Numerical Analysis

Of the One-Dimensional Convection-Diffusion Equation

MEMS1055, Computer Aided Analysis in Transport Phenomena
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1 Introduction

In this report, we consider the one-dimensional convection-diffusion equation given by:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = \nu\frac{\partial^2 T}{\partial x^2} \qquad t \geq 0, \quad 0 \leq x \leq 1 \tag{1}$$

where u, ν, and L are known constants, and periodic boundary conditions at $(0, L)$ are employed:

$$T(0,t) = T(L,t) \tag{2}$$

$$\frac{\partial T}{\partial x}(0,t) = \frac{\partial T}{\partial x}(L,t) \tag{3}$$

We would like to obtain the solution for the scalar $T(x,t)$ for one periodic time of the flow evolution (T). Namely,

$$0 \leq t \leq \frac{L}{u} = T \tag{4}$$

In particular, throughout this report we will:

- Solve both the inviscid ($\nu = 0$) and diffusive ($\nu > 0$) form of Equation 1 via:
  - Forward-Time, Central Space, Explicit Method
  - Forward-Time, Central Space, Implicit Method
  - Forward-Time, First-Order Upwind Method
  - MacCormack Method
- Explain the effect of the stability parameters:

$$CFL = \frac{u\Delta t}{\Delta x}, \quad F = \frac{\nu\Delta t}{\Delta x^2}, \quad Re_\Delta = \frac{u\Delta x}{\Delta\nu}$$

- Comment on grid-dependence of the solution

2 Formulation

2.1 FTCS Explicit Method

In this subsection, the Forward Time, Central Space (FTCS) Explicit Method is derived. Taking forward discretizations in time and central discretizations in space of Equation 1 and dropping truncation error terms yields:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} + u\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x} = \nu\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \tag{5}$$

Rearranging the equation above in terms of T_i^{n+1} yields:

$$T_i^{n+1} = T_i^n + \frac{u\Delta t}{2\Delta x}(T_{i-1}^n - T_{i+1}^n) + \frac{\nu\Delta t}{\Delta x^2}(T_{i-1}^n - 2T_i^n + T_{i+1}^n) \tag{6}$$

By setting the Courant Number, $CFL = \frac{u\Delta t}{\Delta x}$ and the Fourier Number, $F = \frac{\nu\Delta t}{\Delta x^2}$, and rearranging the terms in Equation 6, we obtain:

$$T_i^{n+1} = (1 - 2F)T_i^n + (\frac{1}{2}CFL + F)T_{i-1}^n + (F - \frac{1}{2}CFL)T_{i+1}^n \tag{7}$$

Equation 7 provides explicit means to solve for the temperature at the node $(i, n+1)$.

2.2 FTCS Implicit Method

In this subsection, the Forward Time, Central Space (FTCS) Implicit Method is derived. Taking forward discretizations in time and central discretizations in space of Equation 1 and dropping truncation error terms yields:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} + u\frac{T_{i+1}^{n+1} - T_{i-1}^{n+1}}{2\Delta x} = \nu\frac{T_{i-1}^{n+1} - 2T_i^{n+1} + T_{i+1}^{n+1}}{\Delta x^2} \tag{8}$$

Rearranging the equation above in terms of T_i^{n+1} yields:

$$T_i^{n+1} = T_i^n + \frac{u\Delta t}{2\Delta x}(T_{i-1}^{n+1} - T_{i+1}^{n+1}) + \frac{\nu\Delta t}{\Delta x^2}(T_{i-1}^{n+1} - 2T_i^{n+1} + T_{i+1}^{n+1}) \tag{9}$$

By setting the Courant Number, $CFL = \frac{u\Delta t}{\Delta x}$ and the Fourier Number, $F = \frac{\nu\Delta t}{\Delta x^2}$, and rearranging the terms in Equation 9, we obtain:

$$-(\frac{1}{2}CFL + F)T_{i-1}^{n+1} + (1+2F)T_i^{n+1} + (\frac{1}{2}CFL - F)T_{i+1}^{n+1} = T_i^n \tag{10}$$

This is an implicit scheme, meaning that solving for the term T_i^{n+1} is only possible by solving a system of numerical equations at each time step. To go about solving for the values T_i^{n+1}, we can write the system of equations presented by Equation 10 in matrix form as:

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

or

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & a_{M-1} & b_{M-1} & c_{M-1} \\ 0 & 0 & 0 & 0 & a_M & b_M \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ u_{M-1}^{n+1} \\ u_M^{n+1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_{M-1} \\ d_M \end{bmatrix} \tag{11}$$

where the coefficients of the interior nodes are given by

$$a_i = -(\frac{1}{2}CFL + F) \quad b_i = (1+2F)$$

$$c_i = (\frac{1}{2}CFL - F) \quad d_i = T_i^n$$

for $i = 2, 3, ..., M-1$. This system is efficiently solved for using LU Factorization, and as such this method will be implemented in the code to solve for the values T_i^{n+1}.

