

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

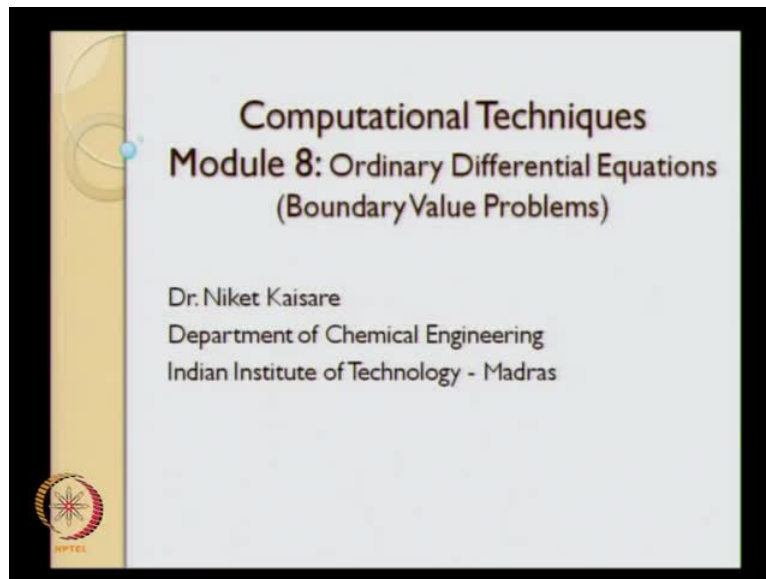
Module No. # 08

Lecture No. # 01

Ordinary Differential Equations (Boundary Value Problems)

Hello and welcome to module 8 **our** for computational techniques course. This particular module concerns with solving numerical methods of solving ordinary differential equations - the boundary value problem.

(Refer Slide Time: 00:22)



In the previous module, we had looked at solving initial value problem. So, what I am going to do in a next few minutes is just motivate this topic of boundary value problems, and how boundary value problems are different from initial value problems and then, we will take a couple of methods to solve boundary value problems. Compared to some of the previous modules, this is going to be slightly shorter module not because this problem is not a problem of importance, but because we are not going to cover some of the more advanced techniques in solving boundary value problems.

(Refer Slide Time: 01:02)

The slide is titled "What is 'Initial Value Problem'?" and contains the following content:

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

To the right of the text is a graph with a vertical y-axis and a horizontal x-axis. A wavy curve starts at a point on the y-axis labeled $y(a)$ and extends to the right. In the bottom left corner of the slide, there is a circular logo with a star-like pattern and the text "NPTEL" below it.

So, let us first motivate this particular topic - the boundary value problems topic. I will first start off with what we mean by an initial value problem, this is what we had done in the previous module of the course. The differential equations - in order to get a unique solution to the set of differential equations, **that** we need to solve the governing equations in addition to that, there are certain auxiliary conditions that need to be satisfied. For example, we had an equation of the form $\frac{dy}{dx} = f(y, x)$ and we had a starting point y at certain point x equal to a , was given as y of a .

So, from starting from this particular starting point **So** as the x progresses how the value of y is going to change. That was what **well** we did in initial value problem; the conditions are specified at one point only. In this particular case, the conditions are specified at x equal to a , the value of y is, y a and we then need to start off from this particular initial value, which is shown as a circular **circular** dart over here.

(Refer Slide Time: 02:40)

The slide is titled "What is 'Boundary Value Problem?'". It contains three main bullet points:

- **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*

There are two diagrams on the right side of the slide. The top diagram shows a 2D coordinate system with a wavy curve. A point on the y-axis is labeled $y(a)$. The bottom diagram shows a horizontal rod supported by two triangular hinged supports at its ends.

We start off at this initial value and then, we progress in one direction. So, we progress along x direction in order to get the solution. So, these are initial value problems; so you can think of this is like a string, and this string is attached only at one end and we are free to move that string; the other end is free to move, depending on how the function value f of x is going to be. If the initial value $y(a)$ is going to change, then the overall curve just shift up or down based on what the value $y(a)$ is going to be. On the other hand, boundary value problems are, you can think of boundary value problems as problems which are hinged at both the ends, both at the left and the right ends they are hinged.

Indeed if you are going to look at buckling of a particular rod under some weight, that will be boundary value problem, and that naturally happens to be a boundary value problem, because the rod is hinged at the initial end as well as the final **final** end. But in general, the boundary value problem consists of the governing equations, but the auxiliary conditions are specified at two different points and not at one single point.

So, the main difference between initial value problems and boundary value problems is that the initial value problems, the auxiliary condition is specified only at one point; whereas in the boundary value problem, the auxiliary conditions **conditions** will be specified at two points at least.

(Refer Slide Time: 03:39)

Reactor with Axial Dispersion

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

So, that is really the motivation behind the boundary value problems. Now, let us look at a general set of examples in which we are going to encounter boundary value problems in chemical engineering system. This is the example that we use in the previous module, this was the model for a plug flow reactor, where F is the total flow rate inside the plug flow reactor. And in the previous module the equation that we had written was $F d C_A$ by $d V$, where V is the volume. And in this particular model, I have just expressed V as the cross sectional area A multiplied by the axial length x .

So, the model that we had in the previous module was F by A multiplied by $d C_A$ by $d x$ equal to some rate of reaction r . And we needed only one condition in order to solve this problem and that was initial condition, the concentration of the species A was specified at the inlet of the reactor. So, C_A at x equal to 0 was specified to be equal to C_0 that was the initial value problem.

Now, this particular model ignores the **the** possibility of actual diffusion or axial dispersion. So, if there is significant axial dispersion in the system, we have a model of reactor with axial dispersion. So, what happens is the overall system remains the same; we only have a dispersion axial dispersion term that comes into this overall model. So, we have this particular convection term, which is because of the mean flow of the system; this is the reaction term, because species A disappears because of the reaction A

giving b , and this is the axial dispersion term or an axial diffusion term which is which has a square dependence which has a second order derivative dependence on C_A .

So, we have $D \frac{d^2 C_A}{dx^2}$ and this is a classical problem of diffusion in reactor and this again, we are specifying the reactor along one direction only. In the next module, we will look at partial differential equations, where the values of C_A are going to change both in x and y direction. So, that will lead to partial differential equations.

Here we are looking at ordinary differential equations only and the things that I have shown in the yellow circles, those are the things that are different in the axial dispersion model compared to the plug flow reactor model. Because this is a second order ODE, we do not require just one boundary condition; we require two boundary conditions.

So, here one condition is specified at the inlet that is the inlet concentration is C_{A0} , this condition is same as the condition that we had before and then, we have to add another boundary condition in order to solve this particular problem. And in this particular case, the boundary second boundary condition that we have used is $\frac{dC_A}{dx} = 0$ at $x = L$ that is at the end of reactor, the $\frac{dC_A}{dx}$ become 0.

(Refer Slide Time: 06:40)

The slide shows a diagram of a horizontal rod of length L between $x=0$ and $x=L$. The left end is at 30°C and the right end is at 80°C . A red wavy arrow labeled $h(T - T_a)$ indicates convective heat loss from the top surface of the rod. Below the diagram, the governing equation is given as $0 = k \frac{d^2 T}{dx^2} - \frac{h}{d} (T - T_a)$. The boundary conditions are $T(0) = 30$ and $T(L) = 80$. A note at the bottom states: "If first end is insulated, then $T'(0) = 0$ ".

