**Western University, Department of Mechanical and Materials Engineering**

**MME 9710: Advanced CFD**

Assignment 1: Introduction to One Dimensional Diffusion Analysis

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# Fortran Solver

Before solving the assignment questions, the Fortran code provided was updated to solve 1-dimensional heat transfer problems. Initially the code was built to solve 1D conduction only, before adding layers for convection and internal generation. Once those processes were verified, a linearization loop was built to include radiation solutions. The updated code can be found in Appendix 1. The following sections outline the changes made to each file and which physical phenomena those changes reflect.

## Discretization Method

### Control Volume Formulation

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The discretization method implemented in the Fortran code is based on the Control-Volume (CV) formulation from the method of weighted residuals. In the CV formulation, the domain of interest is divided into a finite number of control volumes. The differential equation being solved is integrated over each control volume, and the result is solved using piecewise interpolation between the control volume interfaces. This method conserves quantities over each control volume and the entire domain regardless of the number of control volumes used.

This method is implemented by setting the end node value (IE) in the in.dat file. This marks the last node before the ending boundary condition. The difference between the end and beginning node value, plus one, indicates the number of control volumes used.

### Discretization of the Heat Equation for 1D Conduction

For a set of three control volumes West, P, and East (Figure 1), the energy balance excluding any sources reduces to:



Figure 1: Control Volume Set.

Where,

Using piecewise linear approximation of the flux through each control volume, and piecewise constant approximation for the temperature of a given control volume () as the temperature at the center of a control volume is assumed to be representative of the whole volume, the discretized energy balance for a given control volume becomes:

Where each coefficient is discussed in the following sections of code they are represented in.

## main.f

The main routine implements each element of the discretization process by calling the subroutines outlined below. This routine implements a linearization loop that continues iterating on the temperature field until the residuals converge. The main routine begins by initializing the temperature field, calculating an initial set of coefficients, and calculating the temperature field again with those coefficients. Following the first iteration, the routine updates the coefficients with the previous iteration’s temperature field, and calculates the average residual. If the average residual meets the convergence criteria, the main routine ends.

## difphi.f

This subroutine was built to calculate the diffusion coefficient (DE) on the East face of each control volume. A loop was built to calculate the East face DE for each node from IB-1 (the first boundary condition) to IE (the end node). The loop includes IB-1 because diffusion exists on the East face of the initial boundary condition. Diffusion does not exist on the end boundary condition, which is why the loop does not include IE+1. DE was calculated using the following equation:

Where is the thermal conductivity, is the cross-sectional area of the east face of the control volume, is the distance to the center of the East node, and is the distance to the center of the node of interest. Equation (1) results from linear piecewise interpolation of node point temperatures. This method is used to ensure that the discretized equation obeys the conservation law. For conservation to be true,

To satisfy this condition, the flux and temperature distribution at each integration point (e/w) must be the same for control volumes E and P. If a method of order higher than linear is used, the resulting distributions would not be equal, and conservation would not be maintained. If constant flux approximations were used, the resulting integration at each point would approach infinity, as the distribution would not be continuous, resulting in the same outcome.

As a result of the conservation law, the DE of the east face of one node must be equal to the DW of the following node. This allows only the DE of the east face to be calculated for each control volume.

After the loop finishes, the subroutine returns an array of DE values for each control volume.

## srct.f

This subroutine was used to determine the net source terms of each control volume. Source terms are created because of the linearization of each source of heat within a control volume. For each control volume, the total source is given by,

Assuming the control volume has the discrete equation given in (1) and ignoring radiation, the source term reduces to,

Where m is the current iteration of temperature, and and are given by,

Where is the fixed source coefficient, and is the linearized source coefficient. When radiation is not ignored, the source term must be linearized to ensure that piecewise linear flux problems are solved between each control volume. Various linearization techniques are available and give different results, as they break the non-linear problems down in different ways.

The subroutine implements a loop to calculate each source term and over each control volume. Three linearization techniques were included and tested in question 4. An internal generation term is also included in the code, adding to the source term on each control volume. The subroutine returns the two source terms to be used in the active coefficient calculation.

## coeff.f

This subroutine was used to calculate the active coefficients for each control volume. The active coefficients are the coefficients belonging to each temperature term given in equation (1). Each coefficient is given by,

A loop was implemented to calculate the coefficients for each control volume.

## bndct.f

This subroutine was used to assign boundary conditions to the active coefficient arrays. Three types of boundary conditions were derived for common scenarios. Each boundary condition was listed in this subroutine, and updated based on the type of problem being solved.

## resid.f

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This subroutine was used to calculate the residual of each node after a temperature field was solved. The residual describes how closely a linearized problem was solved, and measures the convergence of a solution over multiple iterations. The residual formula is given by,

The residual measures the difference between the updated coefficient calculation, and the previous iterations temperature. The residuals were implemented by comparing the average residual over all the control volumes to a convergence criteria. When the residual reached the criteria, the solution was accepted.

## Code Testing

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Before developing the final solutions to the questions provided, various parameters were tested to determine their effect on the solver. Tests were performed on the 1D conduction problem. It was determined that the initial temperature had no effect on the solution output for various control volume sizes. This implied that the initial guess of the temperature field did not influence the solution. Next, the geometry of the duct was varied. The larger the duct was, the larger the flux was through the duct. This test behaved as expected, and verified the solvers performance. Lastly, the surrounding temperature was varied for the radiation problem using the third linearization technique. It was determined that the surrounding temperature had a large effect on the temperature distribution through the fin. This performance was expected and verified that the linearization loop was performing correctly.

