

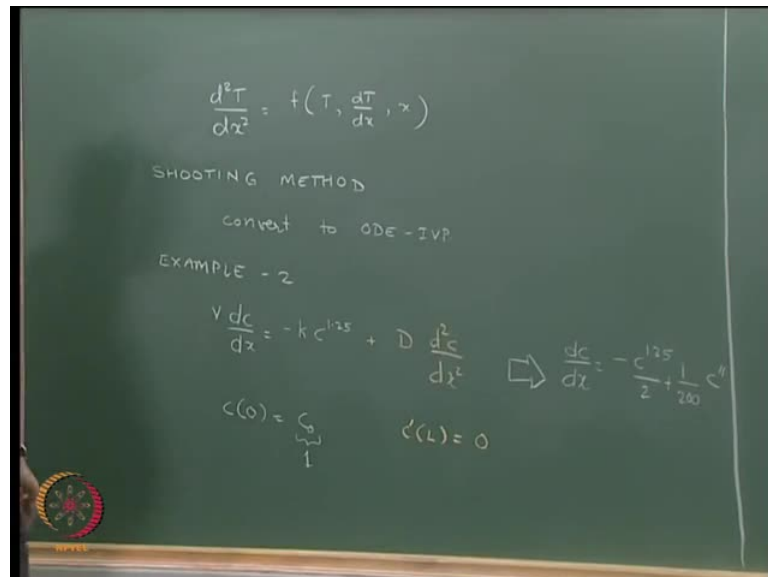
Computational Techniques
Prof. Dr. Niket Kaisare
Department of Chemical Engineering
Indian Institute of Technology, Madras

Module No. # 08

Lecture No. # 03

Ordinary Differential Equations
(Boundary Value Problems)

(Refer Slide Time: 00:19)



Hello and welcome to this lecture 3 of module on ODE, boundary value problems. the type of problems that we have been solving in this particular module are, for example, we have looked at heat conduction in a rod, and that particular case, the problem that we ended up with was $\frac{dT}{dx} = \text{sum function of } T$ or rather $\frac{dT}{dx}$ is sum function of T and x . The way, we said we can solve this particular problem is by two methods. One, which we considered in the previous lecture, was the shooting method and the method that we are going to consider in this particular lecture is through using finite differences.

So, in shooting method, what we did was converted in shooting method, we converted this ODE boundary value problem into ODE initial value problem. In that particular

case, we guess a value for the initial value and based on that guess of the value, we try to see how close we get to the actual boundary value in this particular problem.

If we are far away from the boundary value and not close enough from the boundary value, we use either a bisection rule or a regular false method or Newton's method in order to change our initial values, such that the boundary values are met. That is its strategy that we followed in shooting method. Now, this strategy we saw that work for the heat conduction problem, where we had the problem of $d^2 T$ by dx^2 equal to some linear function. In today's module, first what I am going to do is take up an example where the shooting method is not going to work. The second example that we had spoken about in the first lecture itself was a reactor with axial dispersion and that was our example two.

So, that was based on a modification to the example that we had done in ODE initial value problems. the PFR, the plug flow reactor example, we considered in ODE initial value problem was of the form $v \frac{dc}{dx}$, where c is concentration, is going to be equal to minus k multiplied by c to the power 1.25. So, this was the example that we had taken in the previous module. Now, this we can modify in presence of axial dispersion. We will have another term, which corresponds to the axial dispersion term, and that axial dispersion term will be of the form $D \frac{d^2 c}{dx^2}$, which is the dispersion coefficient multiplied by $d^2 c$ by dx^2

Now, with this the original initial value problem, was what I have written in white, with the initial conditions given as c at 0, is going to be equal to sum value c_0 . Now, with this $d^2 c$ by dx^2 also included, our boundary condition, we will need a second boundary condition and typically the second boundary condition is as we had seen, c dash L equal to 0. So, the first derivative of the concentration c vanishes at the end of the reactor and that becomes our second boundary condition. So, what I have shown in the white color is what we had solved in the previous module. What I am showing in the pink color along with the original equation that is what the problem is we are going to solve in this particular module.

So, I believe the values that we had taken in the previous module were k by v was 1 by 2 and d by v , we can take it as 1 by 200. So, what I mean by that is substituting the values, we can have this as $d^2 c$ by dx^2 equal to minus c to the power 1.25 by 2 plus 1 by 200

multiplied by c double dash. So, that would be the example and $c(0)$ that we had taken in that example was $c(0)$ equal to one. So, what we will do is we will take c to the power 1.25 by 2 on to the left hand side and we will multiply throughout by 200.

(Refer Slide Time: 05:08)

$$\frac{d^2c}{dx^2} = 200 \frac{dc}{dx} + 100 c^{1.25}$$

$$c(0) = 1$$

$$c'(L) = 0$$

$y = c ; z = \frac{dc}{dx}$

\downarrow

$\frac{dy}{dx} = z$, $\frac{dz}{dx} = 200z + 100 y^{1.25}$

$y(0) = 1 ; z(0) = \text{guess}$

\downarrow TO ARRIVE AT c

$c'(L) = 0$

$z(L) = 0$

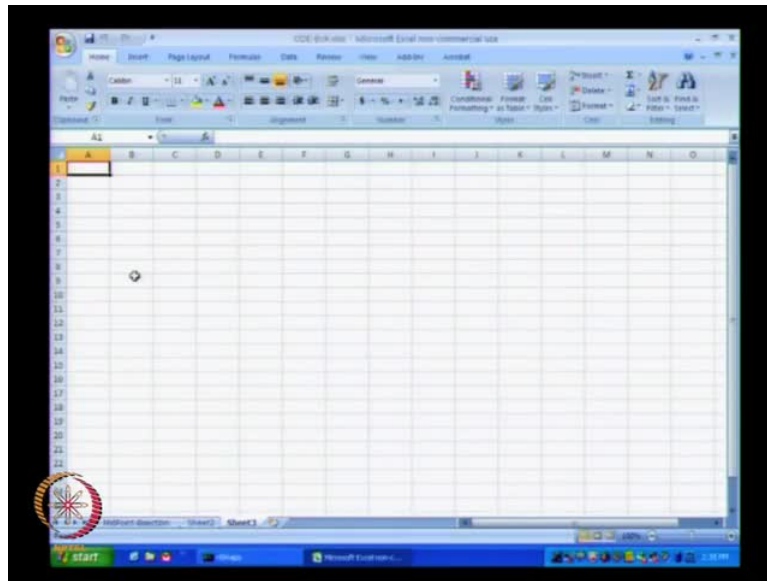
So, we will get the equation of the form d^2c by dx^2 is going to be equal to 200 times dc by dx plus 100 times c to the power 1.25 and this will be subject to the condition c at 0 equal to 1, and c dash at L equal to 0. This is the problem that we intend to solve. As we had done before, we will write y equal to c , and z equal to dc by dx , which will result in two ODEs; the first ODE, **sorry dc by dx , not dz** (Refer Slide Time: 05:55). This will result in two ODEs. The first ODE is going to be dy by dx is going to be equal to z and the second ODE is obtained from over here and that is going to be dz by dx is going to be equal to 200 times dc by dx , which is 200 z plus 100 multiplied by y to the power 1.25.

So, these are going to be our two ODEs: ODE number one, ODE number two, which we are going to solve using our initial condition $c(0)$ equal to 1, and our c dash 0 equal to a guess value. This is going to be our initial value problem that we are going to solve, such that we finally, meet the boundary condition. To arrive at the boundary condition c dash at L equal to 0. So, c at 0 equal to 1, I am going to replace as $y(0)$ equal to 1, c dash 0 equal to guess, I am going to replace that as **$y(0)$. Sorry, not y zero but, z zero** (Refer Slide

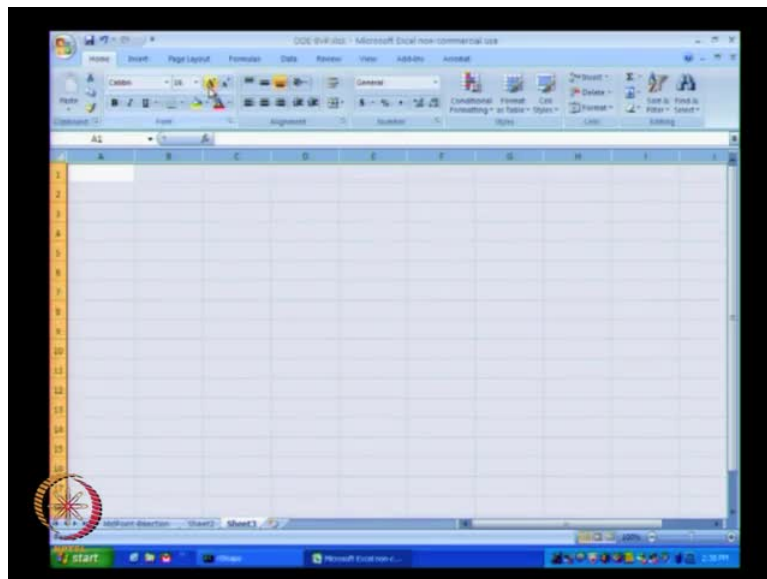
Time: 07:25) equal to guess. We are going to shoot such that we arrive at the boundary condition z at L equal to 0.