Another example let us consider heat conduction in a rod. So, basically we have this rod, one end of the rod is kept at 30 degree Celsius, another end of the rod let say is kept at 80 degree Celsius, because of the temperature difference, there is going to be a heat

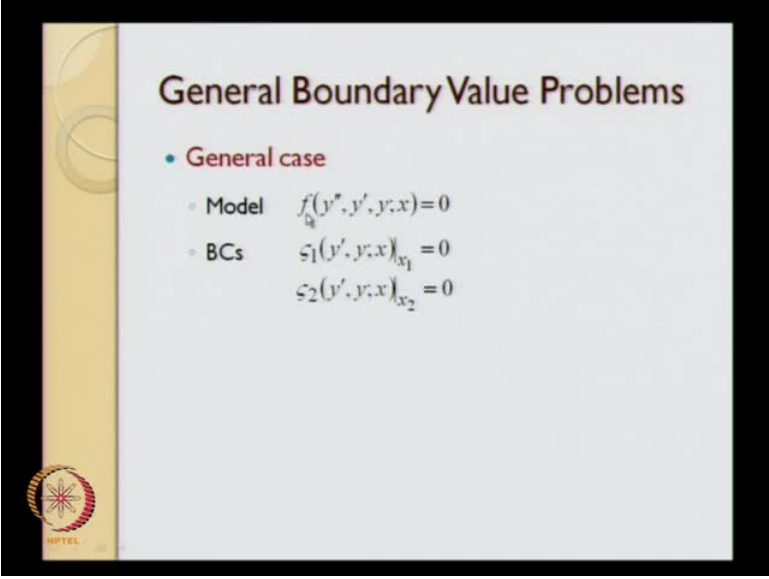
transfer that takes place from this particular hot end to this cold end. So, this is from right to left is the direction of transfer that is going to take place.

Let us say the overall atmosphere is at 30 degrees Celsius, then this rod is going to emit heat or its going to lose heat, rather to the ambient and this loss of heat is governed by the Newton's law of cooling. In other words, we have heat transfer coefficient h multiplied by the cross sectional area multiplied by the difference in the temperature that becomes the total heat loss into joules per unit time. When it comes to the total heat flux **that** that is just h multiplied by T minus T_{ambient} and if we rearrange this equation, we will get this as $d^2 T$ by dx^2 equal to some constant β multiplied by T minus T_a .

And we need two boundary conditions, and the first boundary condition is T at x equal to 0 is going to be 30; T at x equal to L is going to be 80. So, those are the two boundary conditions. Now, if instead, if this particular end was insulated, rather than it been kept at 30 degree Celsius, then we would have the condition - the inlet condition- is $d T$ by dx equal to 0, at x equal to 0 that would have been the inlet boundary condition.

So, what we have seen so far is, one is the most common examples in chemical engineering systems, where we encounter boundary value problem are associated with a diffusion or a conduction type of term, where we get $d^2 T$ by dx^2 type of term. Now, because of $d^2 T$ by dx^2 type of term, we require conditions to be two boundary or two initial conditions to be specified. Now, either the temperature or that particular value may be specified or the T dash, which is $d T$ by dx at a particular end could be specified. So, these are the two different ways of specifying the boundary conditions.

(Refer Slide Time: 09:08)



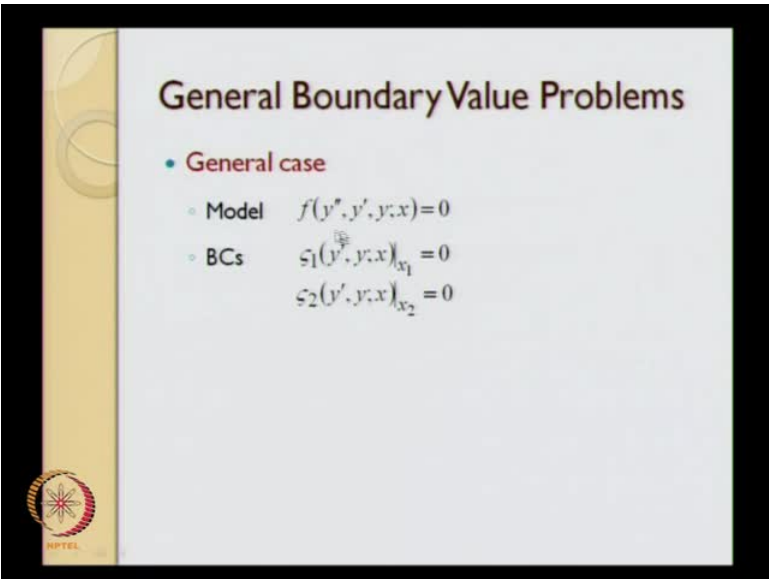
General Boundary Value Problems

- **General case**
 - Model $f''(y, y', y; x) = 0$
 - BCs $\zeta_1(y', y; x)|_{x_1} = 0$
 $\zeta_2(y', y; x)|_{x_2} = 0$

The slide features a yellow vertical bar on the left with a circular logo at the bottom containing a star-like pattern and the text 'NPTEL'.

So, now, to generalize this set of ODE's for **boundary conditions** boundary value problems, this is going to be a very general way of representing any non-linear ODE. So, we will have some function f of y double dash y dash y and x equal to 0 as going to be a model. **in this particular case**. In the previous case, this entire thing is going to be nothing but our f of $d^2 T$ square by $d x$ square, $d T$ by $d x$, (t, x) .

(Refer Slide Time: 09:39)



General Boundary Value Problems

- **General case**
 - Model $f''(y, y', y; x) = 0$
 - BCs $\zeta_1(y', y; x)|_{x_1} = 0$
 $\zeta_2(y', y; x)|_{x_2} = 0$

The slide features a yellow vertical bar on the left with a circular logo at the bottom containing a star-like pattern and the text 'NPTEL'.

So, this is going to be our governing equation subject to boundary conditions, because this is the second order ODE. We require two boundary conditions: one is x_1 of 1 at x_1 equal to 0; the other boundary condition is x_2 at x_2 equal to 0. So, this is a very general way of writing a boundary value problem.

(Refer Slide Time: 10:00)

Common ChE BVP

- Second order ODE
 - Model
$$\frac{d^2y}{dx^2} + p(x,y)\frac{dy}{dx} + q(x,y) = 0$$

Linear if: $p(x)$ and $q(x,y) = r(x)y + s(x)$
 - Boundary conditions
 - Dirichlet: $y|_{x=a} = \alpha; y|_{x=b} = \beta$
 - Neumann: $y'|_{x=a} = \alpha; y'|_{x=b} = \beta$
 - Mixed: $(y + c_1y')|_{x=a} = \alpha$

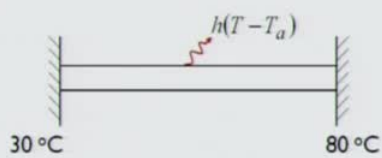
In general, we have $\alpha(x,y)$ and $\beta(x,y)$

Let us look at the more specific case of the type of boundary value problems that we are going to encounter in chemical engineering system. After we rearrange a particular equation, we will get an equation of the form $d^2y/dx^2 + p(x,y)dy/dx + q(x,y) = 0$, where p and q in general can be functions of both x as well as y .