# Question 1: 1D Conduction

This problem analyzed a square fin experiencing pure conduction with prescribed temperature on each end of the fin. The temperature distribution across the fin was solved for. The properties of the problem can be found in Table 1, and the geometry of the problem can be found in Figure 2.

Table 1: Question 1 properties





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Figure 2: Square fin geometry.

## Code Implementation

This problem was implemented by setting the geometry in makgrd.f, setting the boundary conditions in bndct.f, and varying the number of control volumes used in the discretization.

The half height, and half depth Y and Z, were set in makgrd.f to initialize the geometry of the problem. Dirichlet boundary conditions were present in the problem due to specified temperatures at each end of the fin. This boundary condition was set in bndct.f, and can be seen in Table 2. The boundary conditions were initialized at nodes IB – 1 and IE + 1 because the boundary condition control volume has zero volume, and the middle of the control volume is sent to the edges of the IB and IE nodes. The number of control volumes were varied from 1 to 64, doubling in each iteration, to determine the effect of meshing on the temperature distribution.



Table 2: Question 1 boundary conditions

## Results

For each number of control volumes, the average residual and heat flux between the first two nodes were calculated. The heat flux was used as the criterion to determine when the grid had converged. Table 3 summarizes the results of each control volume. The results of each control volume were plotted on a composite plot to visualize the grid convergence. Figure 2 plots the temperature distribution of each control volume iteration.

Table 3: Summary of Question 1 results



Both residual and grid convergence were tested to verify the solution of each number of control volumes. For each number of control volumes, the residuals converged after the first iteration. Since the problem was completely linear, none of the active coefficients were a function of temperature. This caused the active coefficients to remain constant after the first solution, which caused a constant solution over each iteration of the linearization loop. The residuals of 32 and 64 control volumes did not reach the convergence criteria. However, the residuals were still small, and converged after the first iteration as expected, resulting in a reasonable solution.

To measure grid convergence, the heat flux between the IB – 1 and IB nodes was calculated. The heat flux remained relatively constant regardless of the number of control volumes used, as the change in heat flux between each number of control volumes was always below two percent. This indicates that the temperature distribution was completely grid independent, and is reliable over all sizes of control volumes.

One control volume was tested to determine the extreme behavior of the solver. Since the heat flux remained constant, one control volume was a reasonable number to use for this problem. This is a result of the geometry and expected temperature distribution of the problem. Since the problem was completely linear, both in temperature distribution (no source terms) and in geometry (constant cross section), the temperature of the fin was directly proportional to its x distance from the first node. This is responsible for making all control volume sizes reasonable approximations of the temperature distribution. Additionally, since the flux distribution between control volumes was piecewise linear, the interpolation technique used matched the expected physical distribution of temperature, which allowed the distribution to be modelled accurately.

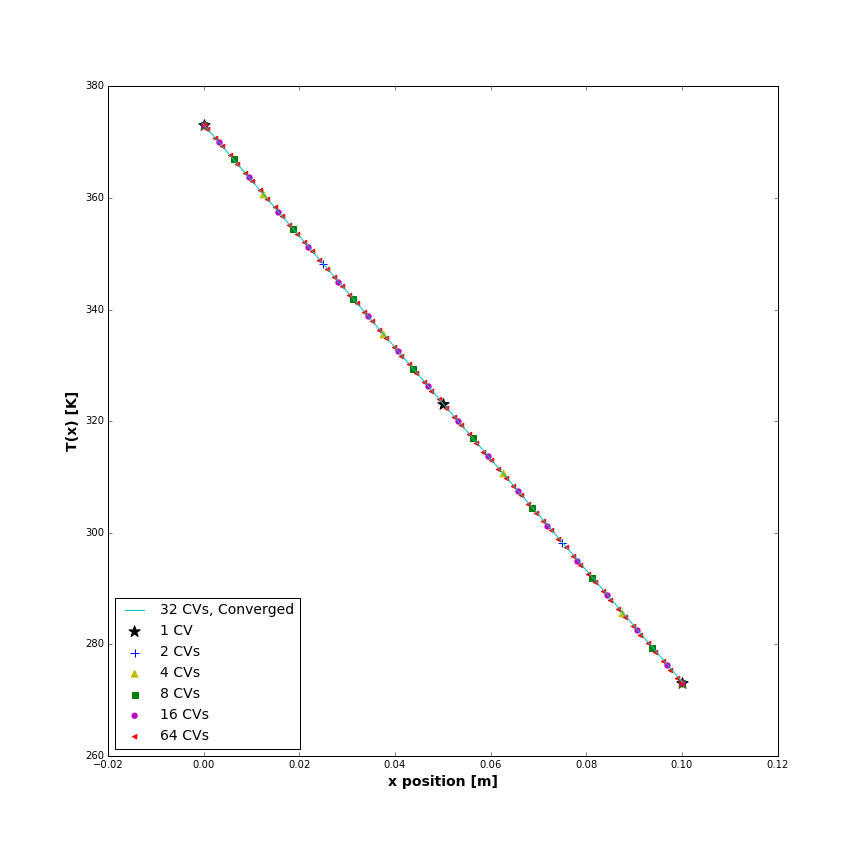


Figure 2: Temperature distribution of square fin with pure conduction

# Question 2: 1D Convection

This problem analyzed a square fin experiencing both conduction and convection with prescribed temperatures on each end of the fin. The temperature distribution across the fin was solved for and compared to the analytic solution. The properties of the problem can be found in Table 4, and the geometry of this problem was the same as problem 1, and can be found in Figure 3.

Table 4: Problem 2 properties



## Code Implementation

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This problem was verified using the same process as problem 1, with the addition of source term calculations for each control volume to account for convection.

