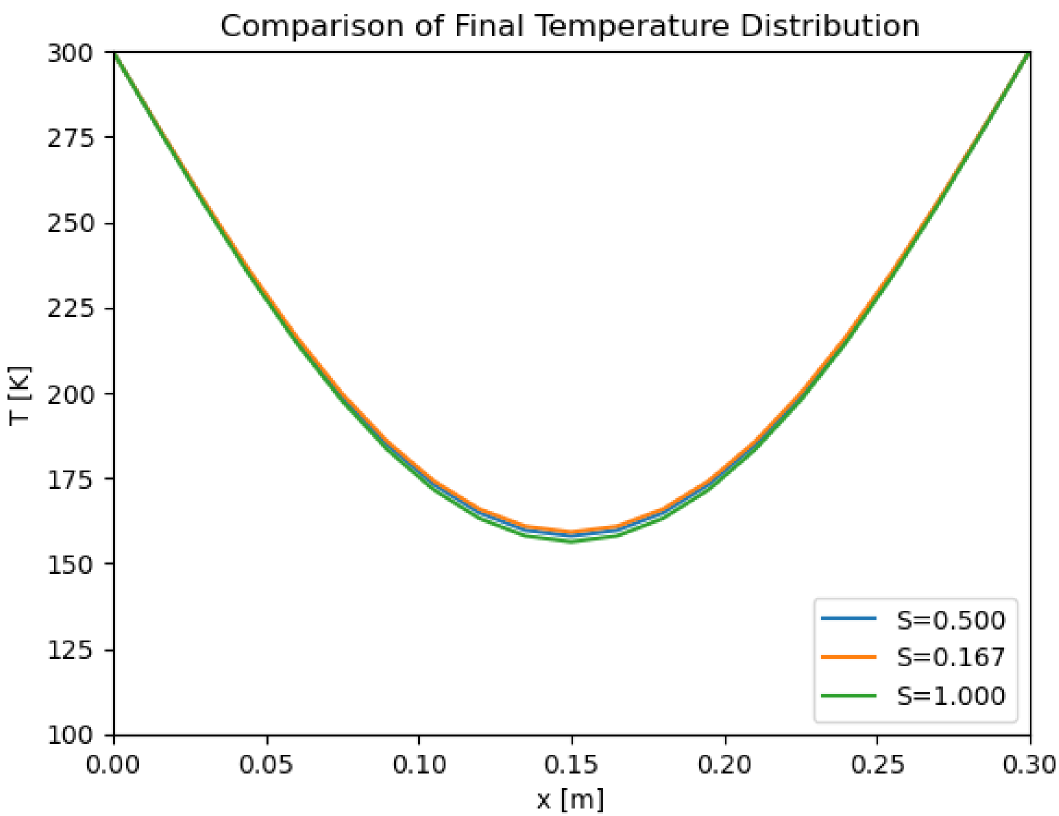

Figure 8.

Ther error for this sweep in *S* value shows a clear trend in decreasing the error with increasing *S* value. This matched the trend mentioned previously.

Table 3.

S	Error
1/6	643.458
½	197.296
1	114.832

4. Dufort-Frankel (DF) Solution

DF Method

The Dufort-Frankel (DF) method is a variation of the Richardson method that is stable at real positive values of the stability factor. This method is essentially central in space and time, where the time derivative skips the step considered in the iteration. For those familiar with the 2/3 time stepping method [2], this is similar, except has a built-in averaging filter. This method applied to the heat equation is in Equation 18.

Equation 18. DF Discretization of1D Heat Equation. n is the time step, and j is the spatial point.

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} = \alpha \frac{u_{j+1}^{n} - u_j^{n+1} - u_j^{n-1} + u_{j-1}^{n}}{\Delta x^2}$$

The TE of the scheme suggests that the method is second (2nd) order in both space and time.

Equation 19. Truncation Error for DF.

$$TE = \left(\alpha \frac{\Delta x^2}{12} - \alpha^3 \frac{\Delta t^2}{\Delta x^2}\right)\frac{\partial^4 u}{\partial x^4} + \left\{\alpha \frac{\Delta x^4}{360} - \alpha^3 \frac{\Delta t^2}{3} + \alpha^5 \frac{2\Delta t^4}{\Delta x^4}\right\}\frac{\partial^6 u}{\partial x^6}$$

Calculation Method

Reforming the discretized 1D equation for DF becomes:

Equation 20. DF Discretization of 1D Heat Equation with Substituted Stability Factor.

$$u_j^{n+1} - u_j^{n-1} = 2S\left(u_{j+1}^{n} - u_j^{n-1} - u_j^{n+1} + u_{j-1}^{n}\right)$$

Taking this a step further, the known values can all be moved to the right-hand side (RHS) of the equation, and the unknowns on the left-hand side (LHS) of the equation.