Now, this particular equation is set to be linear, if this function p is only a function of x ; p is not a function of y , that means, p is just a function of x can be any arbitrary function of x , and this q should be a linear function of y , which basically means the q we should be able to write it as r multiplied by y plus s , where r and s themselves can be functions of x , but they cannot be functions of y . If these conditions are satisfied, then we will get a linear ODE; if these conditions are not satisfied, we will essentially get a non-linear ODE. Another case is the difference between homogenous versus non-homogeneous ODE. If this s of x is equal to 0, we will have a homogeneous ODE; if s of x is not equal to 0, we will have a non-homogeneous ODE. So that is regarding the second order ODE model for this system.

(Refer Slide Time: 11:26)

Example-2: Heat Conduction


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

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

Let us talk about the boundary conditions as we had seen before, if I go to couple of slides earlier, the two types of boundary conditions that we have seen is that the value at boundary is specified or the first differential at one of the boundary is specified.

(Refer Slide Time: 11:40)

Common ChE BVP

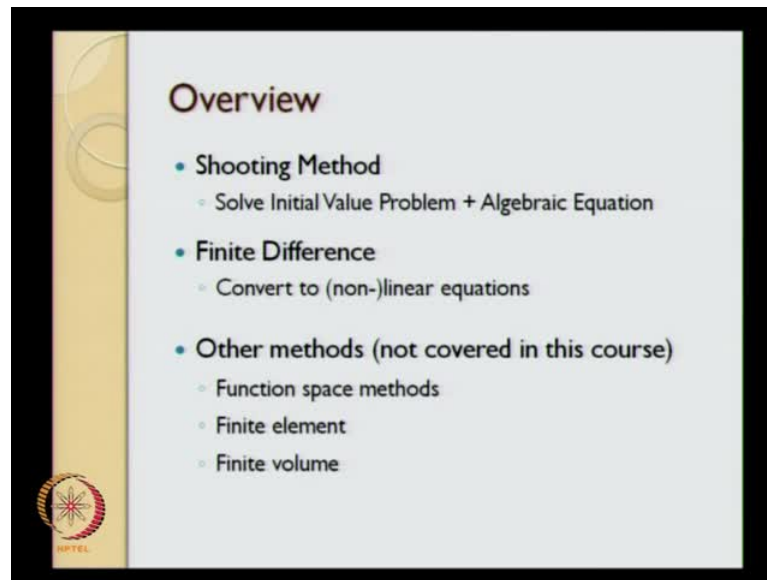
- Second order ODE
 - Model $\frac{d^2 y}{dx^2} + p(x, y) \frac{dy}{dx} + q(x, y) = 0$
Linear if: $p(x)$ and $q(x, y) = r(x)y + s(x)$
 - Boundary conditions
 - Dirichlet: $y|_{x=a} = \alpha; y|_{x=b} = \beta$
 - Neumann: $y'|_{x=a} = \alpha; y'|_{x=b} = \beta$
 - Mixed: $(y + c_1 y')|_{x=a} = \alpha$

In general, we have $\alpha(x, y)$ and $\beta(x, y)$

So, these are two different types of boundary conditions, which are called the Dirichlet or the Neumann boundary conditions respectively. So, the Dirichlet boundary condition is y is specified at some point x equal to a as y of a equal to α ; the Neumann

boundary condition is where the y' is specified, instead of y being specified, and the mixed boundary condition is where both **where** linear combination of y and y' are specified at **one of** one of the ends. And in general, we can have basically α and β to be a functions; in this particular case α and β can be functions of x and y .

(Refer Slide Time: 12:23)



Now, let us get to the overview of this particular module. In this module, we are going to consider two methods to solve boundary value problems the first method is called shooting method, where we are going to convert the boundary value problem in into an initial value problem and then, shoot for the solution I will talk about that a few minutes from now, and second example is to use a finite difference method, where the overall differential equation using numerical **diferential** derivatives is converted from differential equations to either to linear or non-linear equations. If the second order ODE is a linear, ODE we will get a linear set of equations; if it is a non-linear, ODE we will get non-linear set of equations.

So, these are the two methods that we are going to talk about in this particular module - the shooting method and the finite difference method. The shooting method we are going to borrow ideas from ODE initial value problem and solve algebraic equation using either the bisection rule or the Newton-Raphson's rule. In the finite difference, we are going to borrow ideas from numerical differentiation, which was covered in module 6 and the ideas from solving linear or non-linear equations, which was covered in module

3 and 4 respectively. The other methods which we are not going to cover in this particular course are functions space methods or finite element methods. For example this would be an orthogonal Orthogonal collocation method would be an example of this type. And the third example is the finite volume methods; we are not going to cover this in this course, because they are slightly advanced techniques. For our purpose, we are going to limit ourselves to shooting method and finite difference method.

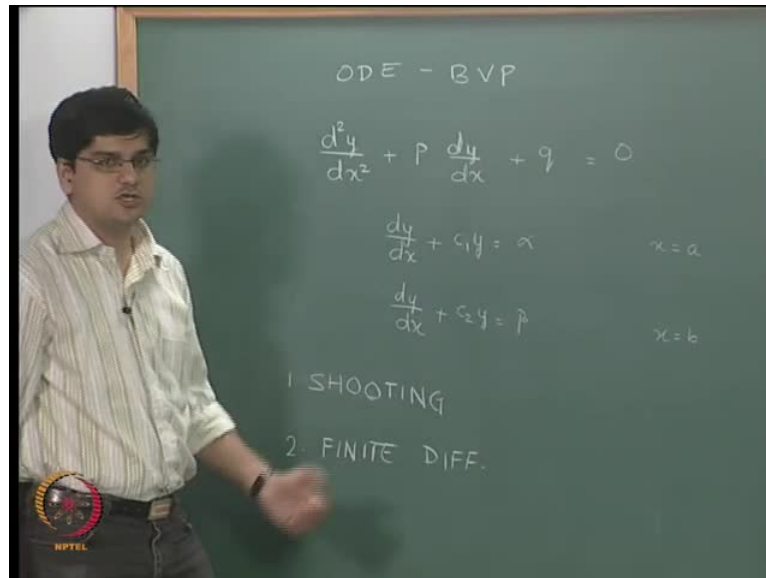
So, now, what I am going to do in the next part of this particular lecture is cover the overall basis behind the shooting method and behind the finite difference method. I will do that in this particular module. In the next module sorry In the next lecture of this module, we will cover solving the one particular example using shooting methods.

So, what I am going to do in that is use one of the ODE solving techniques - the midpoint technique - in order to solve the initial value problem and then, use a bisection rule to show how these two rules can be combined together in order to use them in shooting method. And the same example in the lecture 3 of this module, I am going to use it solve it using the finite difference method.

So, this is going to be a relatively shorter module, because we are not going to do any theoretical developments on ODE initial value problems or on algebraic equation solving; we just going to show a practical way of using the techniques that we have learned in previous modules in order to solve ODE boundary value problem.

So, let us go to our board and let us just look at how what what is involved in solving using the shooting method or using the finite difference method.