The same geometry from problem 1 was kept in makgrd.f. The Dirichlet boundary condition were present in the problem due to specified temperatures at each end of the fin. This boundary condition was set in bndct.f, and can be seen in Table 5. The boundary conditions were initialized at nodes IB – 1 and IE + 1. The number of control volumes were varied from 1 to 63, doubling in each iteration, to determine the effect of meshing on the temperature distribution.

The source term calculation was built into the code by calculating and in each control volume as discussed in section 1.4. This accounted for the convection heat removal over the surface of each control volume.

Table 5: Problem 2 boundary conditions



## Results

For each number of control volumes, the average residual, heat flux between the first two nodes, and the temperature gradient between the first two nodes were calculated. The heat flux and temperature gradient were each used as the criterion to determine when grid convergence had been reached. Table 6 summarizes the results of each control volume. The results of each control volume were plotted on a composite plot to visualize the grid convergence. Figure 3 plots the temperature distribution of each control volume iteration.

Table 6: Question 2 summary of results



IE was selected so that the number of control volumes would be odd. This allowed the center of a control volume to occur in the middle of the fin, where the minimum temperature was expected. The residuals converged regardless of the number of control volumes used. The grid converged to under two percent difference when 15 control volumes were used, which indicates the minimum number of control volumes required to obtain a reliable solution. This convergence process is used to determine when the solver becomes independent of the mesh used. Convergence is required because the solution will not be reliable unless various sizes of control volumes match. Figure 3 illustrates the convergence process. As the number of control volumes increases, the temperature distribution converges to the expected concave shape. The solid line in Figure 3 indicates the minimum grid converged solution.

When grid convergence was achieved, the converged control volume size was compared to the analytic solution (see Figure 4). The analytic solution was determined using fin tip conditions. The fin was modelled using Case C in Table 3.4 of Incropera and Dewitt for prescribed end temperatures. The temperature distribution for this condition is,

Where and are given by,

Isolating for gives,

As Figure 4 illustrates, the grid converged solution matches the analytic solution. The minimum temperature measured was 360.24K, which had less than one percent difference from the analytic temperature. The analytic solution indicates a concave shape which is a result of the convection heat transfer addition to the problem. Since both end temperatures are fixed, heat is removed from the fin along the bars length, and the maximum heat removal occurs at the center as it is the farthest point from the prescribed temperatures. This distribution is matched relatively easily by the solver as convective heat transfer is a linear process related directly to the temperature difference between the control volume of interest and the surroundings. This is reflected in the piecewise linear flux between each control volume, which allows the solver to model the solution accurately.

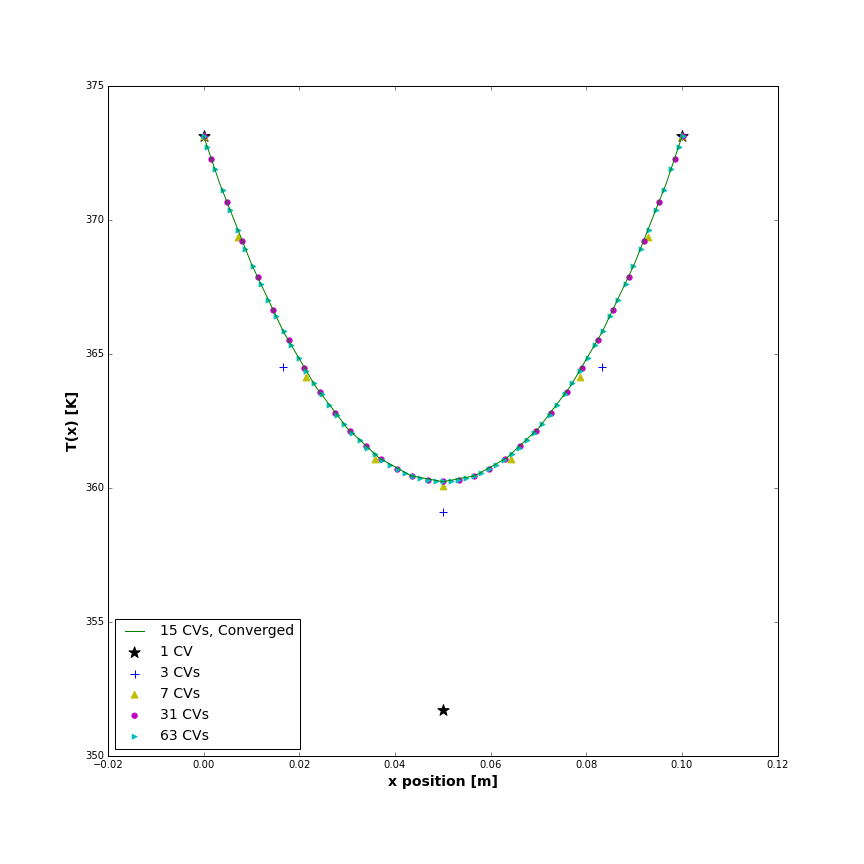


Figure 3: Problem 3 composite of temperature distributions for various control volumes