2.3 Upwind Method

In this subsection, the first-order Upwind Method is derived. Taking forward discretizations in time and backward discretizations in space of Equation 1 and dropping truncation error terms yields:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} + u\frac{T_i^n - T_{i-1}^n}{\Delta x} = \nu\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \tag{12}$$

Rearranging the equation above in terms of T_i^{n+1} yields:

$$T_i^{n+1} = T_i^n + \frac{u\Delta t}{\Delta x}(T_{i-1}^n - T_i^n) + \frac{\nu\Delta t}{\Delta x^2}(T_{i-1}^n - 2T_i^n + T_{i+1}^n) \tag{13}$$

By setting the Courant Number, $CFL = \frac{u\Delta t}{\Delta x}$ and the Fourier Number, $F = \frac{\nu \Delta t}{\Delta x^2}$, and rearranging the terms in Equation 13, we obtain:

$$T_i^{n+1} = (1 - CFL - 2F)T_i^n + (CFL + F)T_{i-1}^n + FT_{i+1}^n \tag{14}$$

Equation 14 provides explicit means to solve for the temperature at the node $(i, n+1)$.

2.4 MacCormack Method

In this subsection, the MacCormack Method is derived. This is also known as the predictor-corrector method. Taking forward discretizations in time and space of Equation 1 and dropping truncation error terms yields:

$$\frac{T_i^* - T_i^n}{\Delta t} + u\frac{T_{i+1}^n - T_i^n}{\Delta x} = \nu\frac{T_{i-1}^n - 2T_i^n + T_{i+1}^n}{\Delta x^2} \tag{15}$$

where T_i^* is known as the *predicted* value. Again setting the Courant Number, $CFL = \frac{u\Delta t}{\Delta x}$ and the Fourier Number, $F = \frac{\nu\Delta t}{\Delta x^2}$, and rearranging the terms in Equation 15, we obtain:

$$T_i^* = T_i^n + CFL(T_i^n - T_{i+1}^n) + F(T_{i-1}^n - 2T_i^n + T_{i+1}^n) \tag{16}$$

Equation 16 is known as the predictor step. The corrector step is then given by:

$$T_i^* = \frac{1}{2}\big[(T_i^n + T_i^*) - CFL(T_i^* - T_{i-1}^*) + F(T_{i-1}^* - 2T_i^* + T_{i+1}^*)\big] \tag{17}$$

Equation 14 provides explicit means to solve for the temperature at the node $(i, n+1)$. Note that for this method there are two calculations at each time step.

3 Results

3.1 FTCS Explicit Method

A plot of the numerical solution, $T(x,t)$, vs. axial position (x), for the inviscid case with

$$CFL = \frac{u\Delta t}{\Delta x} = \frac{1 \cdot 0.001}{0.01} = 0.100$$

is shown in Figure 1.

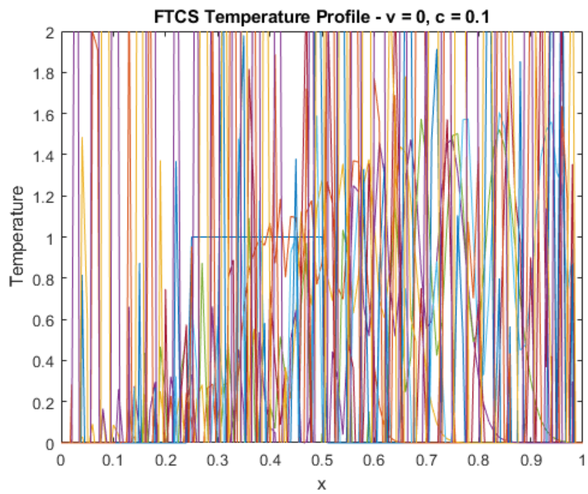

Figure 1: Temperature Solution, FTCS Explicit Method, $\nu = 0$, $CFL = 0.1$

For the inviscid case, we find that this method is *unconditionally unstable.*

Plots for $\nu = 1e-3$, $CFL = 0.1$ and $\nu = 10e-3$, $CFL = 0.1$ are shown in Figures 7 and 8, in the Appendix, Section 5.1. From these plots we conclude that the method is stable under these conditions, however dispersion error accumulates near the edges for low values of diffusivity. Additionally, we find that the stability of the solution for the diffusive case is highly dependent upon the stability parameters (CFL and F). In particular, we find that the stability conditions for the FTCS Explicit Method are as follows:

$$CFL^2 \leq 2F, \quad CFL \leq 1, \quad F \leq \frac{1}{2} \tag{18}$$

For values of CFL and F which do not satisfy these conditions, the solution becomes highly unstable and oscillatory. There are also certain conditions for CFL and F in which the diffusion becomes irrelavent, such as when

$$CFL = 1, \quad F = \frac{1}{2}$$

This result is provided in Figure 9. Hence, we conclude that the FTCS Explicit Method is highly dependent upon the grid and stability parameters, and special care should be given to this method in solving for $T(x,t)$.

3.2 FTCS Implicit Method

A plot of the numerical solution, $T(x,t)$, vs. axial position (x), for the *inviscid* case with

$$CFL = \frac{u\Delta t}{\Delta x} = \frac{1 \cdot 0.001}{0.01} = 0.100$$

is shown in Figure 2.

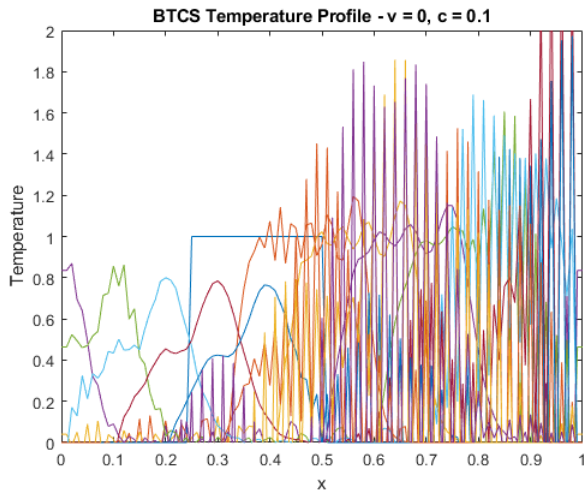

Figure 2: Temperature Solution, FTCS Implicit Method, $\nu = 0$, $CFL = 0.1$

The solution is stable, however it includes an immense amount of sispersion error. As the CFL is increased, the numerical error begins to dissipate, as shown in Figure 3.

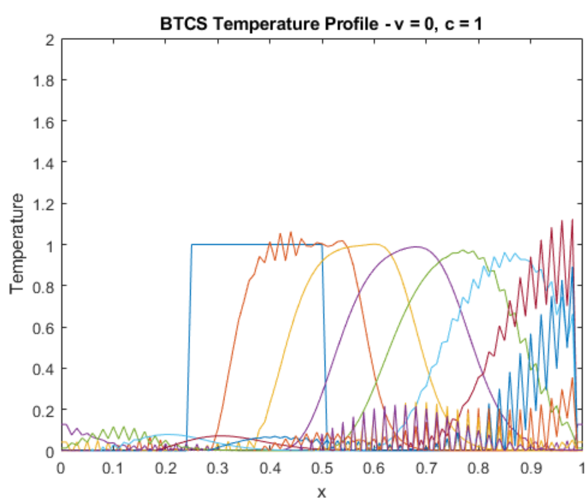

Figure 3: Temperature Solution, FTCS Implicit Method, $\nu = 0$, $CFL = 1.0$

Plots for $\nu = 10e-3$, $CFL = 0.1$, $\nu = 60e-3$, $CFL = 0.1$, and $\nu = 60e-3$, $CFL = 10$ are shown in Figures 10, 11, 12, Section 5.1. From these plots, we conclude that the FTCS Implicit Method is *unconditionally stable*. However, due to the large amount of dispersion error accumulated in the inviscous case, it is recommended that this method is not used for pure convection.

3.3 Upwind Method

A plot of the numerical solution, $T(x,t)$, vs. axial position (x), for the *inviscid* case with

$$CFL = \frac{u\Delta t}{\Delta x} = \frac{1 \cdot 0.001}{0.01} = 0.100$$

is shown in Figure 4.