(Refer Slide Time: 15:37)

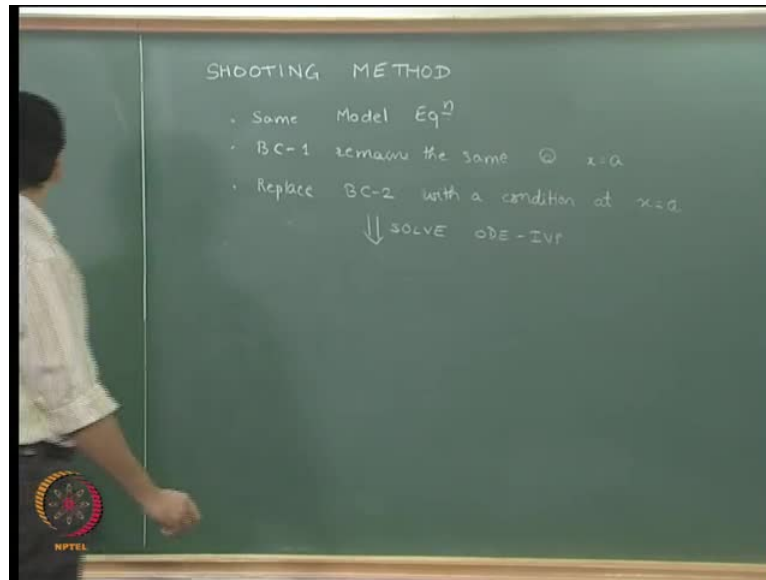


So, let us continue where we left off; we were talking about ODE boundary value problems and the example that we took of the of the of a general ODE boundary value problem was $d^2y/dx^2 + p dy/dx + q = 0$, where p and q in general can be functions of both x and y ; we are not saying that p and q should be linear or non-linear functions, let them be functions of x and y . I have just For simplicity of notation, I am not writing this as p of x, y or q of x, y . And if the constant term in this q if it is 0 that ends of being a homogeneous equation; if the term that does not depend on y if that is 0, it becomes a homogeneous ODE.

So, this is the general way of writing the ODE of our interest. Now, in in case of boundary value problems, we will essentially have... Let us just talk about in general, the case of a mixed boundary value in which case we will have the boundary value problem in the form $dy/dx + c_1 y = \alpha$ at $x = a$, and $dy/dx + c_2 y = \beta$ at $x = b$. Let me write this as $c_1 y = \alpha$ at $x = a$, and $c_2 y = \beta$ at $x = b$.

So, this is the governing equation and these are the two boundary. We are going to solve this general problem using the shooting method or using finite differences. So, let us go and first talk about shooting method; in shooting method what we do is, we convert the ODE boundary value problem into an ODE equivalent - ODE initial value problem.

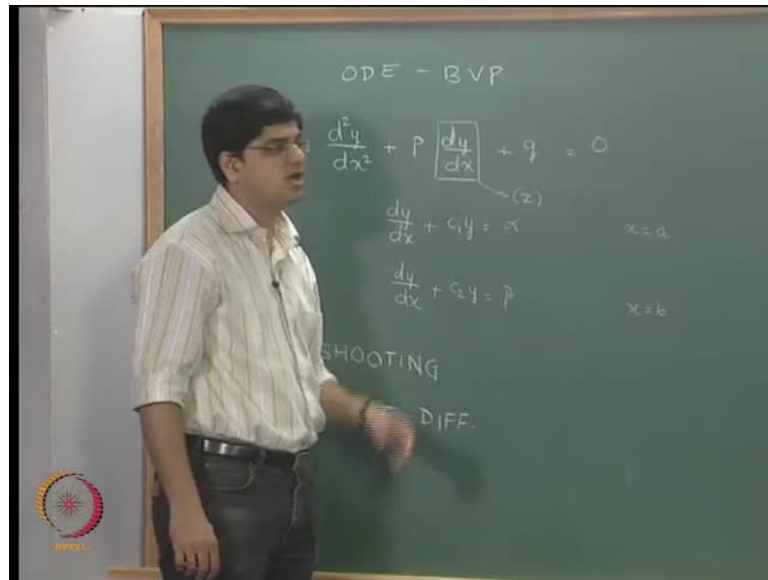
(Refer Slide Time: 18:11)



So, we will have the same ODE d^2y by dx^2 plus p dy by dx plus q equal to 0 that is the ODE that we will have. But instead of having the boundary conditions at two boundaries, we will have both the **boundary** conditions specified at one single boundary. So, we have the same model equation; we will have the boundary condition 1 remains the same at x equal to a . Now, what we do is, we replace boundary condition 2 with another condition at the same point x equal to a .

So, we replace; so with this we have converted our boundary value problem into an initial value problem, because now what happens is, instead of specifying the conditions at x equal to a , and x equal to b we have specified both the conditions at x equal to a , and x equal to a . As a result, this ODE initial value problem is something that we can solve using the initial value problem techniques that we have talked about before.

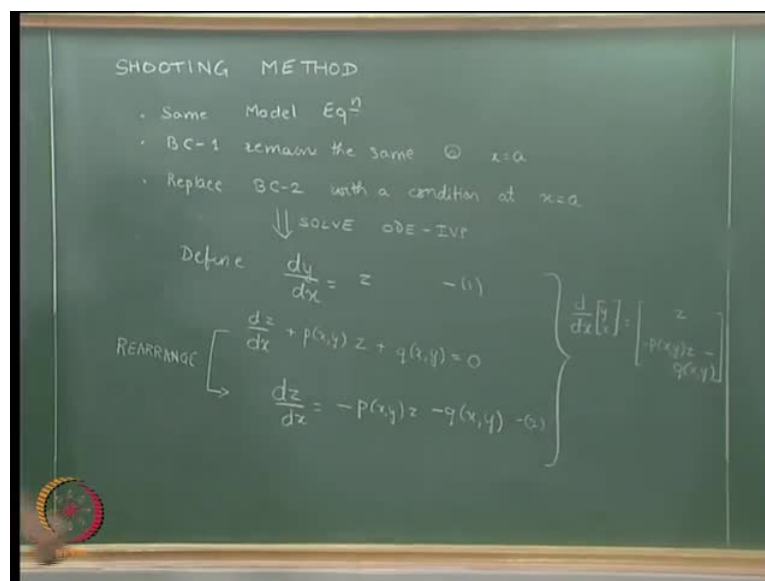
(Refer Slide Time: 20:08)



Now with this and how we will go about solving the ODE IVP is lets go back and look at this particular equation, we had $d^2 y$ by $d x$ squared plus $p d y$ by $d x$ plus q equal to 0; we will define another variable z equal to $d y$ by $d x$.

So, $d y$ by $d x$ we will call that as another variable z . So, with this definition $d^2 y$ by $d x$ squared can be written as $d z$ by $d x$ plus p multiplied by z plus q equal to 0 becomes one ODE, and $d y$ by $d x$ equal to z becomes our second ODE.