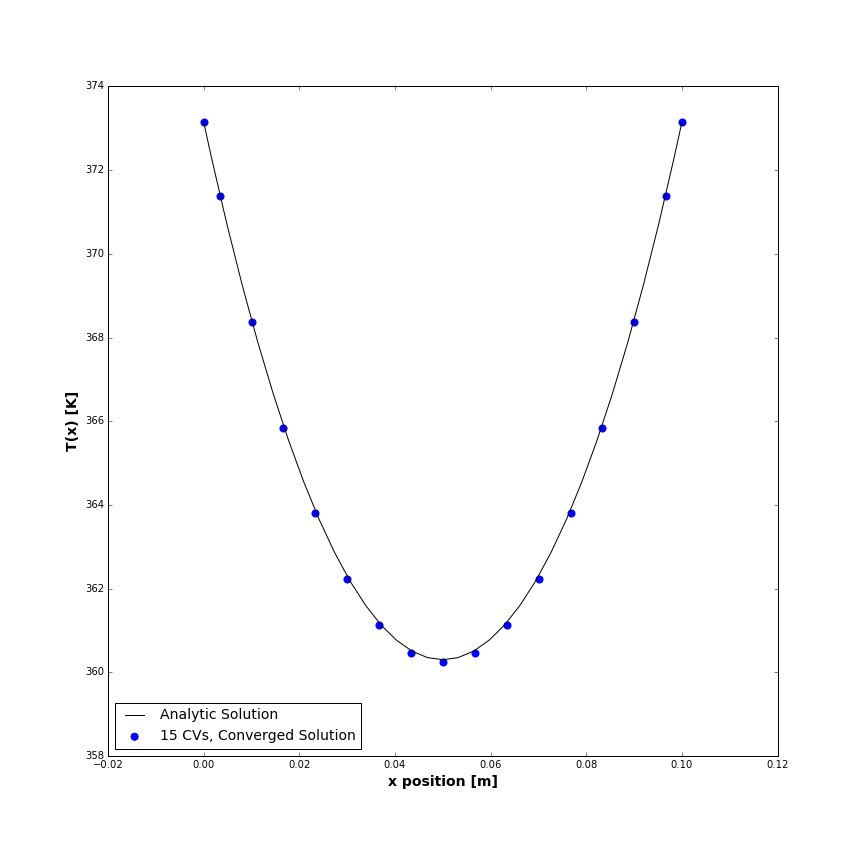


Figure 4: Problem 2 analytic solution (line) compared to the minimum grid converged solution (point)

# Question 3: Internal Heat Generation

This problem analyzed an infinite plane wall experiencing uniform internal heat generation throughout its length and convection on its boundaries. The temperature distribution, surface temperatures, and maximum temperature throughout the wall was solved for and compared to the analytic solution. The properties of the problem can be found in Table 7, and the geometry of this problem can be found in Figure 5.

Table 7: Question 3 properties





Figure 5: Question 3 geometry

## Code Implementation

This problem was verified using a similar process as problem 1 and 2, with the addition of an internal generation source term calculation for each control volume, and a new boundary condition.

The geometry of the problem required the use of the second geometry id type, the plane wall. This geometry does not model a cross section, as the plane wall is assumed to be infinite. The Robin boundary condition was present in this problem due to the convection present at each face of the wall. This boundary condition was set in bndct.f, and can be seen in Table 8. The boundary conditions were initialized at nodes IB – 1 and IE + 1. The number of control volumes were varied from 1 to 64, doubling in each iteration, to determine the effect of meshing on the temperature distribution.

The source term calculation was built into the code in the srct.f subroutine by calculating and in each control volume as discussed in section 1.4. An internal generation flag was added to the subroutine which allowed an internal generation value to be set, or zero if internal generation wasn’t present. This term was added to the existing convection source terms and the surroundings temperature was set to zero in the input file to zero the convective source terms along the length of the wall, as convection was only present at the boundaries. Since does not depend on the surrounding temperature, it was set to zero manually.

Table 8: Question 3 boundary conditions



## Results

For each number of control volumes, the average residual, heat flux between the first two nodes, and the maximum and surface temperatures were calculated. The heat flux was used as the criterion to determine when grid convergence had been reached. Table 9 summarizes the results of each control volume. The results of each control volume were plotted on a composite plot to visualize the grid convergence, found in Figure 6.

Table 9: Question 3 results



### Fortran Solution

For every control volume size the residuals converged. However, the residuals were large relative to the convergence criteria. This was not concerning since the processes in this problem are still linear, which does not cause the residuals to play a large role in the evaluation of the solution.

The heat flux criterion was initially used to determine when the grid converged. It can be seen from Table 9 that the change in heat flux was small across all control volumes. This would indicate that the solution is independent of control volume size regardless of the number of control volumes used. This was because the only heat transfer process in the wall that was affected by x position was conduction, which only depends on the conductivity, area, and x distance. However, since the solution of this problem was regarding the temperature distribution, the distribution of each grid was compared to the analytic solution (section 4.2.2) to determine when the grid was accurately modelling the solution. Table 10 summarizes the surface and maximum temperature convergence. Like the heat flux, there was little change in surface and maximum temperature between control volume sizes. However, it should be noted that one control volume does not correctly model the system, as it implies that the surface temperatures are equal on both sides of the wall. This cannot be true as the difference in surrounding temperature on each side of the wall would cause a temperature gradient through the wall.

Based on both sets of convergence criteria, the solution is independent of meshing for all control volume sizes. However, comparing the shape of the Fortran solution to the analytic solution shows that finer mesh size more accurately predicts the curve expected within the wall. The analytic solution compared to the midrange control volume size can be seen in Figure 7.

Table 10: Question 3 surface temperature summary



### Analytic Solution

The analytic solution was produced by modelling a plane wall with internal generation and prescribed surface temperatures. The surface temperatures were calculated using an energy balance at each face of the wall. The general equations were taken from Tables C.1 and C.2 in Appendix C of Incropera and Dewitt. “L” in the following equations is the half length of the wall. The energy balances at each face give,

Isolating for in the face 2 balances gives,

Substituting into face 1 and solving for and gives,

Using these surface temperatures, the temperature distribution through the wall was found from,

Using this distribution, the maximum temperature was found by setting the derivative equal to zero and solving for x, followed by T(x) at that x value. This gave,

It can be seen from Figure 7 that the Fortran solution accurately reflects the analytic solution as the surface and maximum temperatures for all control volume sizes are within 1% of the analytic solution. This accuracy is again reflected because of the linear nature of the heat transfer within the wall. Inside the wall, the conduction process is linear, and piecewise linear interpolation is used between control volumes. This allows accurate modelling of the temperature distribution regardless of the size of the control volume. This was not changed by the internal generation since the source was constant across each control volume.