Equation 21. DF Discretization of 1D Heat Equation as Used in Linear Equation.

$$(1 + 2S)u_j^{n+1} = 2S\left(u_{j+1}^{n} + u_{j-1}^{n}\right) + (1 - 2S)u_j^{n-1}$$

Becoming a linear equation, it becomes:

Equation 22. DF Discretization Arranged in a Linear Equation.

$$[(1 + 2S)]\left[u_j^{n+1}\right] = [2S, 0{,}2S]\begin{bmatrix} u_{j-1}^{n} \\ u_j^{n} \\ u_{j+1}^{n} \end{bmatrix} + [(1 - 2S)]\left[u_j^{n-1}\right]$$

Von Neumann Stability Analysis

For the von Neumann stability analysis, we need to show the domain of stability factor, S, where the amplification factor, G, is less than one (1). i.e.:

Equation 23. Set for Stability.

$$\mathcal{S} = \{S{:}\, G(S) \in (0, 1]\}$$

[1] provides the amplification factor for the DF method seen in Equation 24.

Equation 24. Amplification Factor for DF Method.

$$G = \frac{2Scos\beta \pm \sqrt{1 - 4S^2 sin^2\beta}}{1 + 2S}$$

When plotted, as in Figure 9, there is a clear trend that forms. There is a value of S, $S = 1/2$, where the DF method is not stable in a real domain when S goes beyond it. For higher values, there is a circular domain that does not extend the full spatial domain. If memory serves, this means that the partial differential equation changes from hyperbolic to elliptical through the parabolic condition. While it is unconditionally stable, it does change nature at some values of S.

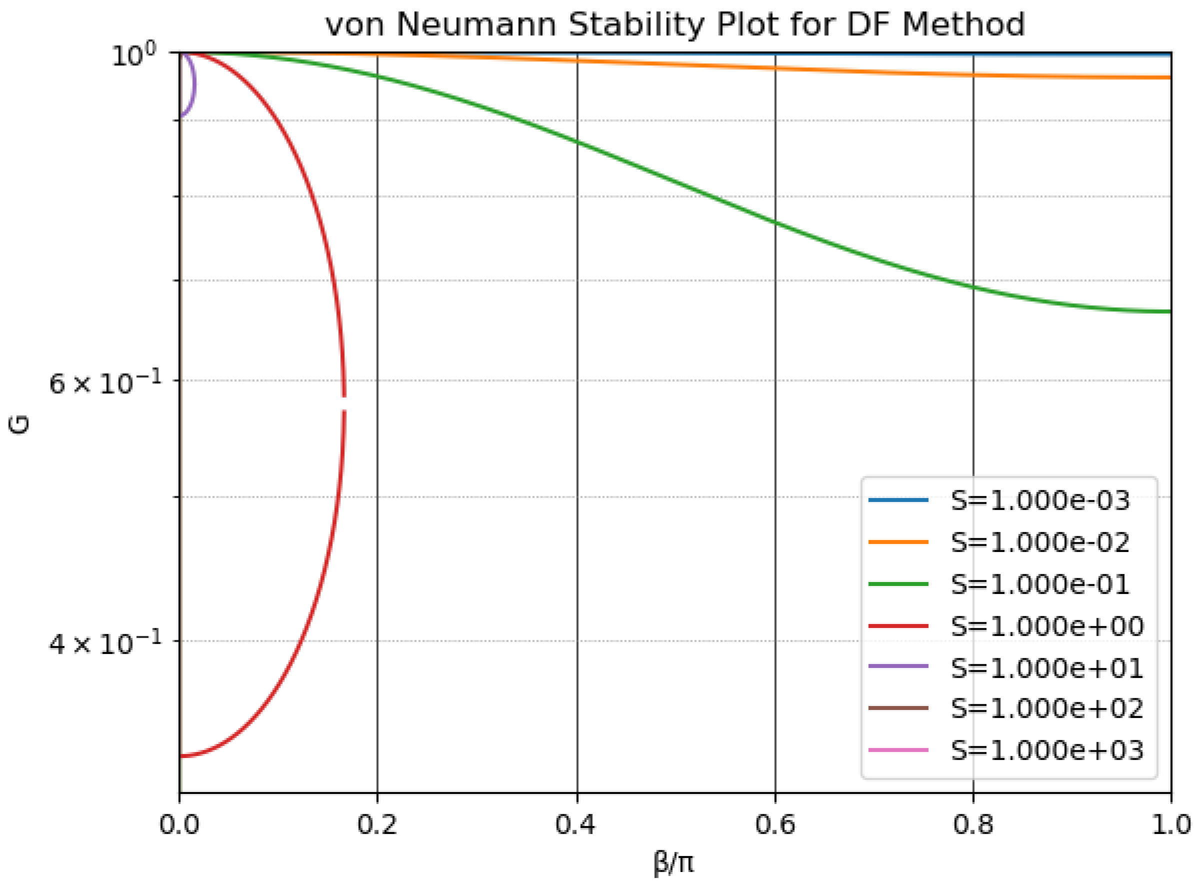

Figure 9.

5. Works Cited

1. Anderson, D. A., Tannehill, J. C, Pletcher, R. H., Munipalli, R., and Shankar, V. (2021). Computational Fluid Mechanics and Heat Transfer. *Series in Computation and Physical Processes in Mechanics and Thermal Sciences.* 4th Edition, CRC Press.
2. Simens, M. P., Jimenez, J., Hoyas, S., and Mizuno, Y. (2009). *A high-resolution code for turbulent boundary layers.* Journal of Computational Physics. Vol 228, pgs 4218-4231.