(Refer Slide Time: 20:45)

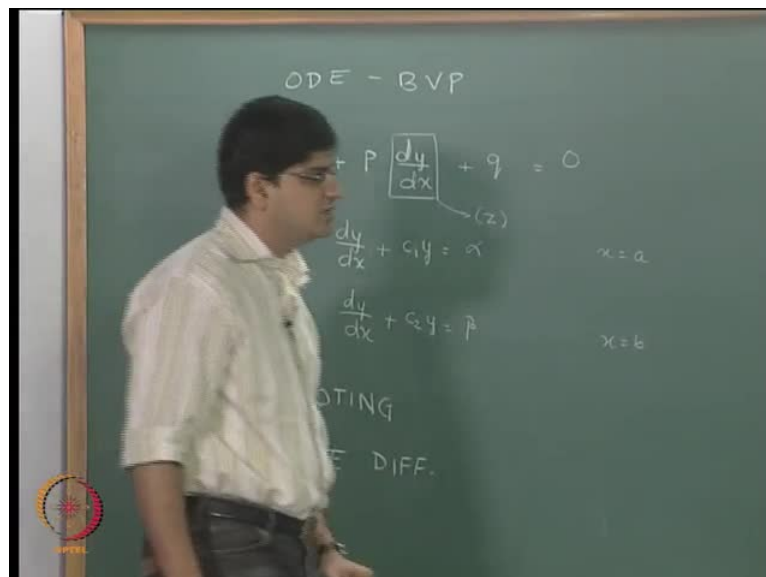


So, what I mean by that is, that becomes our first ODE and the second ODE is going to be d^2y/dx^2 , which is d/dx multiplied by dy/dx , and dy/dx is z . So, we will have that as $dz/dx + p$ multiplied by dy/dx . So, p of (x, y) multiplied by dy/dx , dy/dx is nothing but z plus q of (x, y) equal to 0, which we can rearrange to write this as. So, we have our ODE number 1 and our ODE number 2.

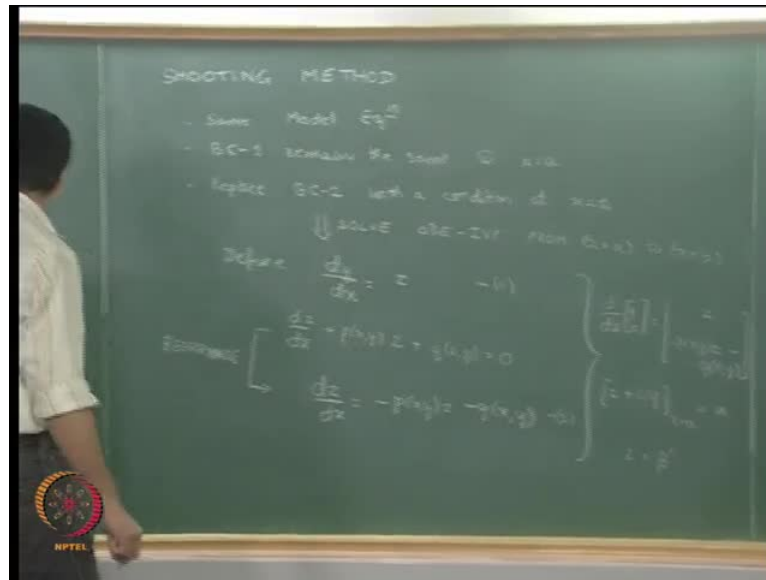
We can combine these two ODE's together and we can write them in the vectorial form. Now, this is the vectorial form that we had looked at during solving ODE initial problem, exactly the same vectorial form **we can use** we are going to use and we are going to write dy/dx of y, z is going to be equal to z is going to be in the first row, and in the second row we have minus $p z$ minus q .

So, we have d of (y, z) equal to some **function** function f_1 and function f_2 and this we can solve them using any of our ODE solving techniques, such as the Runge-kutta method or the midpoint method or the Adam-Moulton's method so on and so forth. So, any ODE's IVP solving technique of our choice we can use them to solve this particular method, subject to the following initial conditions.

(Refer Slide Time: 23:25)



(Refer Slide Time: 23:37)

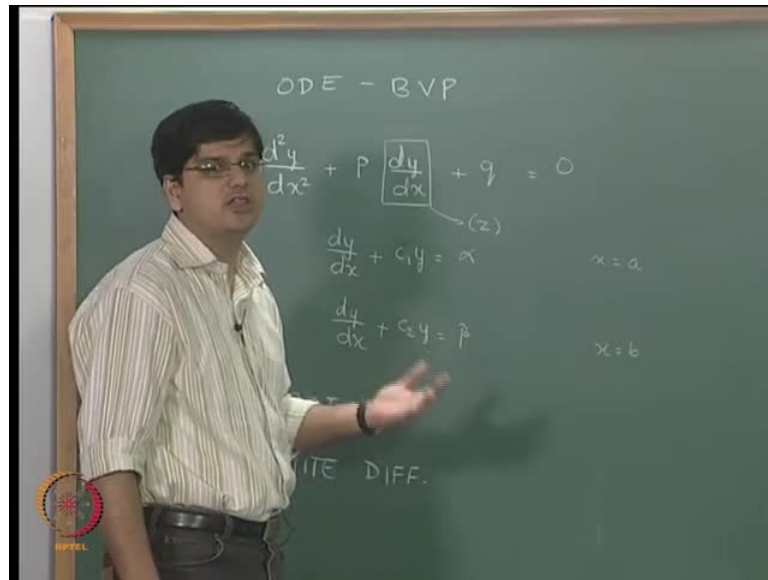


The first initial condition was $\frac{dy}{dx} + c_1 y = \alpha$, $\frac{dy}{dx}$ is now nothing but z ; $c_1 y$ is going to remain as $c_1 y$ that is going to be equal to α . So, our first initial condition becomes $z + c_1 y$ computed at the initial point $x = a$ equal to α , and second is what we had written is, we are going to replace the boundary condition $BC-2$ with a condition at $x = a$, and let say the condition we are going to choose at $x = a$ depending on this particular overall condition.

We can probably let say choose say $z = \beta$. Now, this is a problem that we can solve because this is an initial value problem in variables y and z and we can solve it using two initial conditions and when we solve them using two initial conditions, we will solve them from $x = a$ to $x = b$.

So, replace $BC-2$ with this, solve ODE IVP from $x = a$ to $x = b$. Once we have solved this ODE IVP going from $x = a$ to $x = b$, then we check the final condition at $x = b$, whether this particular condition is satisfied or not.

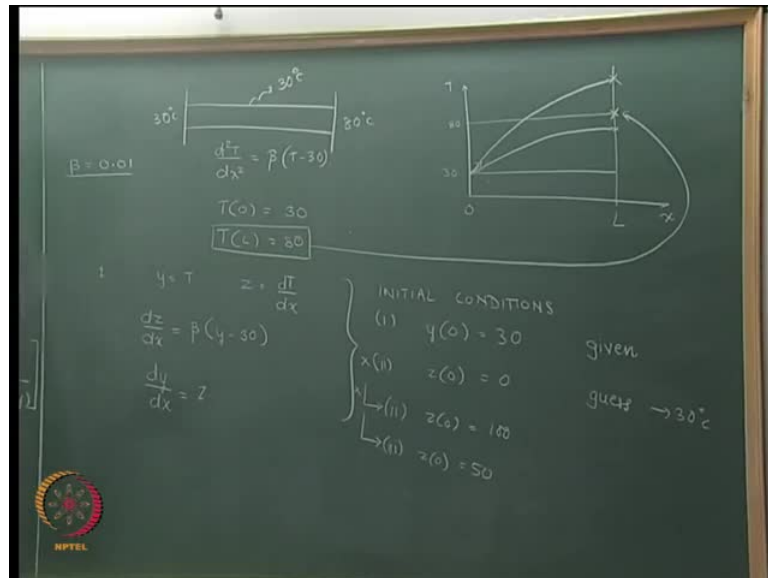
(Refer Slide Time: 25:13)



Now, if this condition is not satisfied, then we use any of our non-linear solution techniques in order to find out how to get **ours** our initial value to change in order to satisfy this condition. When this condition gets satisfied, at that time we know that the solution that we have come up with the chosen initial guess that is the true solution for the system.