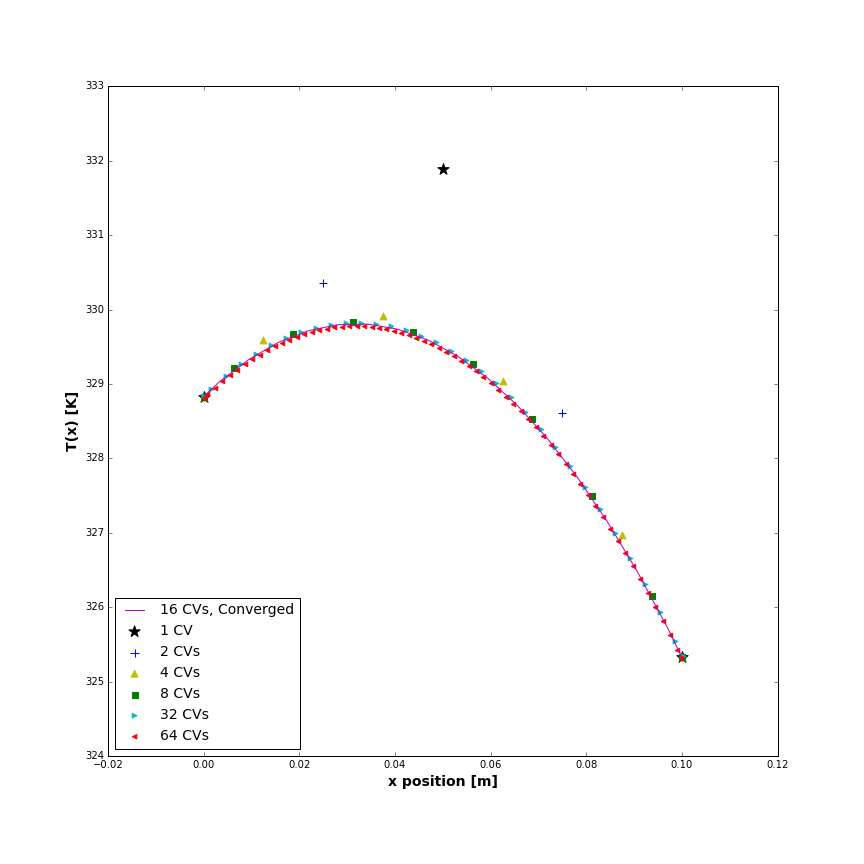


Figure 6: Question 3 temperature distributions for various control volume sizes

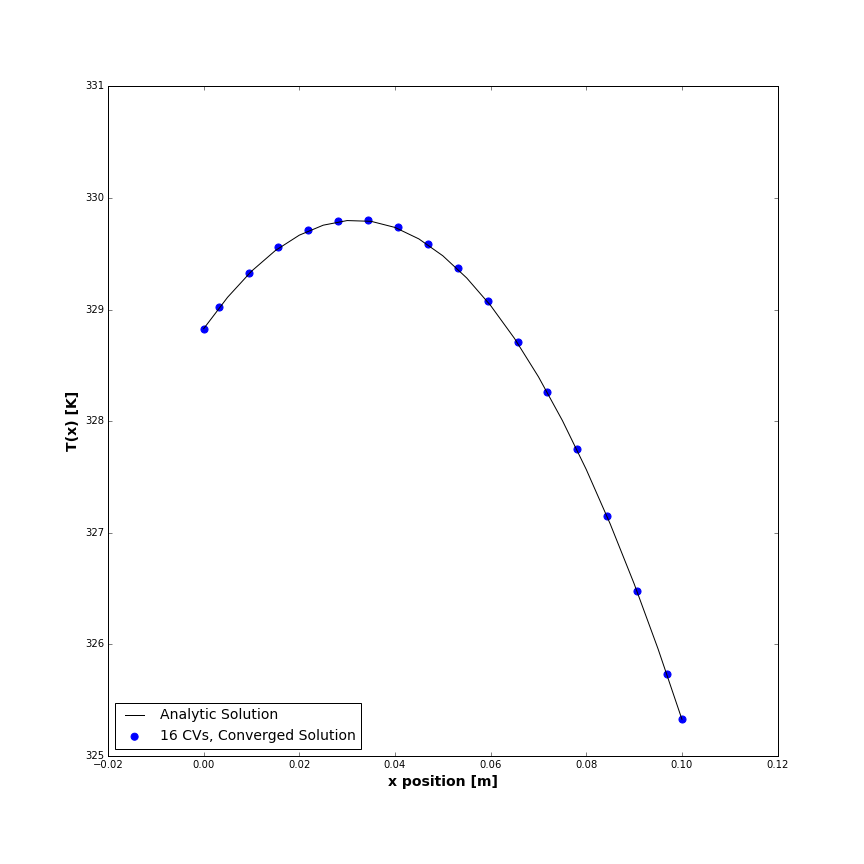


Figure 7: Question 3 analytic solution (line) compared to the grid converged solution (point)

# Question 4: Linearization Techniques

This problem analyzed a square fin experiencing conduction and radiation with prescribed tip temperatures; the temperature distribution was solved for. The properties of the problem can be found in Table 11, and the geometry of this problem is the same as questions 1 and 2 (see Figure 2). Three linearization techniques were tested on two different materials to determine which linearization techniques were most successful. Residuals were analyzed to determine when the non-linearity caused by the radiation source was correctly linearized.