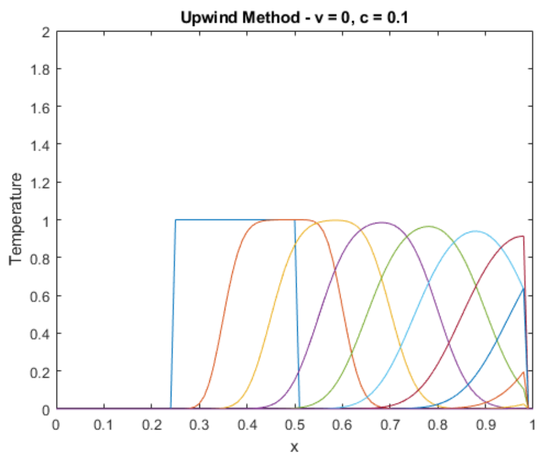

Figure 4: Temperature Solution, Upwind Method, $\nu = 0$, $CFL = 0.1$

We see that in this case the Upwind Method introduces *false diffusion* into the numerical solution. Note that from Equation 14, this false diffusion should disappear with CFL = 1. A plot of the numerical solution for the inviscid case with CFL = 1 is shown in Figure 5.

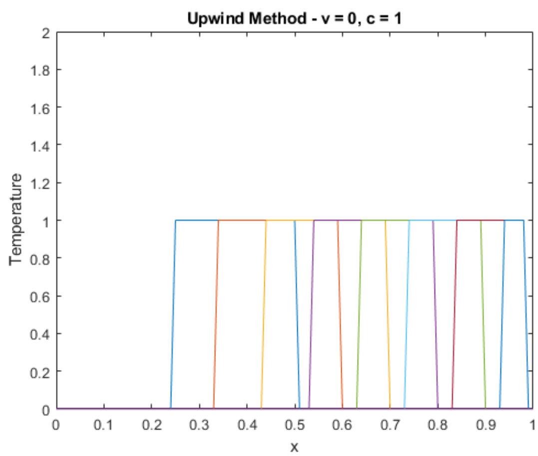

Figure 5: Temperature Solution, Upwind Method, $\nu = 0$, $CFL = 1.0$

Indeed, the false diffusion disappears in this case. From analyzing the numerical solution, we find that the stability parameters for the inviscid, upwind method are as follows:

$$CFL \leq 1 \tag{19}$$

Plots for $\nu = 45e-3$, $CFL = 0.1$ and $\nu = 46e-3$, $CFL = 0.1$ are shown in Figures 13 and 14, in the Appendix, Section 5.1. From these plots, we can conclude that the stability guideline for the viscous, Upwind Method is:

$$CFL + 2F \leq 1 \tag{20}$$

3.4 MacCormack Method

A plot of the numerical solution, $T(x,t)$, vs. axial position (x), for the inviscid case with

$$CFL = \frac{u\Delta t}{\Delta x} = \frac{1 \cdot 0.001}{0.01} = 0.100$$

is shown in Figure 6.

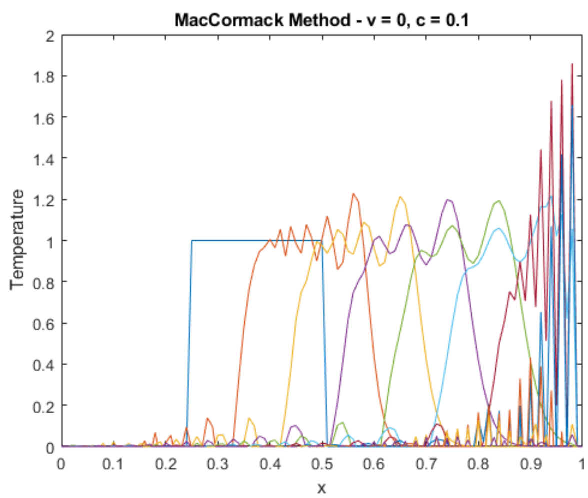

Figure 6: Temperature Solution, MacCormack Method, $\nu = 0$, $CFL = 0.1$

We see that in this case, the method is stable, however dispersion error accumulates near the edges of the domain. As the CFL number is increased, as in Figures 15 and 16, Section 5.1, the dispersion error dissipates. For values of CFL > 1, the solution becomes unstable. Thus, as in the Upwind Method, the inviscid MacCormack Method is subject to the following stability guideline:

$$CFL \leq 1 \tag{21}$$

Plots for $\nu = 1e-3$, $CFL = 0.1$, $\nu = 10e-3$, $CFL = 0.1$, and $\nu = 50e-3$, $CFL = 0.1$ are shown in Figures 17, 18, and 19 in the Appendix, Section 5.1. From these plots, we see that at low diffusivity, numerical error accumulates near the edges of the domain. As the diffusivity is increased, the numerical error dissipates, but the solution becomes highly innacurate/unstable. It is rather difficult to get a sense of the stability conditions for the viscous MacCormack Method, however, empirical stability guidelines have been established throughout the field. Namely, from Tannehill's[1] work in 1975, an emperical stability condition is as follows:

$$\Delta t \leq \frac{\Delta x^2}{u\Delta x + 2\nu} \tag{22}$$

From this equation, we see that the stability conditions reduces to $F \leq \frac{1}{2}$ for the viscous condition when $u = 0$, and reduces to $CFL \leq 1$ for the inviscous case when $\nu = 0$. Thus, it would be suggested that the MacCormack Method is not used for problems involving high values of diffusivity.