So this is the problem that we are going to try to solve using Microsoft excel. Basically, what I want to show you is how this particular way of solving this problem could lead to certain issues that we need to be aware of.

(Refer Slide Time: 08:13)

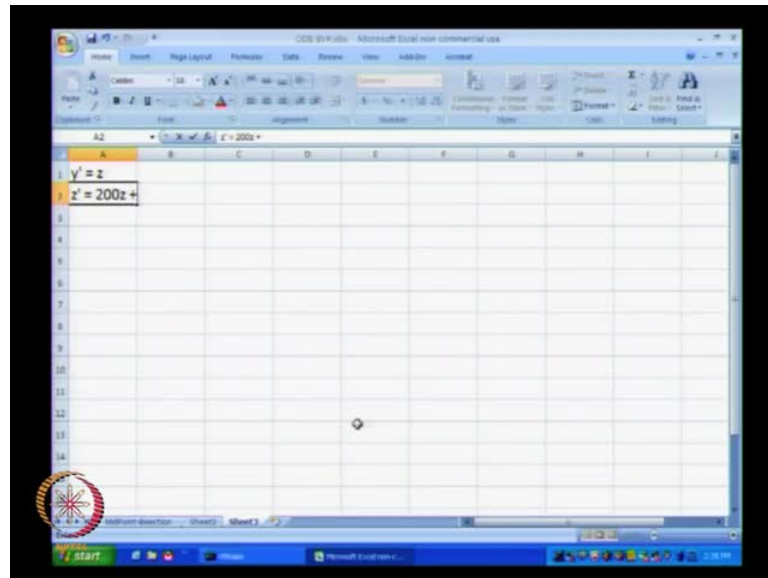


(Refer Slide Time: 08:16)

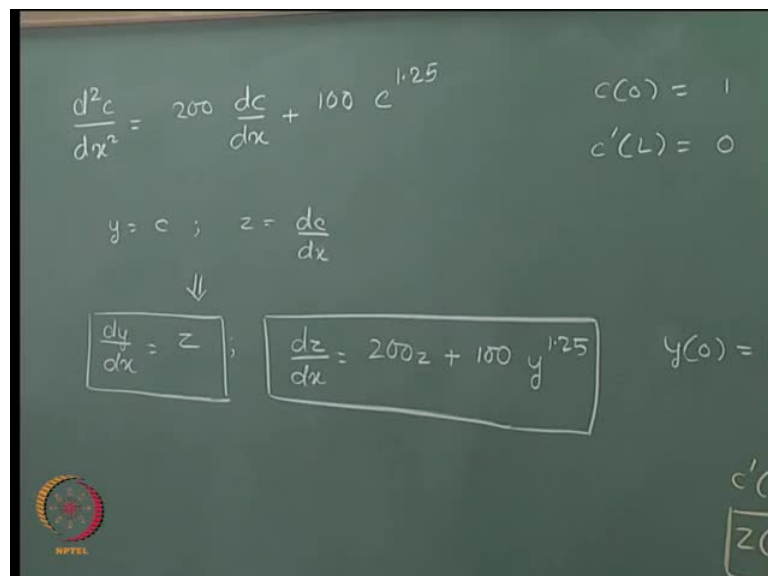


So, let us create a new problem, new spread sheet, where we are going to solve this particular problem. Let us go to a new sheet, **sorry** and what we are going to do is solve the problem that I just showed on the board. We will increase the size of font size and all those we will increase.

(Refer Slide Time: 08:31)

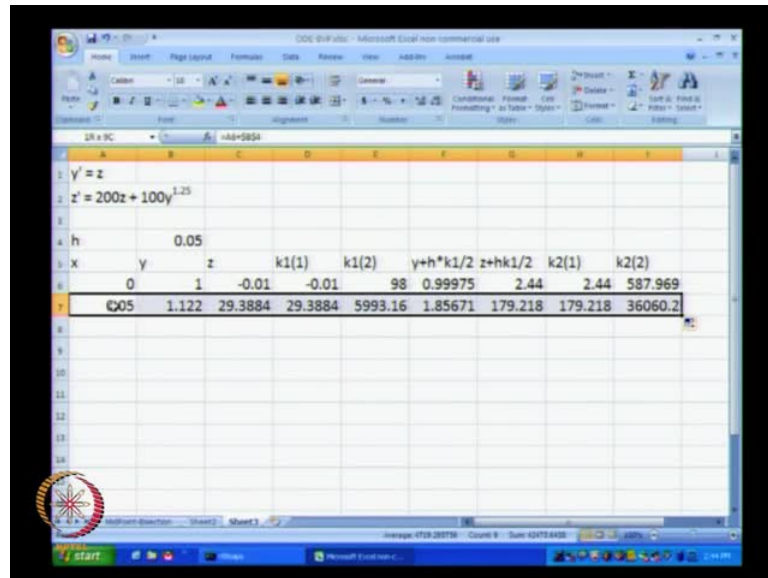


(Refer Slide Time: 08:52)



So, let us try to solve the problem the problem that we wanted to solve we would write that as y dash equal to z and z dash is going to be equal to 200 z plus 100 y to the power 1.25.

(Refer Slide Time: 08:58)



So, I will just do format cells, and I will just beautify it little bit. So, this is the problem that we are going to solve with the initial values, y_0 equal to 0, and let us try certain other initial value. We will try that for a bunch of initial values and see what happens.

We will choose our h less, choose our h as 0.01 as we did previously, or let us choose it as 0.05, let us say. And x we are going to start with 0 and over x_{i+1} , is going to be equal to the previous x plus h . I will do function f_2 and put dollar signs over there so that we are fine. Now, we require y and we require z , y is known to us, the initial y is 1. Let us say initial z is going to be minus 0.01, which is what z we are going to start off with. Now, y' is equal to z , so we will have k_{11} , it is just going to be equal to z ; y' is equal to z , k_{12} is going to be equal to 200 multiplied by z plus 100 multiplied by y to the power 1.25.

That is going to be our k_2 . 200 multiplied by z , plus 100 multiplied by y to the power 1.25. Next, we want y plus $k_{11}h$ by 2. So, y plus h multiplied by k_{11} by 2, and we want z plus h k_{12} by 2. So, this is essentially what we want and so that is going to be equal to y plus and again this is what we have done in the previous lecture of this module also. So we have y plus h multiplied by k_{11} , divided by 2 and I press f_2 over here, and edit this by putting dollar sign, so that when I drag and drop our h value does not change. This I can just drag it to z plus h k_{12} by 2 and I will press f_2 to figure out that is indeed we have z , so that is c_6 plus h multiplied by k_{12} multiplied by k_{12} divided by 2.

So, we will just drag this, until we think it should be enough. So, that is x equal to 1 and let us just go down. And so let us do this up to x equal to 2, let us not even go up to 10. That is enough for me to show you what the problems are. So, let us say, we choose the value of z equal to minus 0.01, and quickly you will see that this particular method is diverging. This, why we get this as an error over here, is because the number that we would get over here based on the numerical value should be infinity.

Let us try another value z equal to 0. We will see the same problem. Let us try z equal to 5 and we will see the same problem. So, let us say z equal to 0, we will see that after about 1.2 meters of length, we get the concentration predicted as infinity. Now, if z let us say we increase it to 5, which is not a correct value, because of reaction the concentration should be decreasing but, if you go and check again, we have this guy as going to a very large value again.

So, what that means is basically if our initial guesses are not in the correct ballpark or not in the correct direction, there is no way for the method that we are going to follow, the shooting method to really figure out that this is the wrong steps that we are trying to take, and there is no way that one could recover from these type of errors, simply because the method has not converged and indeed it has diverged.

So, what we need is z should be the fairly large negative value, so let us try to make this value as minus ten, and if we make this value of as minus ten, our y value becomes negative. So, immediately our k_1 becomes **square root of** we are trying to take a square root of a negative number and therefore, it does not work. So, maybe we have gone too negative, so let us try to go to say minus 5. Minus 5, also does not work, because this value immediately has got a negative. Let us say minus 2, see how it works. Minus 2, well this value sounds reasonable but, this value has immediately gone negative again minus 2 is not working.

So, let us try minus 1.5. Again, we have the same point type of problem. Let us try minus 1; again we have a problem, after the second iteration. Let us try minus 0.5 and with minus 0.5 it work for two iterations but, it did not work beyond this two iterations.

(Refer Slide Time: 17:15)

x	y	z	k1(1)	k1(2)	y+h*k1/2	z+hk1/2	k2(1)	k2(2)	
0	1	-0.5	-0.5	-0.5	0	0.9875	-0.5	-0.5	-1.56005
0.05	0.975	-0.578	-0.578	-18.7157	0.96055	-1.04589	-1.04589	-114.086	
0.1	0.92271	-6.28228	-6.28228	-1166.02	0.76565	-35.4329	-35.4329	-7014.95	
0.15	-0.84894	-357.03	-357.03	#NUM!	-9.77469	#NUM!	#NUM!	#NUM!	
0.2	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.25	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.3	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.35	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.4	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.45	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.5	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.55	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	
0.6	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	#NUM!	

So, what I am trying to show over here is we take smaller and smaller values and still now with minus 4 we are going to infinity, but with minus 5, if we see, with minus 0.4 we are going to infinity, but minus 0.5 we are going to a square root of a negative number and the method cannot continue. So, this is one of the biggest problems with the shooting method, is that it is a method that is often times it fails in order to converge.