Table 11: Question 4 Properties



## Code Implementation

This problem was verified using a similar process to problems 1 and 2, with the addition of source term calculations for each control volume to account for radiation, and a linearization loop.

The same geometry from problem 1 was kept in makgrd.f. A Dirichlet boundary condition was present in the problem due to specified temperatures at each end of the fin. This boundary condition was set in bndct.f, and can be seen in Table 12. The boundary conditions were initialized at nodes IB – 1 and IE + 1. The number of control volumes were varied from 1 to 64, doubling in each iteration, to determine the effect of meshing on the temperature distribution.

Table 12: Question 4 Boundary Conditions



The source term calculation was built into the code by adding a flag for the linearization technique in srct.f. The flag was used to specify which linearization technique would be used for the solution. Within each condition, the specific linearization terms were added to the existing and structure, to create a general solution based on the type of heat transfer present. This accounted for the radiative heat removal over the surface of each control volume for all linearization techniques.

The residual calculation and linearization loop was especially important in this problem, as the residuals did not remain constant over all iterations. This occurred because the linearization terms for radiation are a function of temperature, causing the active coefficients and to update after each solution iteration. The loop ended when the residual reached the convergence criteria for non-linearities, 1x10-5.

## Results

For each number of control volumes, the average residual over all control volumes and the heat flux between the first two nodes was calculated. The heat flux was used as the criterion to determine when grid convergence was achieved. This process was conducted for all linearization techniques and both materials. The results of each material are discussed individually.

### Steel Results

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Table 13 summarizes the results of each control volume for all three linearization techniques. The results of each control volume were plotted on a composite plot to visualize the grid convergence, found in Figures 8 through 10.

The temperature distribution through the steel fin was constant for each linearization technique. The temperature distribution was completely linear despite the presence of radiation, and the grid converged after four control volumes were used. The temperature distribution was completely linear due to the high conductivity of steel. The high conductivity allows the heat to diffuse between the control volumes more than it is removed by radiation. This allows all linearization techniques to perform well as the effect of radiation is negligible relative to the conduction of the material, and causes the temperature distribution to be linear.

The average residuals for each linearization technique reached the convergence criteria except for 64 control volumes. The third linearization technique was the most efficient way of linearizing the problem, as it converged in four iterations compared to six for the other two techniques. The Newton – Raphson method is more efficient than the first two linearization techniques because it approximates the non-linear function as a combination of tangent lines at various points throughout the function. This method converges on the tangent lines that accurately model the roots of the non-linear equation, resulting in an accurate linear representation of the non-linear function. The other two methods are not built this way, and are not stable techniques.

Table 13: Question 4 steel results



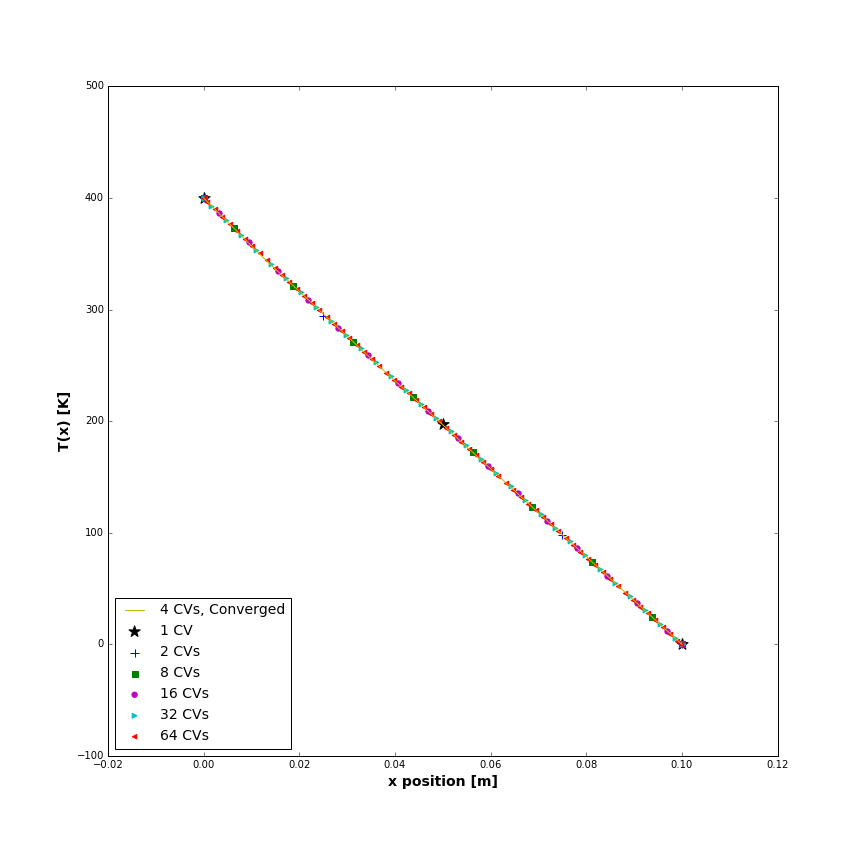


Figure 8: Steel, linearization 1. Converged (line).