3.5 Relation to Reynold's Number

Another useful stability parameter that arises when solving Burger's Equation is the *Mesh Reynolds Number*, which is given by:

$$Re_\Delta = \frac{CFL}{F} = \frac{u\Delta x}{\nu} \tag{23}$$

We note that this is a dimensionless parameter and defines the ratio between convective and diffusive terms. Let us analyze this quantity for the FTCS Explicit Method, whose results are given in Section 3.1. From Equation 18, we first have that:

$$CFL^2 \leq 2F$$

$$\frac{CFL}{F} \leq \frac{2}{CFL}$$

Thus,

$$Re_\Delta \leq \frac{2}{CFL} \tag{24}$$

Furthermore, since

$$F \leq \frac{1}{2}$$

it follows that:

$$\frac{1}{F} \geq 2$$

$$\frac{CFL}{F} = Re_\Delta \geq 2CFL \tag{25}$$

Combining Equations 24 and 25, it follows that the stability restrictions on the Mesh Reynolds Number become:

$$2CFL \leq Re_\Delta \leq \frac{2}{CFL} \tag{26}$$

For values of Re_Δ that do not lay within this range, the numerical solution will become unstable and oscillatory in nature. Similar analyses for the Implicit, Upwind, and MacCormack methods could be performed, but will not be discussed in this report. Overall, we have obtained a relationship between the Courant Number (CFL), Fourier Number (F), and Mesh Reynolds Number Re_Δ, and it is easy trivial to see that they are dependent upon one another.

4 Conclusion

In this report, we obtained the solution $T(x,t)$ for one periodic time of the flow evolution for the one-dimensional convection-diffusion equation presented by Equation 1. The scalar $T(x,t)$ was solved for using four different methods, including the Forward-Time, Central Space Explicit and Implicit Methods, the Forward-Time, First-Order Upwind Method, and the MacCormack Method, for both inviscid and diffusive cases. The stability requirements for each of the aforementioned cases are summarized in Table 1.

Method	Inviscid	Diffusive
FTCS Explicit	*Unconditionally Unstable*	$CFL^2 \leq 2F, \quad CFL \leq 1, \quad F \leq \frac{1}{2}$
FTCS Implicit	*Unconditionally Stable*	*Unconditionally Stable*
Upwind	$CFL \leq 1$	$CFL + 2F \leq 1$
MacCormack	$CFL \leq 1$	$\Delta t \leq \frac{\Delta x^2}{u\Delta x + 2\nu}$

Table 1: FTCS Optimization of Δt, $n = 100$

A few general comments about each of the methods are also outlined below:

- **FTCS Explicit:**
  - In the viscous case, for $CFL = 1$ and $F = \frac{1}{2}$, the diffusion term cancels out and there is no diffusion present in the numerical solution.
  - Dispersive errors for low values of diffusivity.
  - Performs rather poorly, in general.
- **FTCS Implicit:**
  - High dispersion error for the inviscid case and for the viscous case with low values of diffusivity.
  - Performs very well for high values of diffusivity and/or large time steps.
- **Upwind:**
  - In the inviscid case, the numerical solution introduces false diffusion. False diffusion dissipates with $CFL = 1$. However, at this point the solution is on the borderline of stability.
  - Little to no dispersion error in any case.
- **MacCormack:**
  - High dispersive error for both the inviscid and viscous cases.
  - Inherent false diffusion in the inviscid case.
  - Performs poorly for high values of diffusivity.

It has also been established that, in general, the solution is highly dependent upon the stability parameters, and thus highly dependent upon the grid sizing. Grid sizing should be chosen to ensure stability is achieved based on the guidelines presented in Table 1. Overall, considering the fragile nature of the each method's accuracy and stability, results should be checked carefully for a problem of this nature.