The initial value problem that we can get through a shooting method, the initial value problem itself may not be solvable. The reason that initial value problem may not be solvable is because the eigen values of the problem that we will end up with, might either one of the eigen values or multiple of these eigen values might be positive, which basically means, once we start off with a solution that solution is going to diverge and at certain point that solution is going to diverge too infinity or minus infinity.

Unless, we can get a solution or we can guarantee a solution of an initial value problem, we will not be able to proceed with the shooting method. This is not actually limited to just this particular problem that I showed you, it is not just limited to the axial dispersion problem. This type of problems does happen. For example, in the heat conduction problem, if we add up say a heat generation term. Let us say there is some kind of a heat generation, because of electrical heating at the center of the rod or something like that. Some of those heat generation term themselves might lead to the same type of instability that we saw with the reactor.

Likewise, if there is a radiation within this particular system, the radiation problem itself has certain amount nonlinearities associated with t to the power 4 terms. Those radiation nonlinearities are also going to cause some problems with the shooting method. So, the overall crux of the matter is that while shooting method is indeed going to work in certain specific examples, shooting method does not work in certain other examples.

The method of analysis that we took up in the ODE initial value problem in the previous module that is the method of analysis that you need to choose in order to figure out whether the ODE initial value problem is going to converge or not. Typically, the problem in shooting method happens because of the ODE initial value problem not converging. Usually, if the ODE initial value problems are going to converge to certain solutions, then we can actually get the algebraic equations part to converge.

For example, we can use a bisection method, which is guaranteed to converge, or even the Newton-Raphson's method or Fixed point iteration type of a method, if we are going to use. Those problems tend to be often well behaved that we can indeed go ahead and use the shooting method. So that is all I have to say about the shooting method. Now, let us go to the second method that we talked about using the finite differences and we will take up an example of using the finite differences after I show how to use the finite differences on the board.

(Refer Slide Time: 20:21)

$$\frac{d^2 T}{dx^2} = \beta (T - 30) \quad T(0) = 30 \quad T(L) = 30$$

DOMAIN EQUATIONS (at Node "i")

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} = 0.01 [T_i - 30]$$

$$\frac{1}{\Delta x^2} T_{i-1} - \left[\frac{2}{(\Delta x)^2} + 0.01 \right] T_i + \frac{1}{(\Delta x)^2} T_{i+1} = -3 \quad \text{for } i=2 \text{ to } n$$

At $i=1$ $T_1 = 30$ $T_{n+1} = 30$

So, we had started we had introduced ourselves to using the finite difference method for the heat conduction problem. The heat conduction problem, if we stated again was $d^2 T / dx^2 = \beta (T - 30)$, where β value was equal to 0.01. So, that was the problem that we wanted to solve with the boundary conditions $T_0 = 30$, and $T_2 = 80$. So, we have a 2 meter long rod. Now, this 2 meter long rod, we are going to divide it into n intervals. These are going to be n equally spaced intervals, so we will call this node as 1, this node as 2, this node as 2, and so on up to n th node and $n + 1$ th node.

We are going to write all the domain equations for all of these nodes, and the boundary equations for node number 1, and node number $n + 1$. As we had seen, because we have Dirichlet type of boundary conditions, we do not need any ghost point method. We can only go with the usual method of solving that is have the domain conditions for the nodes 2 to n and boundary conditions for the node 1 and $n + 1$. So, the domain conditions or rather the domain equations for node i , is going to be now $d^2 T / dx^2 = \beta (T_i - 30)$. We will be able to write that as $T_{i+1} - 2T_i + T_{i-1} = \beta \Delta x^2 (T_i - 30)$.

So, we are going to take a 0.01 multiplied by T_i on to the left hand side and finally, we are going to get $T_{i+1} - 2T_i + T_{i-1} = \beta \Delta x^2 (T_i - 30)$. And this equation is going to be true for $i = 2$ to n . And for $i = 1$, the equation that we are going to have is $T_1 = 30$, because T_1 is nothing but, T at the initial point, we have a Neumann boundary condition.

So, $T_1 = 30$ is one equation and the final equation is $T_{n+1} = 80$. Now, we have 2 to n that means there are $n - 1$ equation over here. 1 and 2 equations over here, so there are total $n - 1 + 2$, which is $n + 1$ equations; $n + 1$ equation and $n + 1$ unknowns. These are linear equations and we can solve them using the Tridiagonal matrix algorithm that we had looked at in the linear algebra course.

(Refer Slide Time: 24:48)

$$\begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_n \\ T_{n+1} \end{bmatrix} = \begin{bmatrix} 30 \end{bmatrix}$$

Now, if we were to write this in the tridiagonal form, what we get is basically let us just try to write this overall equation in the form of a x equal to b and continue writing this. Now, the x bar is going to be nothing but, T 1, T 2 and so on up to T n and T n plus 1 equal to b bar. The first equation we said was T 1 equal to 30, which was our first equation. So, with the equation T 1 equal to 30, we will write it as one multiplied by T 1 plus 0 multiplied by T 2, plus 0 multiplied by T 3, and so on up to 0 multiplied by T n and 0 multiplied by T n plus 1 equal to 30. So, that is going to be the first row.

(Refer Slide Time: 25:43)

$$\frac{d^2 T}{dx^2} = \beta (T - 30) \quad T(0) = 30 \quad T(L) = 30$$

DOMAIN EQUATIONS (at Node "i")

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{(\Delta x)^2} = 0.01 [T_i - 30]$$

$$\frac{1}{\Delta x^2} T_{i-1} - \left[\frac{2}{(\Delta x)^2} + 0.01 \right] T_i + \frac{1}{(\Delta x)^2} T_{i+1} = -3 \quad \text{for } i=2 \text{ to } n$$

At $i=1$ $T_1 = 30$ $T_{n+1} = 30$

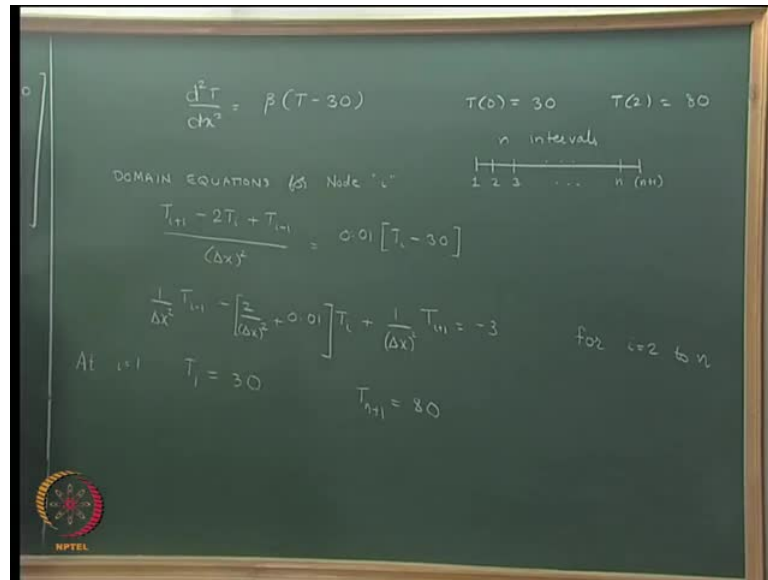
The second row we had 1 by Δx squared T_i minus 1 . So, that is going to be. So, in the second row, if we look at this particular equation, in the second row what we will have is i equal to 2 . So, this becomes T_1 , this is T_2 and this is T_3 . So, the coefficient of T_1 is 1 by Δx squared, coefficient of T_2 is -2 by Δx square plus 0.01 , the coefficient of T_3 is Δx squared and all other coefficients are 0 .

(Refer Slide Time: 26:11)

$$\begin{bmatrix}
 1 & 0 & 0 & \dots & 0 & 0 \\
 \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} + 0.01 & \frac{1}{\Delta x^2} & \dots & 0 & 0 \\
 0 & \dots & \dots & \dots & \dots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & \dots & \dots & 0 \\
 0 & \dots & \dots & \dots & \dots & 0
 \end{bmatrix}
 \begin{bmatrix}
 T_1 \\
 T_2 \\
 \vdots \\
 T_n \\
 T_{n+1}
 \end{bmatrix}
 =
 \begin{bmatrix}
 30 \\
 \vdots \\
 \vdots \\
 \vdots \\
 \vdots
 \end{bmatrix}$$

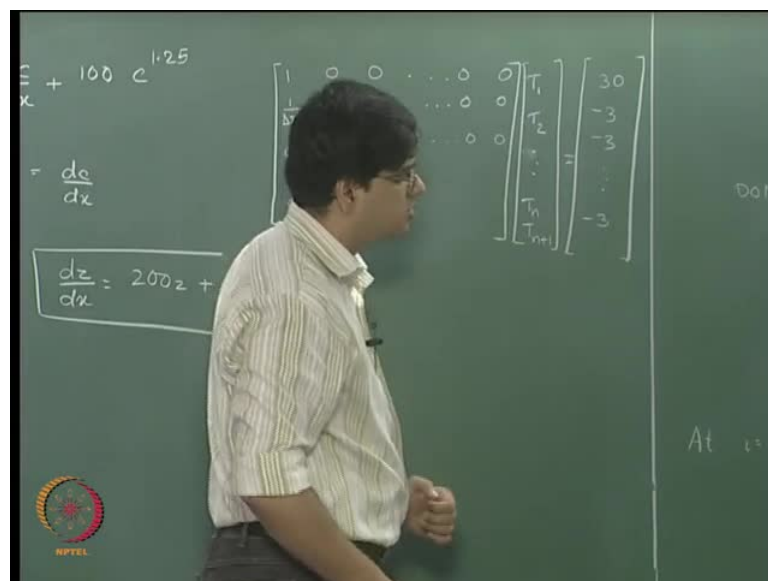
So, we will write that down over here. It is 1 by Δx squared is the coefficient for T_1 . The coefficient for T_2 is -2 by Δx squared minus 0.01 . That is the coefficient for T_2 . The coefficient for T_3 is again 1 by Δx squared and everything else is 0 that is what we will get in the second row. Likewise, in the third row, we will have 0 , we will have 1 by Δx square over here, -2 by Δx square, -0.01 over here, 1 by Δx square over here and rest everything would be 0 .