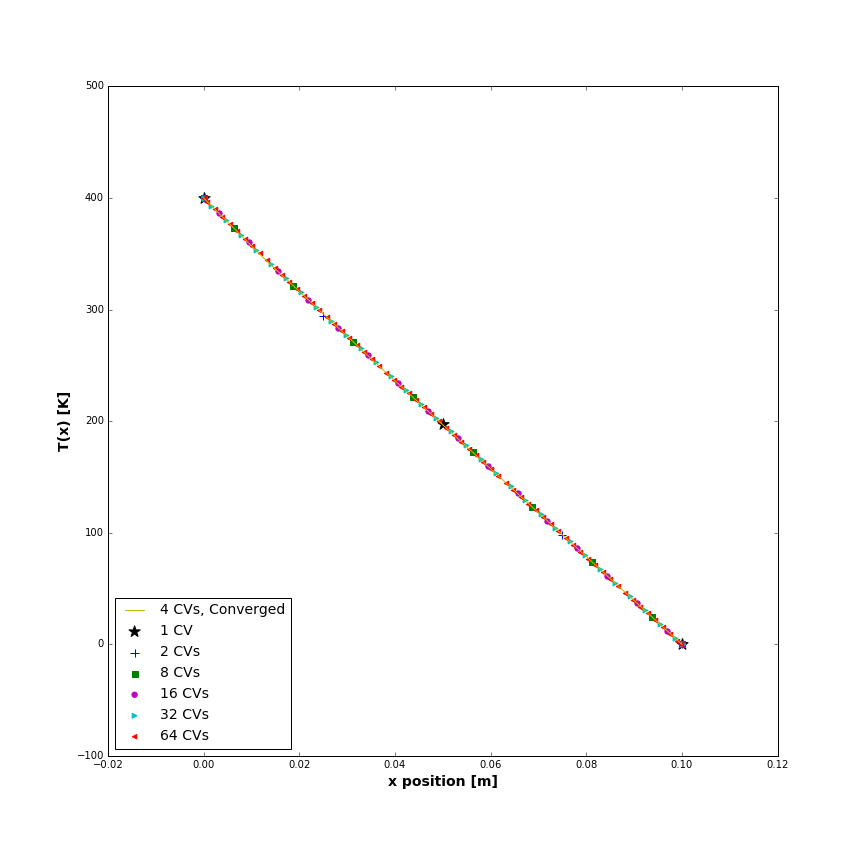


Figure 9: Steel, linearization 2. Converged (line)

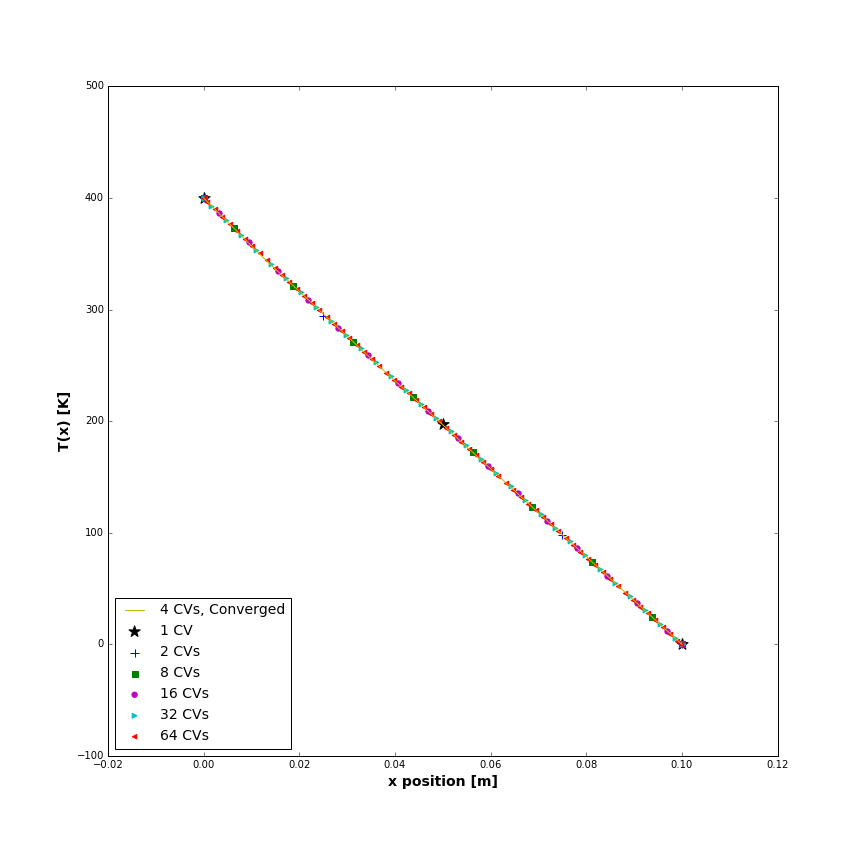


Figure 10: Steel, linearization 3 (NR). Converged (line)

### Wood Results

Table 14 summarizes the results of each control volume for all three linearization techniques. The results of each control volume were plotted on a composite plot to visualize the grid convergence, found in Figures 11 and 12.

Since the thermal conductivity of wood is much lower than steel, only one linearization technique was successful. The low thermal conductivity made the heat loss due to radiation closer to the heat diffusion through the control volumes, causing instability in the first two linearization techniques.

The first linearization technique did not successfully return a solution for the wooden fin. As seen in Table 14, the residuals diverged for all control volume sizes. This is because this technique relies on one coefficient, , to linearize the radiation source, making it very unstable.

The second linearization technique returned a solution (Figure 11), but the solution was not meaningful. The residuals did not converge for this linearization technique and were well above the criteria. Additionally, the grid did not show signs of convergence, as the difference in heat flux spiked at 16 control volumes. This was caused by the sensitivity of the second technique to large values of radiative heat transfer relative to conduction. Since the thermal conduction was low, the technique was not able to converge.