5 Appendix

5.1 Additional Figures

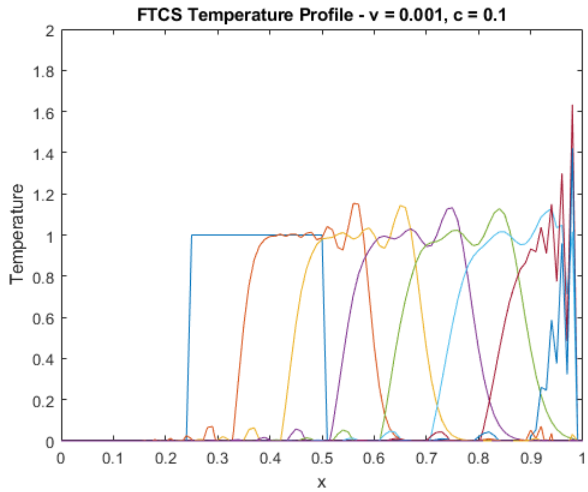

Figure 7: Temperature Solution, FTCS Explicit Method, $\nu = 1e-3$, $CFL = 0.1$

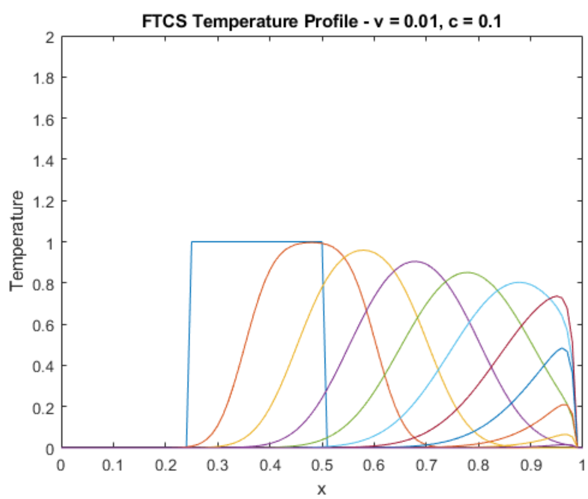

Figure 8: Temperature Solution, FTCS Explicit Method, $\nu = 10e-3$, $CFL = 0.1$

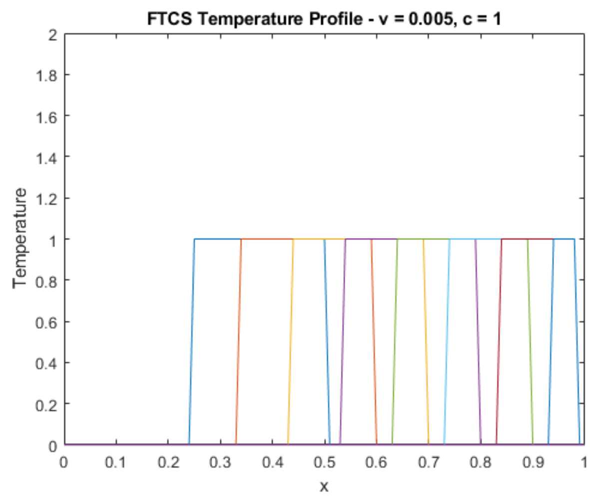

Figure 9: Temperature Solution, FTCS Explicit Method, $\nu = 0.5$, $CFL = 1.0$

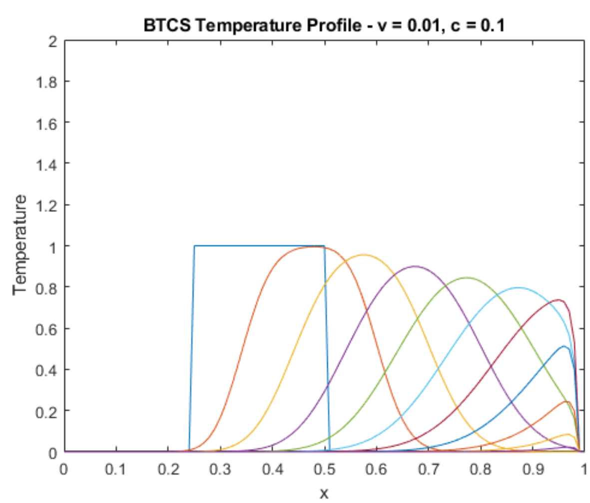

Figure 10: Temperature Solution, FTCS Implicit Method, $\nu = 10e-3$, $CFL = 0.1$

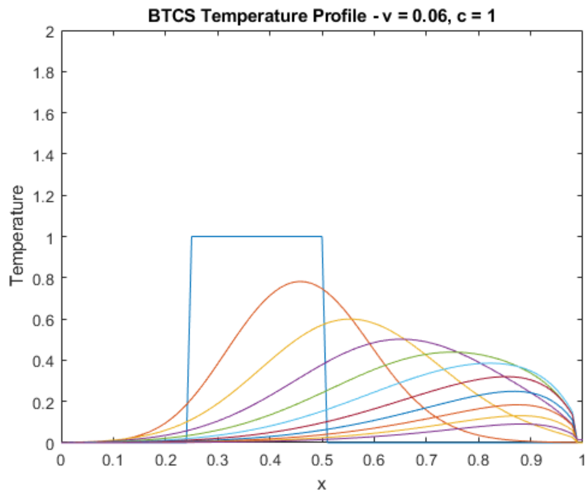

Figure 11: Temperature Solution, FTCS Implicit Method, $\nu = 60e-3$, $CFL = 0.1$