(Refer Slide Time: 26:54)

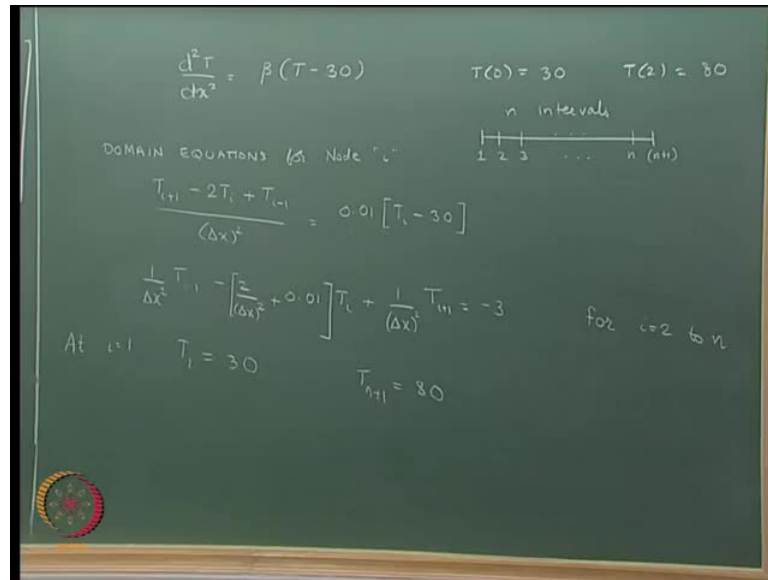


Let us go back to the equations and this is all going to follow for all of those rows and let us look at what we are going to get at the nth row. In the nth row that means where i equal to n, we will have a coefficient for T n minus one. We will have a coefficient for T n; we will have a coefficient for T n plus 1. All other coefficients are going to be 0 and the value on for the right hand side b is going to be minus 3.

(Refer Slide Time: 27:23)

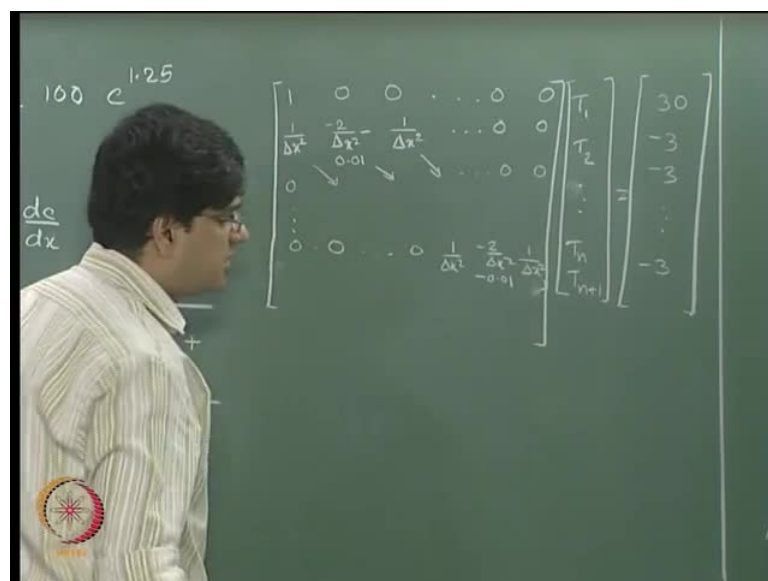


(Refer Slide Time: 27:47)

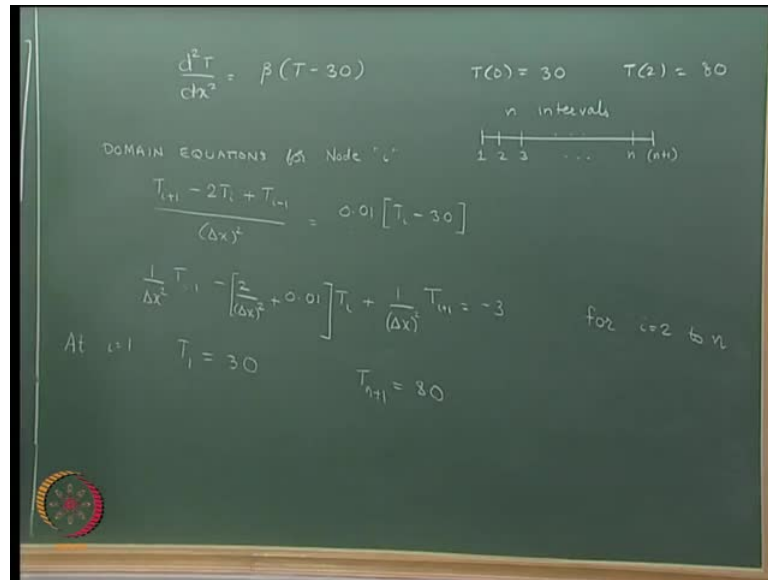


So, also in the previous examples, we will have the value as minus 3 in all of the rows from 2 to n. So, what we said is going to be happen in the row n, is going to be that we are going to have 0 initially, and we will have non-zero terms for T n minus 1. We will have a non-zero term for T n, and we will have a non-zero term for T n plus 1. These non zero terms correspond to T n minus 1. This is the term for T n and this is the term for T n plus 1.

(Refer Slide Time: 27:58)

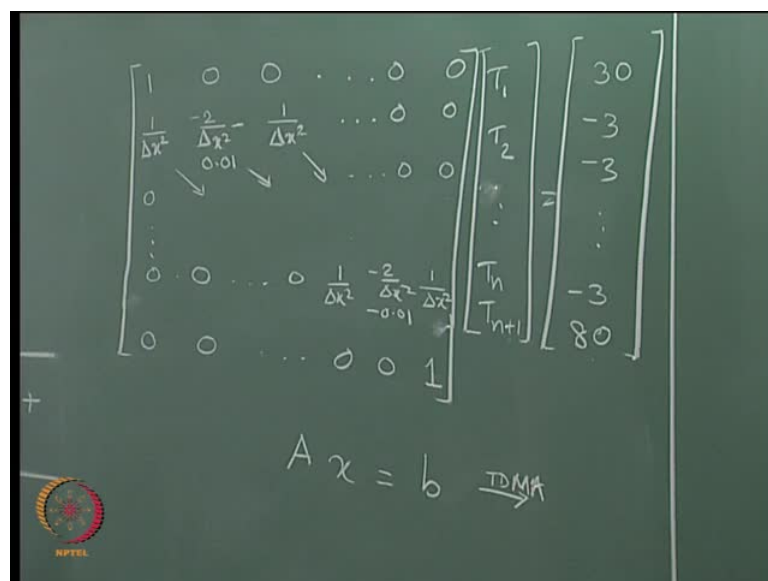


(Refer Slide Time: 28:33)



So, if we notice, it is exactly the same term that is going to repeat. It is 1 by delta x squared minus 2 by delta x squared minus 0.01 and 1 by delta x squared. So, I will just write the last two terms over here; minus 2 by delta x squared minus 0.01, and over here again we have 1 by delta x squared, and everything else is zeros. The last row is going to correspond to the boundary condition and the last boundary condition if we look at it is 1 multiplied by T n plus 1 equal to 80.

(Refer Slide Time: 28:41)

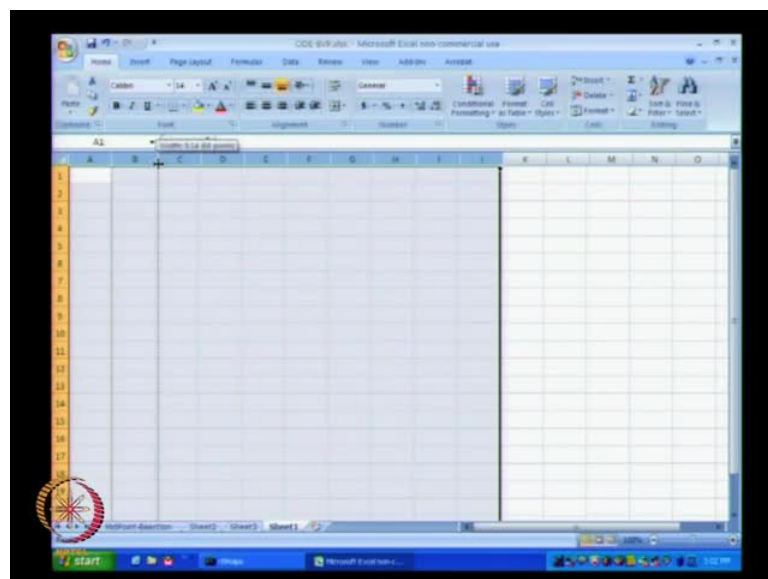


So, we substitute that over here and we will get everything else is going to be zeros and we will have 1 over here. So, 1 multiplied by T_{n+1} is going to be equal to 80. So, to recap for this particular example, what we have is the first row has one corresponding to the T_1 term and zeros everywhere. So, we will have T_1 plus 0, plus 0, plus 0, is going to be equal to 30. So, T_1 equal to 30 is our first equation. Our last equation is we have 0 multiplied by T_1 plus 0 multiplied by T_2 , bla bla bla so, plus 1 multiplied by T_{n+1} .