To show this particular method better, we will look at the heat conduction problem - heat conduction in a rod problem - and we will try to go through these steps **themselves** and we will see how the heat conduction in the rod problem can be solved using the shooting method.

(Refer Slide Time: 26:01)



So, let us look at the heat conduction in the rod. So, what we had said is **there was** this rod with this end kept at 30, the other end kept at 80 degree celsius and the overall governing equation in this system was $d^2T/dx^2 = \beta(T-30)$, where 30 degrees C was the temperature of the ambient.

So, what we have is basically this **this** is probably going to be a rod and this end of the rod is kept at the ambient temperature of 30 and outside temperature is also 30 and this end is kept at 80, because this end is actually heated; the heat transfer will take place from this end to this end of the rod through conduction, in addition to conduction taking place, there will be heat losses from either ends of the rod to the surroundings.

So that is what is going to happen in this overall problem and **we had we had seen in this problem thus this beta is...** so there is a k term going to be over here, that k is really the thermal conductivity of this particular rod and we have $4h/d$ term over here, where h is the heat transfer coefficient and d is the diameter of the rod. So, β is going to be nothing but $4h/d$ that is what our value of β is going to be. Typical values of β are of the order of 10^{-2} to 10^{-3} .

So, let us take the value of β to be 0.01. So, this is the example, **in the next lecture** in this module I am going to use this particular example to solve it using the shooting method on **microSoft** Microsoft excel that is what I am going to do in the next lecture. In

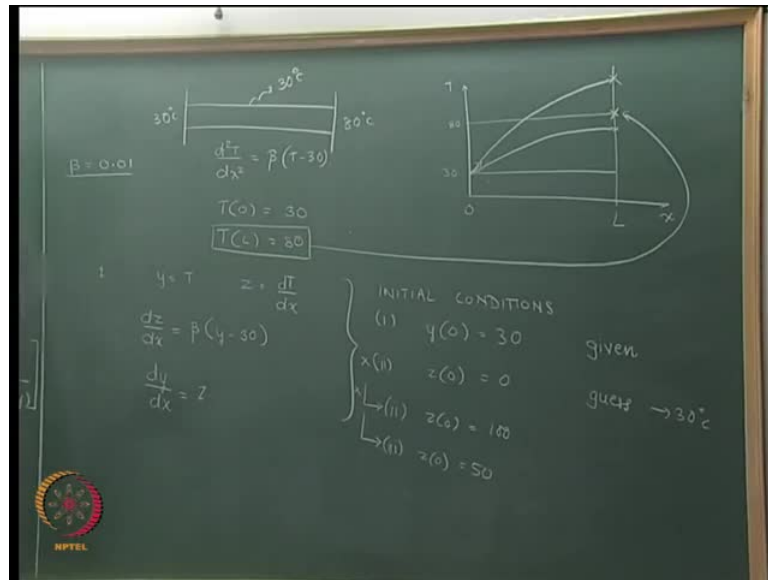
this lecture, I am just going to show the idea behind solving this particular problem using the shooting method.

So, now, we have $\frac{dT}{dx}$ squared equal to $\beta T - 30$ with the condition that T at x equal to 0 equal to 30, and T at x equal to L is 80, where L is the length of the rod. Let us take the length of the rod as say two meters or one meter, whatever it might be, we will look at that particular problem later.

So, this is the overall problem, where the boundary conditions are specified at two different ends. As we said, the first issue is to convert this particular problem into an initial value problem, because the temperature is specified at this end; we cannot specify another temperature at this end. So, what we will do is, we will specify a guess of the $\frac{dT}{dx}$ at that particular end so that is what we are going to do and before going to do that, we will define our y as our temperature and z as $\frac{dT}{dx}$.

So, with this definition our model equation becomes $\frac{dz}{dx}$ of $\frac{dT}{dx}$, which is $\frac{dz}{dx}$ is going to be equal to $\beta T - 30$, which is $y - 30$. So, this is going to be our one equation. The second equation is nothing but z is $\frac{dy}{dx}$ or $\frac{dy}{dx}$ is going to be equal to z . So, this is equation number one; this is equation number two and subject to the boundary conditions or sorry subject to the initial conditions, the first initial condition is $T(0) = 30$ given, and $T(0) = 30$ basically means that $y(0) = 30$. So, I will write this as $y(0) = 30$ as the given initial condition and the second now, because y is specified, let us specify z at the initial condition. So, that would be our second initial condition; so $z(0) = 0$, let say it is a guess. So, these are the initial conditions that we are going to start off with and we will then see how this particular temperature in this rod varies under these conditions.

(Refer Slide Time: 26:01)



So, let us just consider what it really means by **by** these two initial conditions when we are trying to solve this problem. So, now, what we have is, we have this rod; this end of the rod is kept at 30 degrees Celsius; outer atmosphere is also at 30.

So, this rod, if it is a temperature T , it is going to lose heat to the surrounding which are at 30 degree Celsius, with this end kept at 30. Now, $z(0) = 0$ basically means that there is no temperature gradient at the rod, which basically means that this end of the rod and the location next to that end of the rod are at the same temperature which essentially is going to come keep the overall temperature in the system constant at 30 degree Celsius. As long as we have no gradient, we are going to have this overall temperature constant at 30 degree Celsius.

So, what we will do is, we will just plot our temperature versus x ; we start our temperature at 30 degrees Celsius and this is 80 degree Celsius; this we will start at the 0 and this is our L and this is our target. So, now, **we've** with these conditions, we solve the initial value problem, and by solving the initial value problem we will get our temperature profile something like this. And the temperature that is predicted by solving the initial value problem at the end of this particular iteration - end of this particular ODE solving procedure - we will get it as 30. So, with this particular guess, we will get the exit temperature, the temperature at length L is going to be 30. Now, this temperature is less than the temperature at the actual temperature at the other end. So, **with a guess**, it

is like with this guess, we are trying to hit a dart and when we have hit the dot, the dart has hit below the bull side location.

So, what we are going to do is, we are to going to try and hit once once more we are going to try and hit the dart and this time, rather than throwing it flat, we will throw the dart with certain angle. So, what this means is, we are going to throw this dart with z_0 or d_t by d by d_t by d_x at 0 as some large positive value.

So, let say we are going to choose. So, because with this guess we get 30 degrees celsius if we throw the dart downwards, we are going... if this is going to be the direction with which we throw the dart, it is going to hit this board even lower. So, let us not hit the dart downwards, but let us hit the dart upwards, which basically means because this particular thing did not work; we are going to choose z_0 as let say 100, with z_0 chosen as 100, we are probably going to get a temperature profile like this.