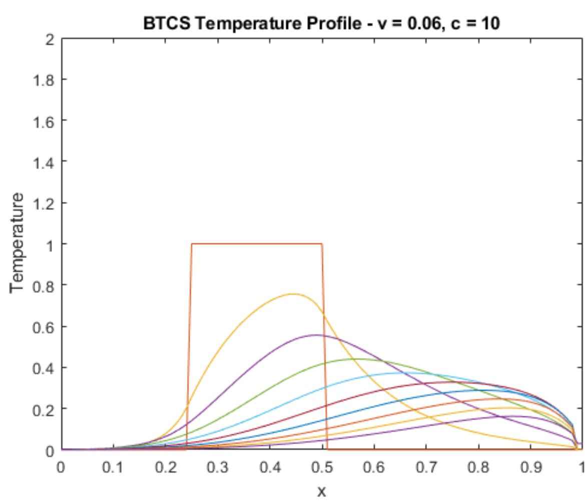

Figure 12: Temperature Solution, FTCS Implicit Method, $\nu = 60e-3$, $CFL = 10$

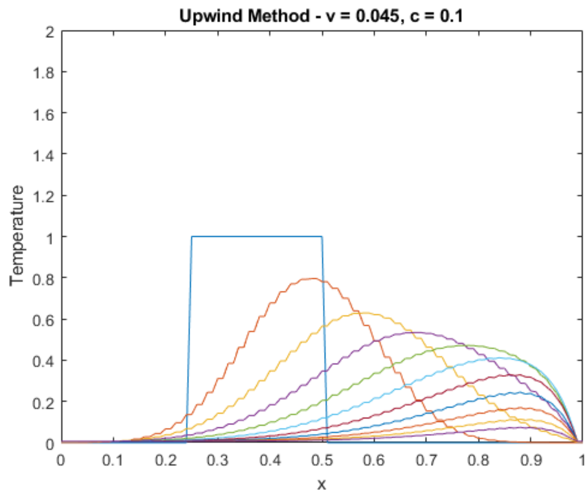

Figure 13: Temperature Solution, Upwind Method, $\nu = 45e-3$, $CFL = 0.1$

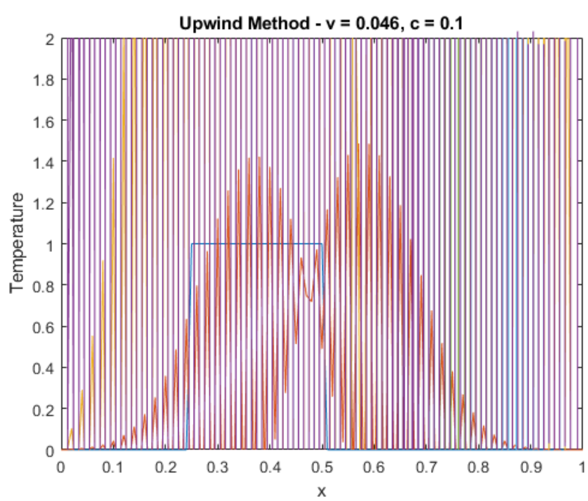

Figure 14: Temperature Solution, Upwind Method, $\nu = 46e-3$, $CFL = 0.1$

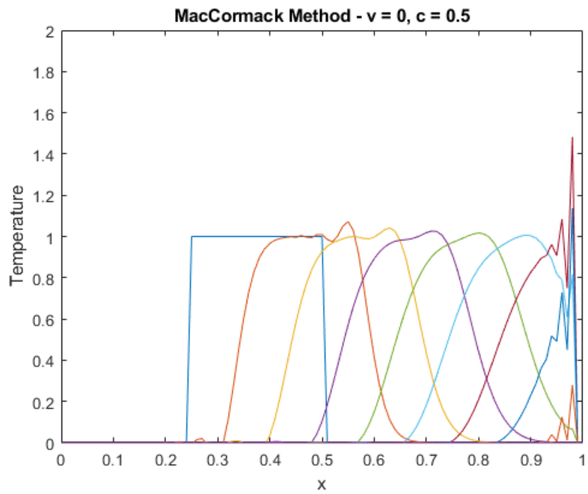

Figure 15: Temperature Solution, MacCormack Method, $\nu = 0$, $CFL = 0.5$

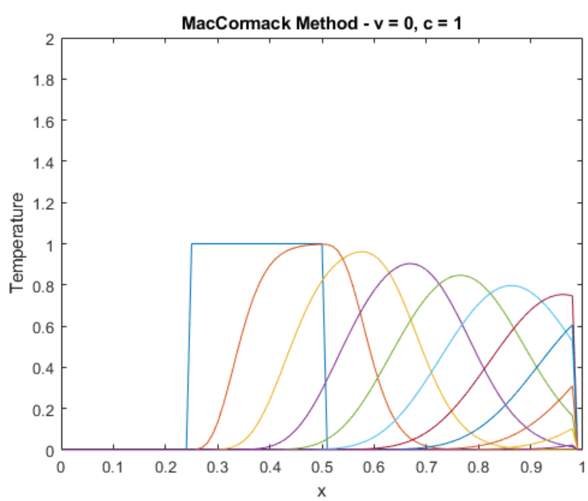

Figure 16: Temperature Solution, MacCormack Method, $\nu = 0$, $CFL = 1$