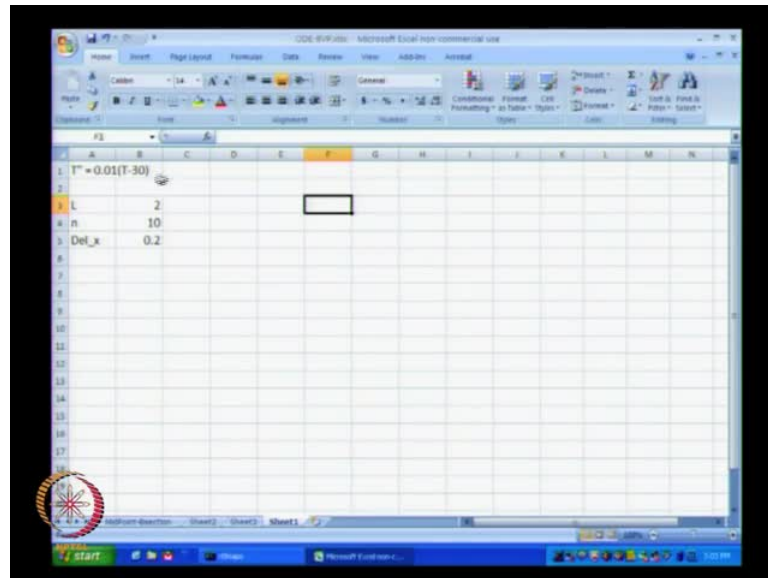
So, our last equation is going to be T_{n+1} equal to 80, and all the middle equations are going to be $1 \times \Delta x^2 \times (i-1) - 2 \times \Delta x^2 \times i + 1 \times \Delta x^2 \times (i+1)$. So, that becomes our matrix A. This is our matrix X and this becomes our matrix b, and we can solve this particular module using the tridiagonal matrix algorithm or any of the other methods that we saw in the linear algebra part of the course.

So, what I am going to do next is go on to the Microsoft excel and show how this particular problem can be solved. I am not going to use the tridiagonal matrix algorithm but, I will use the matrix inversion method that Microsoft excel provides us. So, that is what I am going to do but, the way it will be solved, way this problem would be solved in any kind of a computer implementation of this is indeed to exploit the structure of the tridiagonal matrix that we end up with and we exploit that structure and we get that overall solution, using the T D M A algorithm.

(Refer Slide Time: 30:40)

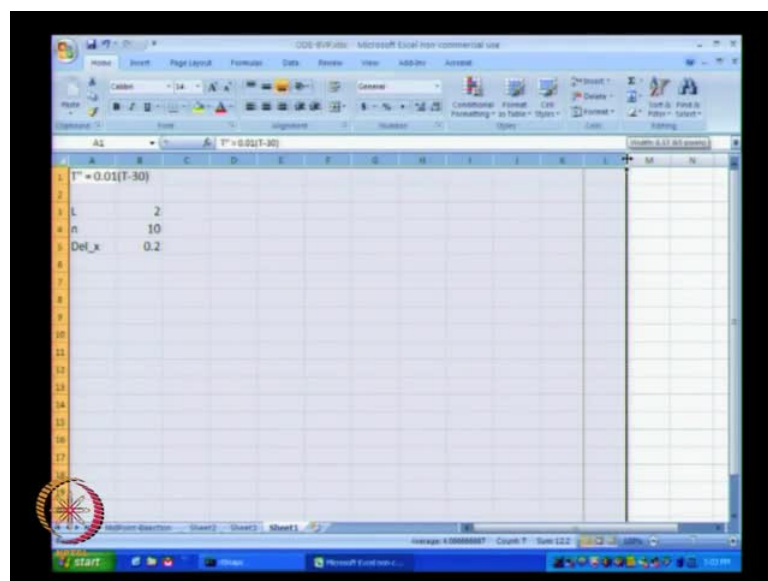


(Refer Slide Time: 30:55)



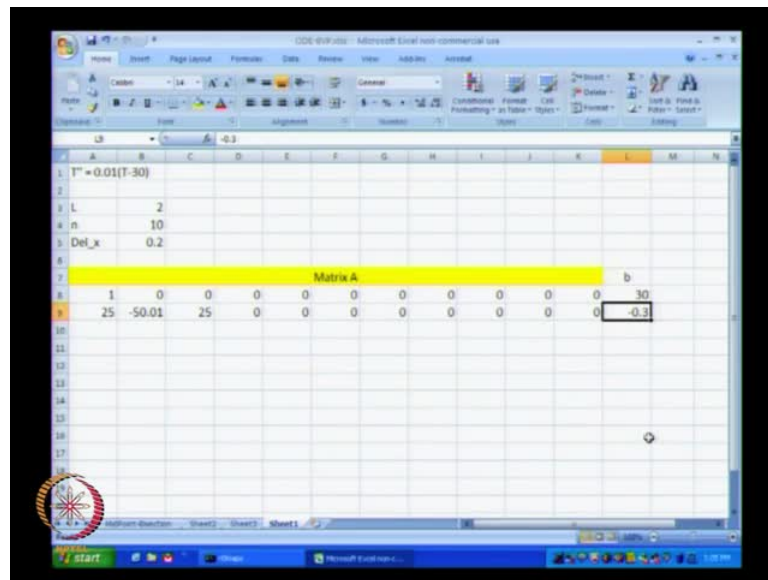
So, let us go to Microsoft excel and try to solve this problem. We will try to solve the same problem again. (No audio between: 30:44-30:55) So, the problem that we are trying to solve is $T'' = 0.01(T-30)$. This is the problem that we are going to solve. We will first define our length and that goes from 0 to 2. So, our length is going to be 2. Our number of steps that we are going to take as n. let us defined this as 10 and our delta x or del x is going to be equal to length divided by n.

(Refer Slide Time: 32:07)



So, those are the parameters for solving this particular problem, using the tridiagonal matrix algorithm. When we say that we have n equal to 10, basically means that the matrix A is 11 by 11 dimensional matrix and matrix b will be another 11 by 1 dimensional vector.

(Refer Slide Time: 32:20)



So, we will need all of them. So, let us just go and increase the font sizes. So, this is what we have. So, the 11 rows are going to represent the matrix A, so I will just merge them. Matrix A and this is going to represent our vector b. And the matrix A will have 11 rows. As we had seen the first row is 1 multiplied by T 1 plus 0 multiplied by T 2 and so on and so forth. So, we will put zeros everywhere else, is going to be equal to 30. That was our initial condition.

Let us look at what the next condition was. It is 1 by delta x squared so it is going to be 1 divided by del x squared. That is going to be this value. The next value is going to be minus 2 divided by del x squared minus 0.01. recall, what we had written over here, the minus 2 divided by del x square comes in because of the T double dash term and minus 0.01 comes in because of 0.01 multiplied by T is taken to the left hand side.

That is what we get and this is the value that we are going to get over here. And this term is going to be 1 divided by delta x squared again, because that is the coefficient that multiplies T i plus 1, and then we have 0 0 0 0 0 0 and 0, and the b value that we had is

what is left on to the right hand side. So, if you look at this expression, what this T once we take to the left hand side, the thing that is the left on the right hand side is 0.01 multiplied by minus 30 that is equal to minus 0.3.

(Refer Slide Time: 34:33)

$$\begin{bmatrix}
 1 & 0 & 0 & \dots & 0 & 0 \\
 \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x^2} & \dots & 0 & 0 \\
 0 & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \dots & 0 & 0 \\
 \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
 0 & 0 & \dots & 0 & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x^2} \\
 0 & 0 & \dots & 0 & 0 & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x^2} & 1
 \end{bmatrix}
 \begin{bmatrix}
 T_1 \\
 T_2 \\
 \vdots \\
 T_n \\
 T_{n+1}
 \end{bmatrix}
 =
 \begin{bmatrix}
 30 \\
 -3 \\
 -3 \\
 \vdots \\
 -3 \\
 80
 \end{bmatrix}$$

$Ax = b$ TDM

(Refer Slide Time: 34:41)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
2														
10														
Del_x		0.2												
	Matrix A											b		
1	1	0	0	0	0	0	0	0	0	0	0	0	0	30
25	-50.01	25	0	0	0	0	0	0	0	0	0	0	0	-0.3
0	25	-50.01	25	0	0	0	0	0	0	0	0	0	0	-0.3
0	0	25	-50.01	25	0	0	0	0	0	0	0	0	0	-0.3
0	0	0	25	-50.01	25	0	0	0	0	0	0	0	0	-0.3
0	0	0	0	25	-50.01	25	0	0	0	0	0	0	0	-0.3
0	0	0	0	0	25	-50.01	25	0	0	0	0	0	0	-0.3
0	0	0	0	0	0	25	-50.01	25	0	0	0	0	0	-0.3
0	0	0	0	0	0	0	25	-50.01	25	0	0	0	0	-0.3
0	0	0	0	0	0	0	0	25	-50.01	25	0	0	0	-0.3
0	0	0	0	0	0	0	0	0	25	-50.01	25	0	0	-0.3
0	0	0	0	0	0	0	0	0	0	25	-50.01	25	0	-0.3
0	0	0	0	0	0	0	0	0	0	0	0	1	80	

So, that is what we will have left on to the right hand side and I think while writing on the board I had made a mistake on the right hand side (Refer Slide Time: 34:37), I had written all of those values as 3. Actually, they should not be 3; they should be 0.3, because it corresponds to 0.01 multiplied by 30, which is 0.3. Now, the third row

concerns the equation for T 3. The equation for T 3 is 1 by delta x squared multiplied by T 2. So, that is going to be equal to 1 by delta x squared multiplied by T 2 minus 2, by delta x squared equal to minus 2, by delta x squared minus 0.01 multiplied by T 3, and same 1 by delta x squared multiplied by T 4.