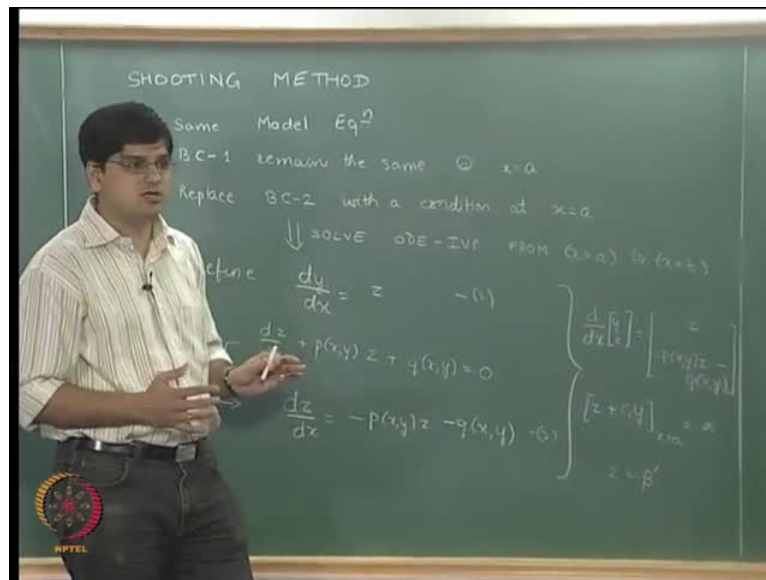
So, what has opened over here is that with z_0 equal to 100, the dart has hit above the bull side. So, what we have done is we have chosen the first initial condition as z_0 equal to 0; we have chosen the second initial condition had z_0 equal to 100. Those two initial conditions when we throw the dart, hit on either side of the true solution, which we are which we are intending to find. The true solution that we are intending to find is that the temperature at the end of the reactor is 80. Where do we get that from? We get that from the boundary condition.

So, we are hitting the darts on the board, the board is nothing but the temperature at the end of the rod; we are hitting the darts on the board and that is why the name of the method is shooting method. The first dart lands below the desired temperature; the second dart lands above the desired temperature. We can then use either the bisection method or the Regula Falsi method or any method of our choice in order to find, where we are going to hit the dart the next time.

So, the using let say the bisection method, we decide, our this guess is also not good enough so we will replace; the third thing we are going to try is z_0 equal to 50, and with z_0 equal to fifty let say that dart hits over here. So, basically z_0 equal to 0 and z_0 equal to 50 or both below the desired target.

So, we are going to retain 50 and 100 as the two guesses and discard 0 as the guess. So, the next guess is going to be 75 so on and so forth. So, what we are doing over here is, we are using the bisection rule in order to find out our true Solution, which is going to ensure that the other boundary condition is met.

(Refer Slide Time: 37:00)

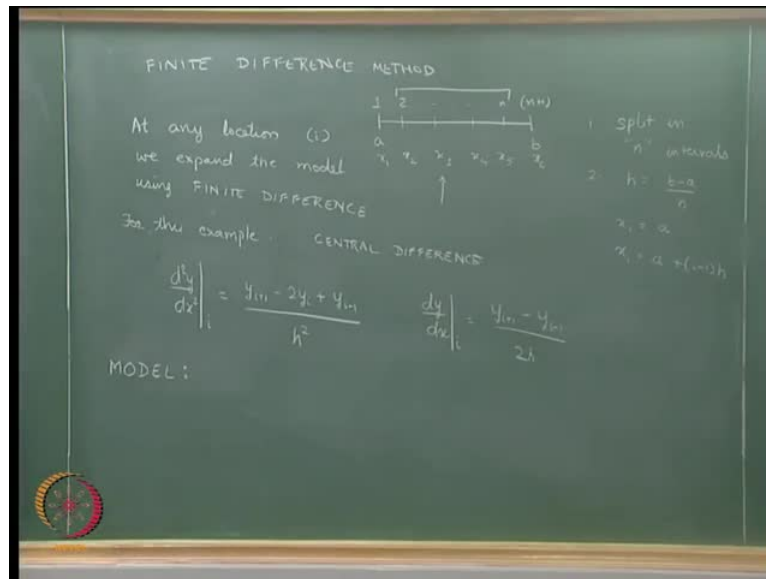


So, this is the shooting methods. So, the idea in shooting method is first to convert the ODE, which is the second order ODE into to first order ODE's. So, we have the same model equation, convert them into two first order ODE's; keep the first boundary condition the same, vary the second boundary condition.

So that we get an initial value problem by specifying the conditions at the same **same** end with the initial value problem **as the** as specified over here; we then go on in order to solve this particular problem using any of the initial value problem solution techniques we covered in the previous module. We check how far we are away from meeting the boundary condition BC-2; if we reach the boundary condition BC-2, we stop our procedure and that is our solution. If we do not meet the boundary condition BC-2, we are going to use either a bisection rule or the Regula Falsi rule or may be the **Newton's** Newton-Raphson's method in order to find out various values of the condition at x equal to a such that the boundary condition BC-2 is satisfied.

So that is going to be our overall procedure. What I am going to do in next module is take up a numerical example of using the shooting method and show you how the shooting method is going to work, for exact same example that I have shown **shown** over here. Now, this was about the shooting method. The second method that we spoke about was the finite difference method.

(Refer Slide Time: 38:34)



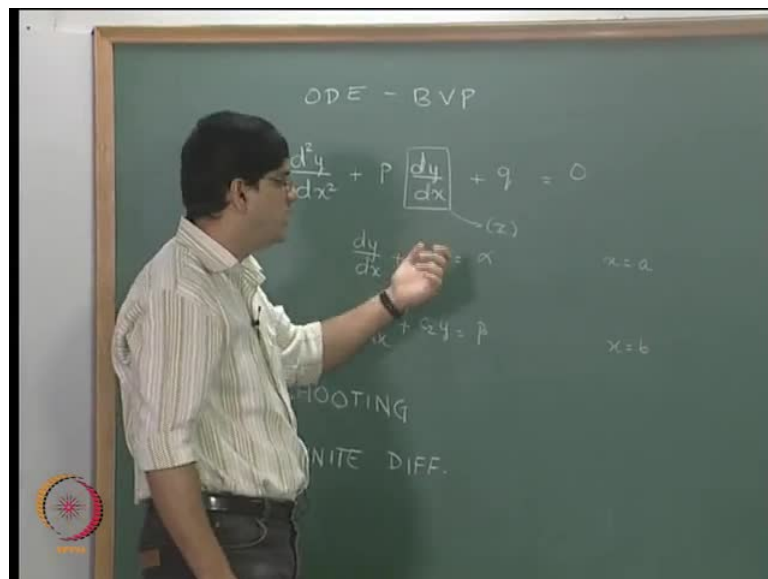
So, let us look at how to solve the boundary value problem using finite difference method. Now, in the boundary value problem, this **this** is the **same boundary value problem that we** general boundary value problem that we saw few minutes earlier; the conditions were specified at x equal to a and x equal to b . So, our domain starts from x equal to a and ends at x equal to b . So, that particular domain we are going to split into n intervals, a to b we have going to split into n intervals, let say n equal to 5. So, 1, 2, 3, 4, 5, let us presume for a moment that these are equivalent intervals. So, this particular guy, we will call this as x_1 ; this is x_2 , x_3 , x_4 x_5 and x_6 .

So, the domain is split in n intervals. Our difference between two consecutive intervals is going to be h is going to be equal to b minus a divided by n ; our x_1 is going to be equal to a and x_i is going to be nothing but a plus i minus 1 multiplied by h . So, x_2 is going to be a plus h ; x_3 is going to be a plus $2h$ a plus $3h$ and so on up to b . So, these are going to be our definitions.

Now, what we are going to do is at any location, we are going to write our model equation using the **the** numerical derivatives expansion. So, our model equation, if we look at that, if we go back over here, our model equation was $d^2 y / dx^2 + p dy / dx + q$. If we recall from our module 6, $d^2 y / dx^2$, we can write that using a finite difference approximation; dy / dx we can use write again using a finite difference approximation.