The Newton-Raphson method was the most effective technique (Figure 12). The residuals were well below the criteria for all control volumes, indicating that all solutions were physically meaningful. The solution was grid independent after 64 control volumes. However, this was using a doubling convergence process. It is likely that between 32 and 64 control volumes could be used to reach grid independence, but the process of determining that number would not be systematic.

After performing analysis on two types of fins with all linearization techniques, the Newton-Raphson technique is the only method of accurately modelling non-linear problems. The other two techniques will not be used in future analysis, and will be removed from the srct.f subroutine.

Table 14: Question 4 wood results



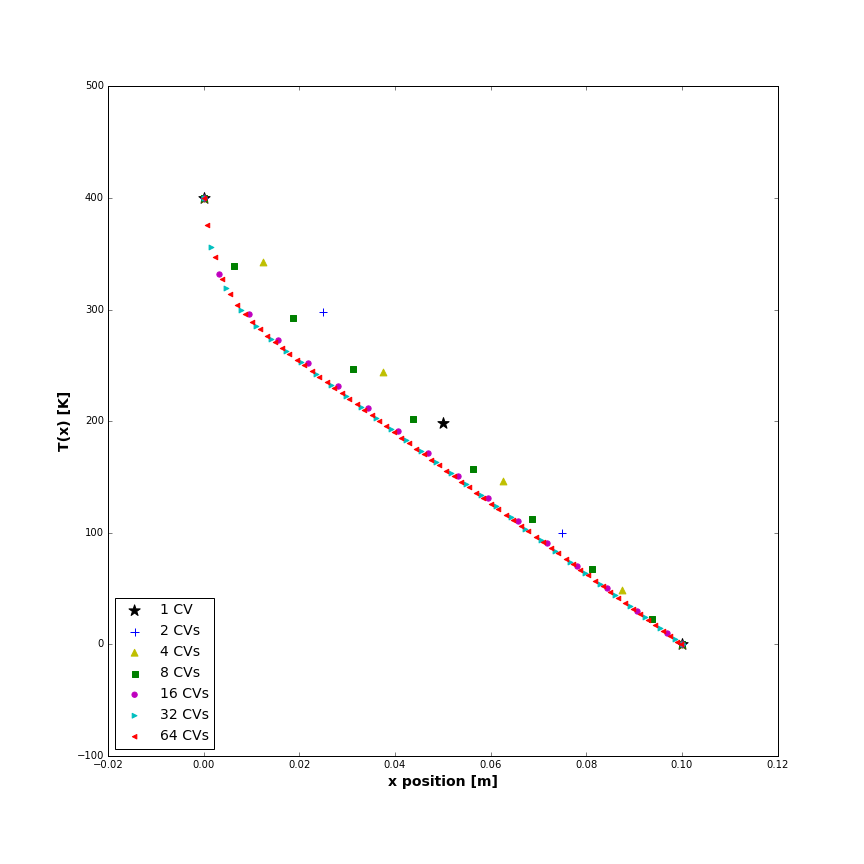


Figure 11: Wood results, linearization 2. Grid did not converge.

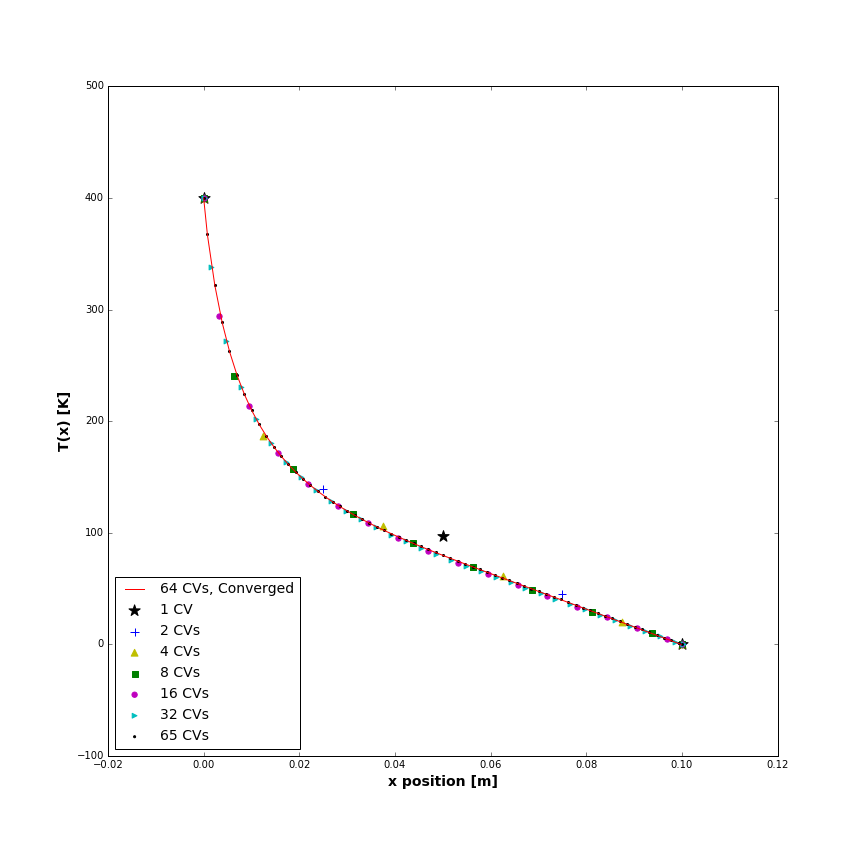


Figure 12: Wood, linearization 3. Converged grid (line)

# Appendix 1: Modified Subroutines

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See following pages for the subroutines that were modified.