So, what we had is T double dash was 1 by delta x squared, multiplied by T 2 minus 2, by delta x squared multiplied by T 3 plus 1, by delta x squared multiplied by T 4. Then when we took this **minus** where 0.01 T on to the left hand side, we got this as 2 by delta x squared minus 0.01, minus 2 by delta x square minus 0.01. Rest everything else is 0, so we will just put 0 over here, 0, 0, 0, 0, 0, 0, 0 and 0, and this should be minus 0.3. That is what we will get. Now, a pattern emerges. What is happening is that if you look at the three diagonals those three diagonals tend to be equal.

Whatever, values that we are going to get along these particular diagonals, are going to equal, because those values are not changing with the equation. So, this is going to be equal to the value on the previous row and previous column and we can just copy it throughout the entire thing, and this should be fine. So, 25, 25, 25 is repeated again, 25 will be repeated at the bottom, so on and so forth. This value will be equal to 0 and this guy is going to be equal to minus 0.3. So, that is going to be our fourth row, and this will repeat up to the tenth row, nth row, where n equal to 10 so forth. Then it will repeat for the fifth, sixth, seventh, eighth, ninth and tenth row.

This is an incorrect thing. So, this should be equal to **0, sorry**. So, the first row should be equal to zero all throughout, and this is what we are doing just drag and drop. So, this is the fourth row, fifth, sixth, seventh, eighth, ninth and tenth. So, we will drag it down up to the tenth row, and this is what we get and we will check those values again and minus 0.3. So, these are the first 10 rows and we need also the eleventh row, corresponding to n plus 1 but, let us check the tenth row. The tenth row is for the temperature T 10, so we have 0 multiplied by T 1, plus 0 multiplied by T 2, and so on, up to 0 multiplied by **T 9 T 8**, plus 1 by delta x squared multiplied by T 9, minus 2 by delta x squared plus 0.01 multiplied by T 10, plus 1 by delta x squared multiplied by T 11. That is going to be equal to minus 0.3.

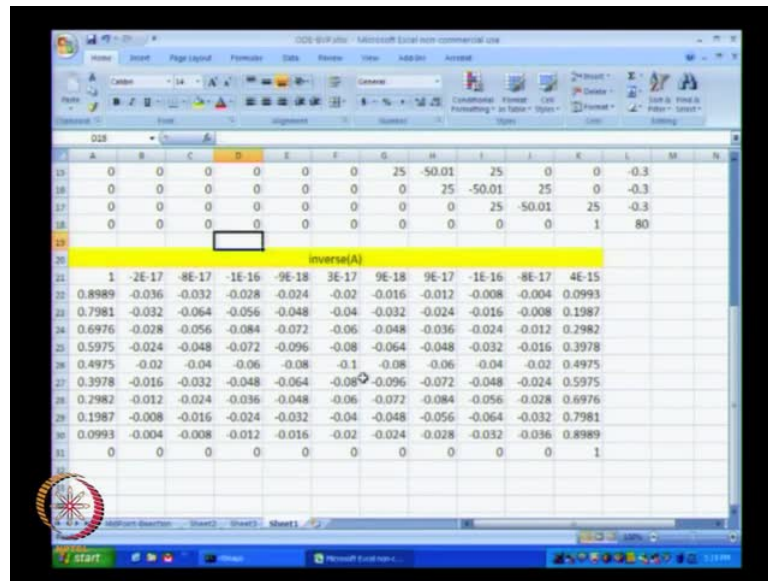
(Refer Slide Time: 34:41)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	L	2												
4	n	10												
5	Del_x	0.2												
7	Matrix A										b			
8	1	0	0	0	0	0	0	0	0	0	0	0	0	30
9	25	-50.01	25	0	0	0	0	0	0	0	0	0	0	-0.3
10	0	25	-50.01	25	0	0	0	0	0	0	0	0	0	-0.3
11	0	0	25	-50.01	25	0	0	0	0	0	0	0	0	-0.3
12	0	0	0	25	-50.01	25	0	0	0	0	0	0	0	-0.3
13	0	0	0	0	25	-50.01	25	0	0	0	0	0	0	-0.3
14	0	0	0	0	0	25	-50.01	25	0	0	0	0	0	-0.3
15	0	0	0	0	0	0	25	-50.01	25	0	0	0	0	-0.3
16	0	0	0	0	0	0	0	25	-50.01	25	0	0	0	-0.3
17	0	0	0	0	0	0	0	0	25	-50.01	25	0	0	-0.3
18	0	0	0	0	0	0	0	0	0	25	-50.01	25	0	-0.3
19	0	0	0	0	0	0	0	0	0	0	0	0	1	80

And the last row is going to have zeros everywhere except the last element, where we are going to have one over here. So, this represents T_{11} equal to 80 degrees. So, this is what we are going to get. So, that is matrix A; this is vector b. Now, what we need to do is invert the matrix. So, I will have this particular row where I will call this is as inverse of matrix A. Now that we have constructed matrix A and we have constructed the vector b. Just give me a minute or so I will just recap. Sorry about that so, we cut the last four minutes and we re-shoot from here, so I will go on for nine more minutes from now.

Now, that we have matrix A and our vector b, that we have obtained for this particular system, lets now go ahead and calculate the inverse of matrix A. Again, when you are trying to solve this particular problem using a numerical technique, it is for this particular problem, where we have a tridiagonal system of equations, it is not computationally sound method to calculate the inverse and then calculate x. Simply, because we can exploit the structure of a tridiagonal matrix, in order to calculate the value of x, the solution x that we are going to get from the system. However, because we do not want to go into using a tridiagonal matrix algorithm, instead of that I will just use matrix inverse in order to solve this problem.

(Refer Slide Time: 40:31)



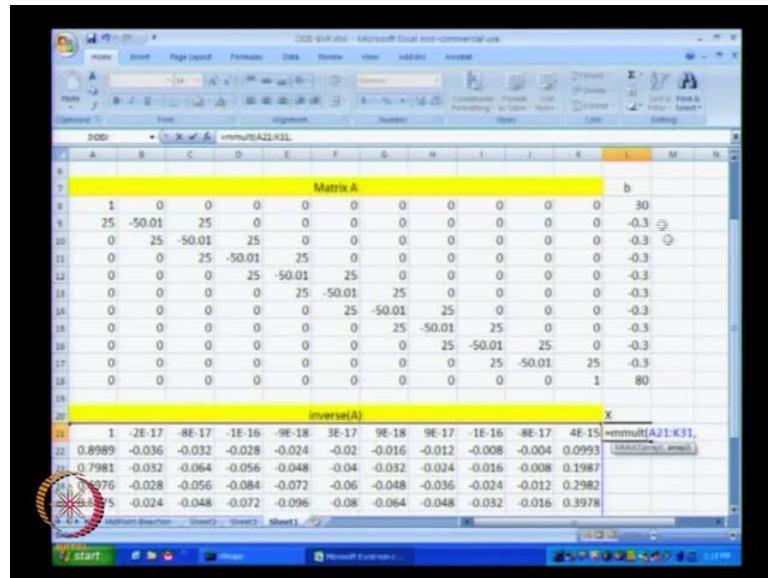
So, what I will do is in the next 11 rows, I am going to compute the inverse of the matrix over there. So, equal to m inverse and we choose the entire 11 by 11 array. When we choose this array, just to the right hand bottom of the choice of that array, you will see a small thing that will popup which says 11 r cross 11 c. That means that right now I have chosen an 11 by 11 array, 11 rows and 11 column arrays.

So, I will just complete the bracket and press enter. Now, what I have is the inverse is computed in one of these rows, and we want to one row and one column and what we want to do is copy this as a matrix inverse for the entire 11 rows and 11 columns. So, I will now select 11 columns. This is the first row; second, third, fourth, fifth, sixth, seventh eight, nine, ten and eleven. So, now I have chosen 11 rows and 11 columns, and now I want to copy this as a matrix inverse. So, at this stage I will press f 2 and control shift and enter. Remember, this is what we had done earlier, control shift enter is going to do a matrix computation in this particular row.