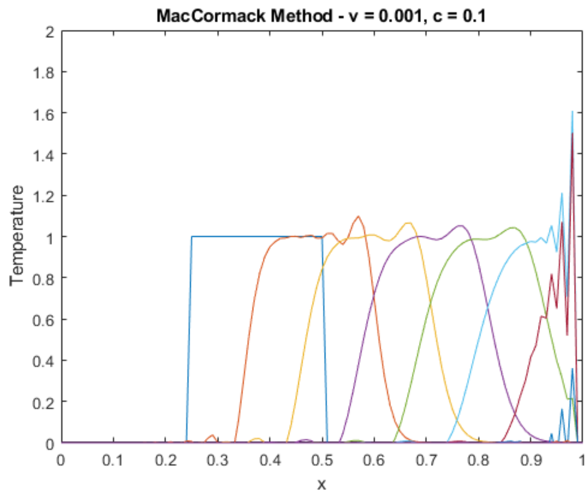

Figure 17: Temperature Solution, MacCormack Method, $\nu = 1e-3$, $CFL = 0.1$

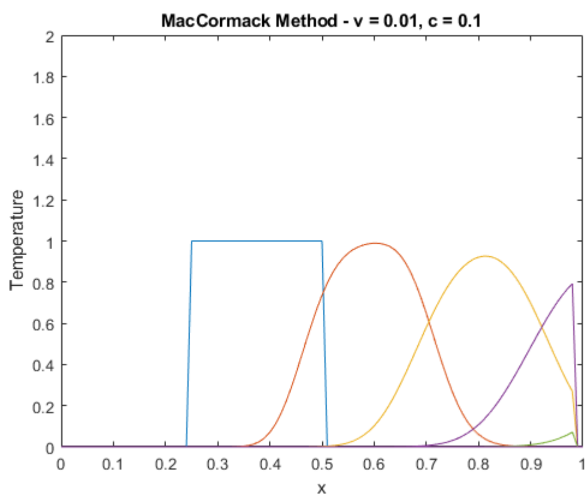

Figure 18: Temperature Solution, MacCormack Method, $\nu = 10e-3$, $CFL = 0.1$

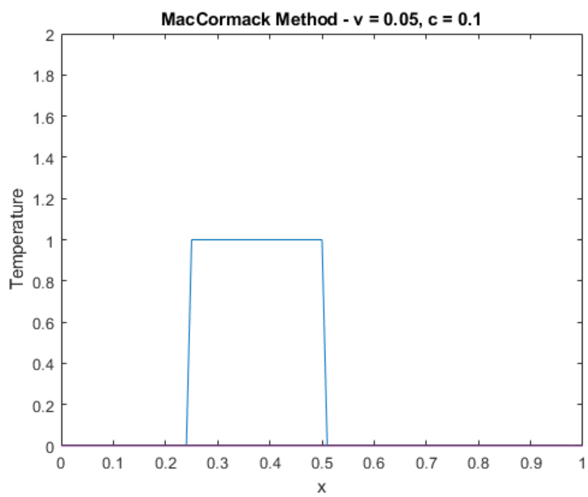

Figure 19: Temperature Solution, MacCormack Method, $\nu = 50e-3$, $CFL = 0.1$

5.2 References

[1] Tannehill, John C., et al. Computational Fluid Mechanics and Heat Transfer. Taylor & Francis, 1997.

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