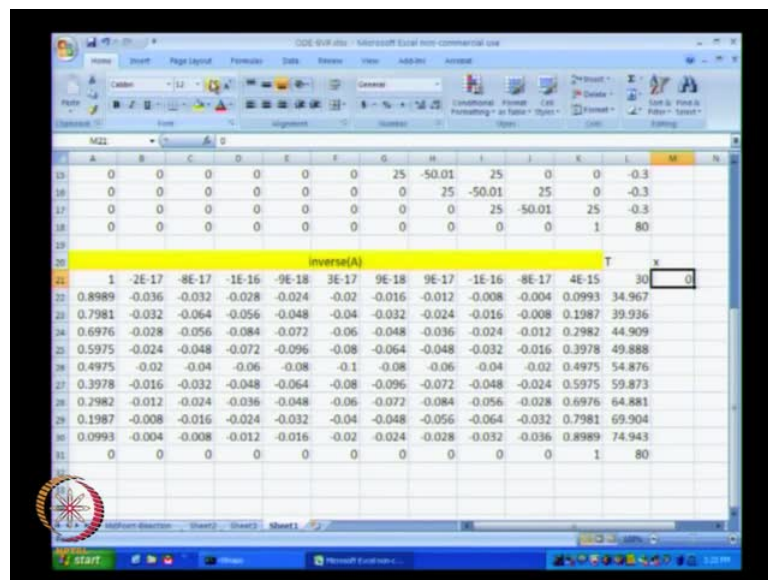
And if you go and press f 2 at any of the row and column within that system, what you will see is that it has copied m inverse A 8 to K 18 over here, and **when you go to the first...** When you look at the actual formula, you will have this A 8 to K 18 put inside these curly braces. What these curly braces actually signify is that it is actually a matrix inverse and it is not just a simple formula. With this matrix inverse, we can now calculate our solution x , our T matrix. So, x is going to be equal to inverse of A

multiplied by b and that we can do by doing m mult; m mult is a matrix multiplication where we required two arrays array 1 and array 2.

(Refer Slide Time: 43:04)

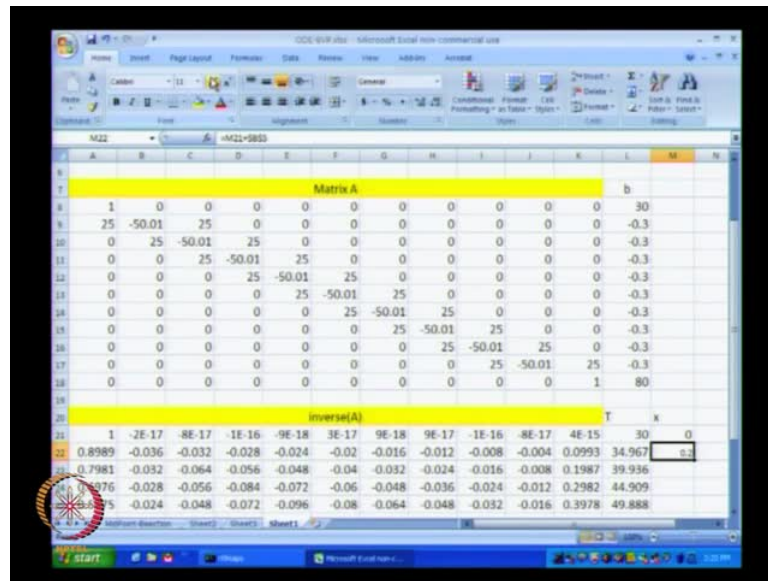


(Refer Slide Time: 43:12)



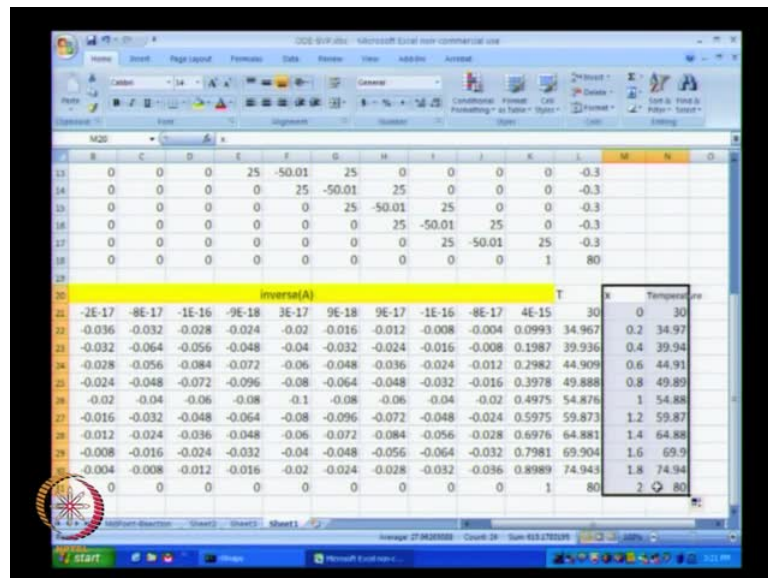
Array 1, we are going to give as the first array over here, comma array 2 is nothing but, the vector b. So, we will just choose the vector b over here, and then close the bracket. That should give us the x and this x, we need to again. We cannot copy, paste this x. What we need to do is we need to select the 11 dimensional vector, press f 2 and then press control, shift and enter and this will give us the overall temperature.

(Refer Slide Time: 43:59)



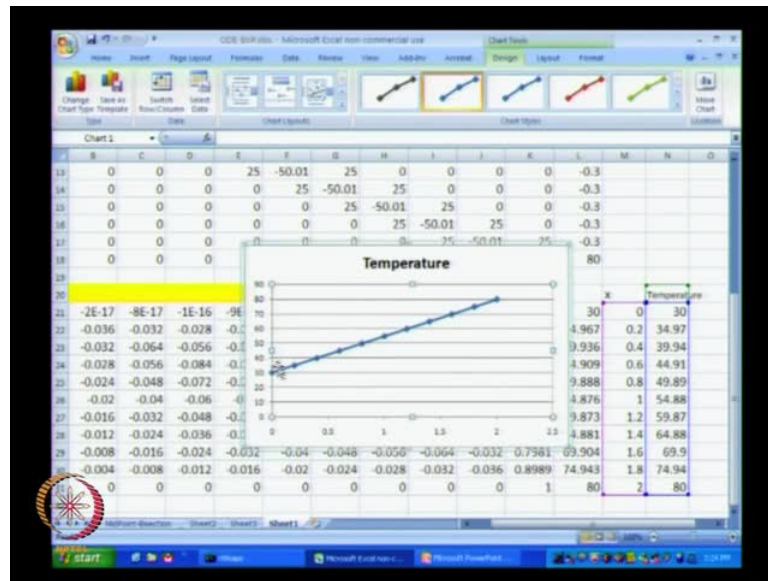
So, I will call rather than calling it x, I will call this as T and I will have another vector called x, which is going to represent the locations. This location is going to start with x equal to 0 and the next one is going to be previous guy plus h or plus delta x and press f 2, put dollar signs and that should be the trick, and I will copy paste it.

(Refer Slide Time: 44:18)

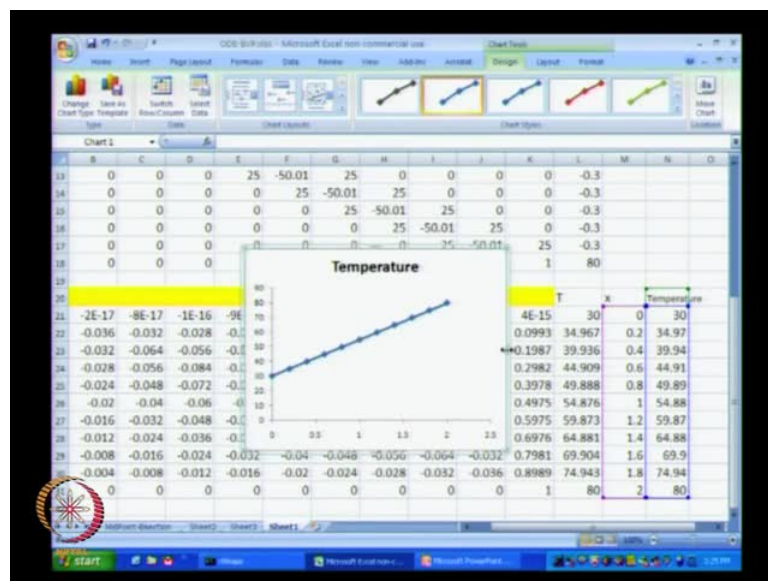


So, this is our x and the temperature I will just copy it again, once again. So, that I can then plot it easily, temperature equal to this guy and we will plot temperature against x by going to insert and inserting a scatter plot.

(Refer Slide Time: 44:48)

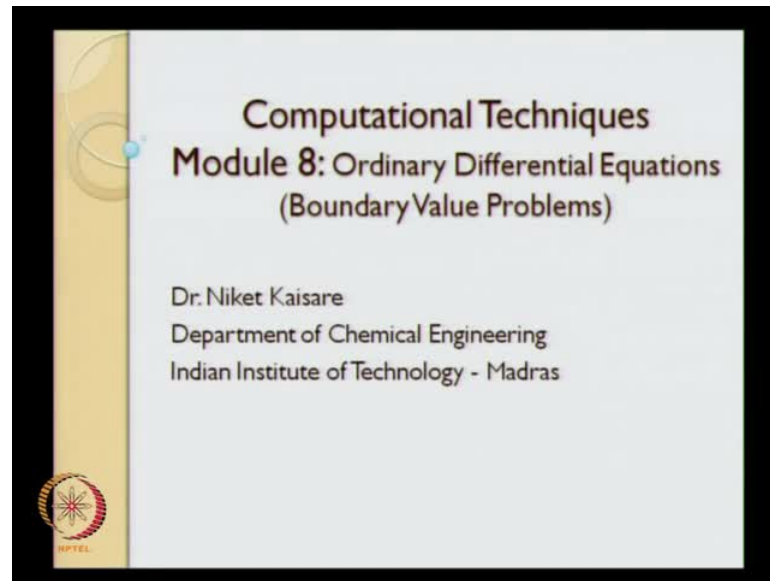


(Refer Slide Time: 45:07)




So, what we have done is we have just plotted the x versus temperature and you can see that the x versus temperature is looks exactly similar to what we had when we used the previous method of solving that is the shooting method. So, this is how we can solve this particular problem using the finite difference algorithm.

(Refer Slide Time: 45:15)

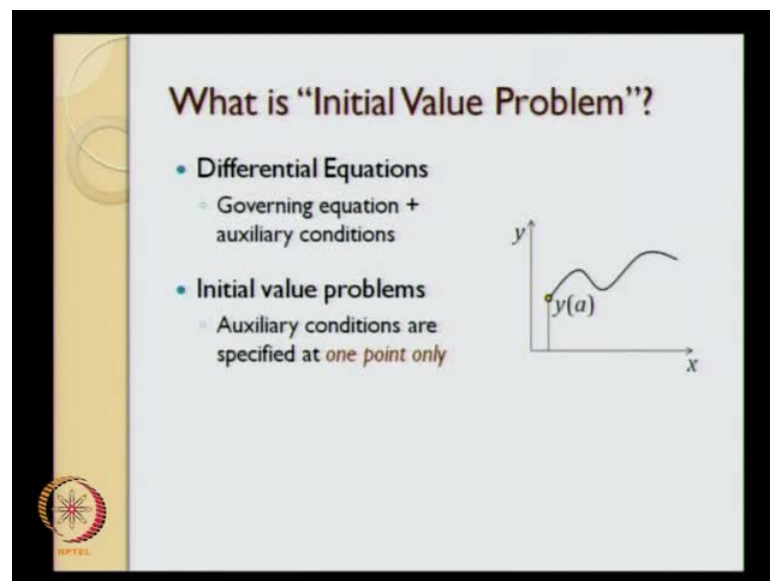


Computational Techniques
Module 8: Ordinary Differential Equations
(Boundary Value Problems)

Dr. Niket Kaisare
Department of Chemical Engineering
Indian Institute of Technology - Madras


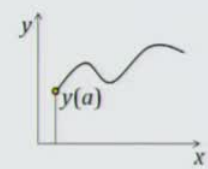


(Refer Slide Time: 45:22)



What is "Initial Value Problem"?




- Differential Equations
 - Governing equation + auxiliary conditions
- Initial value problems
 - Auxiliary conditions are specified at *one point only*



(Refer Slide Time: 45:25)

What is "Boundary Value Problem"?

- Differential Equations
 - Governing equation + auxiliary conditions
- Initial value problems
 - Auxiliary conditions are specified at *one point only*
- Boundary value problems
 - Auxiliary conditions are specified at *two points*




So, let me now go on to conclude this particular module of ODE boundary value problems. What we covered in the ODE boundary value problems? We covered the difference between boundary and initial value problems. In initial value problems, we had the conditions specified only at one location. Whereas, in the boundary value problems, we had the condition specified, the initial boundary conditions specified at two boundaries.

(Refer Slide Time: 45:39)

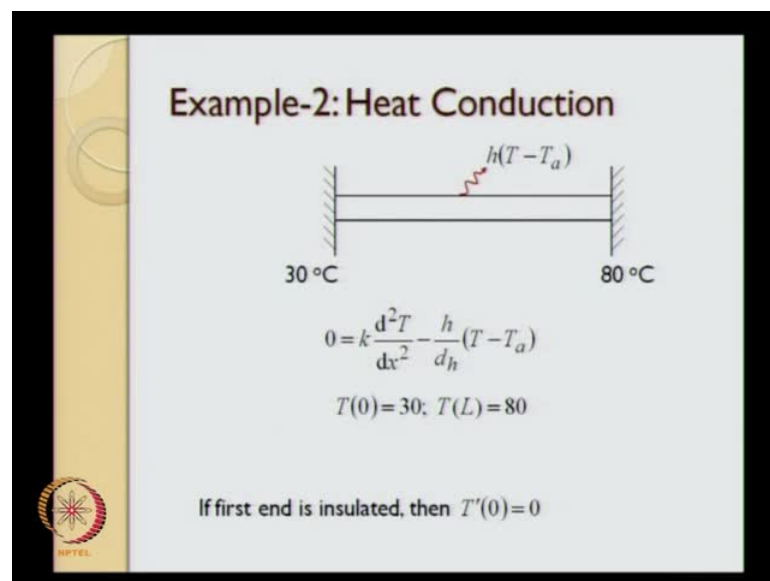
Reactor with Axial Dispersion

- Model for a Plug Flow Reactor
 - Model: $\left(\frac{F}{A}\right) \frac{dC_A}{dx} = -r(C_A)$
 - Initial Condition: $C_A|_{x=0} = C_0$
- With Axial dispersion
 - Model: $\left(\frac{F}{A}\right) \frac{dC_A}{dx} = D \frac{d^2 C_A}{dx^2} - r(C_A)$
 - Boundary Conditions: $C_A|_{x=0} = C_0$; $C_A'|_{x=L} = 0$



An example that we took for the boundary value problem was a reactor with axial dispersion. We took this particular example using the shooting method and showed that shooting method indeed has problems, because of nonlinearities. As long as the ODE initial value problem that we get is going to work, as long as that condition is satisfied, our system of equations is going to be solvable. If that condition is not satisfied we will not be able to solve the system of equations.

(Refer Slide Time: 46:12)



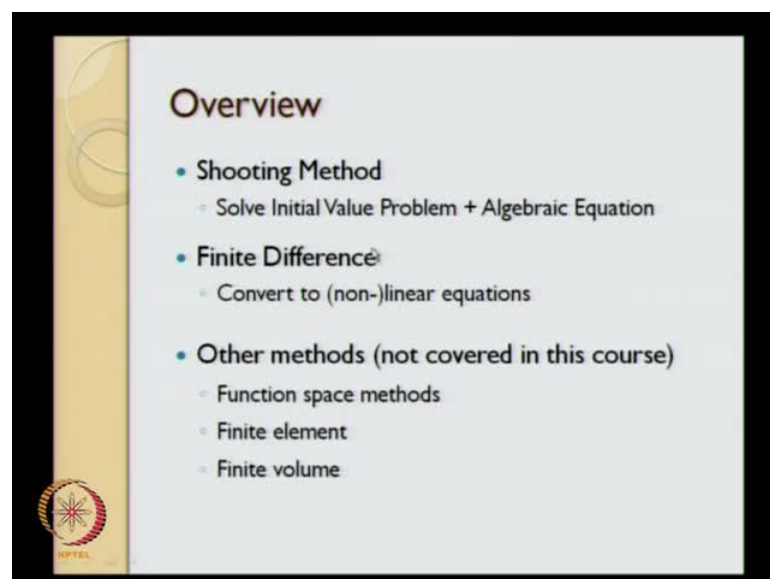
Example-2: Heat Conduction

Diagram of a reactor with boundary conditions: 30°C at the left end and 80°C at the right end. A red wavy arrow labeled $h(T - T_a)$ indicates heat loss from the top surface.

$$0 = k \frac{d^2 T}{dx^2} - \frac{h}{d_h} (T - T_a)$$
$$T(0) = 30; T(L) = 80$$

If first end is insulated, then $T'(0) = 0$

(Refer Slide Time: 46:21)



Overview

- Shooting Method
 - Solve Initial Value Problem + Algebraic Equation
- Finite Difference
 - Convert to (non-)linear equations
- Other methods (not covered in this course)
 - Function space methods
 - Finite element
 - Finite volume

Then we took up the second example of heat conduction and this is the example that we solved using two different methods. Those two different methods were the shooting method and the finite difference algorithm. A final piece of statement about the shooting method and the finite difference algorithm is shooting method as we saw does have a certain limitations, but is relatively simpler to use compared to the finite difference algorithm. That is because ODE initial value problems tend to be often easier to use and there are certain software that are available to solve the ODE initial value problem.

However, the finite difference algorithm is going to be a much more powerful method in order to solve a general ODE boundary value problem. Now, the finite difference algorithm that we have seen has one of the problems, with the finite difference algorithm ends up being that some of the methods especially to handle the boundary of conditions tend to be first order accurate and not higher order accurate. But, going to higher order accuracy methods is going to be straightforward in a boundary value problem.

For example, $d^2 T$ by dx^2 , we represented by a central difference formula which is a second order accurate formula. $d T$ by dx , if we represented using a first order formula using either the forward or backward differences that is going to be order h to the power 1 accurate. But, if we use a central difference, it is going to be h^2 accurate. So, that is where we stop with this particular module and I will see you in the next module.