So, at any location i , we expand the model using finite difference approximation. If you recall from module 6, the central difference formula gives us a second order accurate method. So, **we will use** for this particular example; we will use central difference formula. What we mean by using the central difference formula is our $d^2 y / dx^2$ at location i , will be written as basically $y_{i+1} - 2y_i + y_{i-1}$ divided by h^2 .

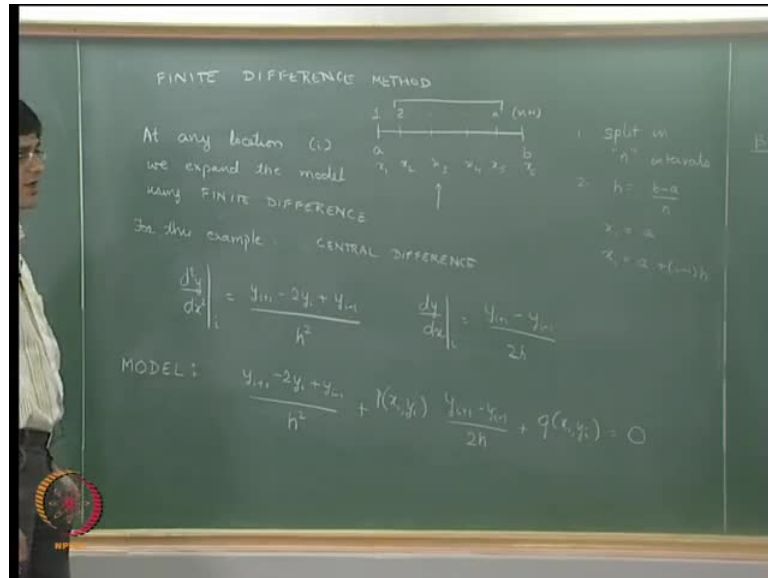
(Refer Slide Time: 43:53)



And likewise, our dy / dx will be written as dy / dx at x_i will be written as $y_{i+1} - y_{i-1}$ divided by $2h$. So, this is how we will write these two guys and for $i = 2$ to 5 or $i = 2$ to n **2 to n minus 2** to n **sorry** because we have n intervals, we are going to go from $1, 2$ and so on up to $n + 1$. For all the internal nodes, that means, for the nodes 2 to n , we are going to just substitute this particular guy and this particular guy in the overall model equation. So, substituting in the model equation what we are going to get, **we will get** basically we will if **you** look at this particular equation, this will

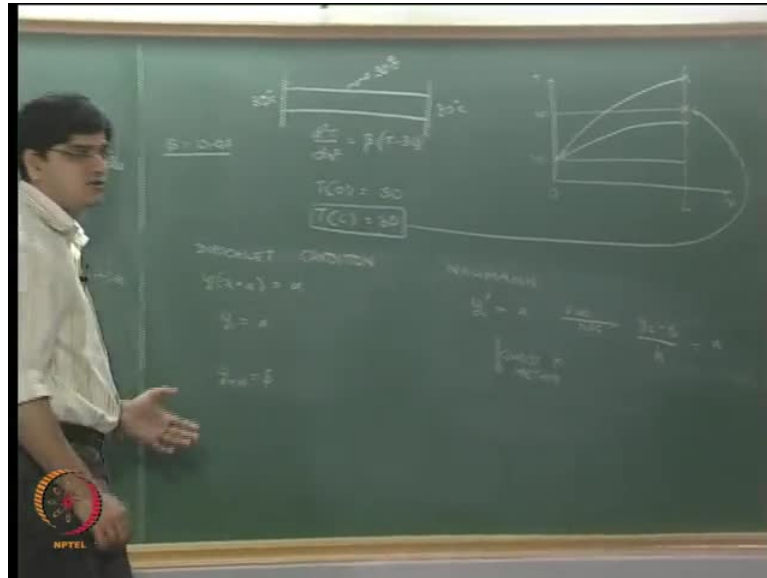
be replaced by $y_{i+1} - 2y_i + y_{i-1}$ divided by h^2 , this will be replaced by $y_{i+1} - y_{i-1}$ divided by $2h$ and remaining terms remain the same.

(Refer Slide Time: 44:14)



So, we will get $y_{i+1} - 2y_i + y_{i-1}$ divided by h^2 plus $f(x_i, y_i)$ multiplied by $y_{i+1} - y_{i-1}$ divided by $2h$ plus $q(x_i, y_i)$ equal to 0. So that is going to be our model. Our boundary conditions are going to be - if we have the Dirichlet type of boundary conditions, they are going to be very straight forward to handle; if we have the Neumann type of boundary conditions, they are going to be a little bit more trickier to handle.

(Refer Slide Time: 45:09)



The Dirichlet condition for example is going to be y at x equal to a is going to be equal to some value α . It is very easy to handle this is nothing but $y_1 = \alpha$; likewise, at the other end, if we had Dirichlet boundary condition, we will get y_{n+1} equal to β .

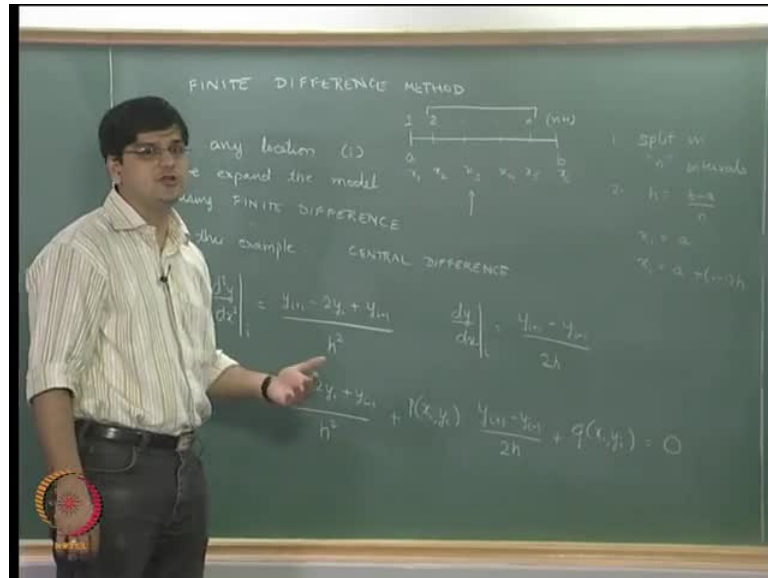
So, those are going to be our two boundary conditions that we can use. Now, we have our first equation as $y_1 = \alpha$; our second to n th equations are going to be these guys, and our $n+1$ th equation will again come from the boundary condition. If it is a Dirichlet boundary condition again, we will get $y_{n+1} = \beta$ and that is exactly what we are going to get in this particular example, where we will get $y_1 = 30$ and we will get $y_{n+1} = 80$ as the two Dirichlet boundary conditions.

But instead of Dirichlet boundary conditions, if we had a Neumann boundary condition, **the Neumann boundary condition**, let us say we have a Neumann boundary condition at this particular end, the Neumann boundary condition is going to be **$y_i - y_{i+1}$ is going to be equal to some value α sorry $y_i - y_{i+1}$ is going to be equal to some value α** .

Now, this boundary condition we can handle in two different ways: we can use a forward difference formula and the other way to handle this is using a ghost point method.

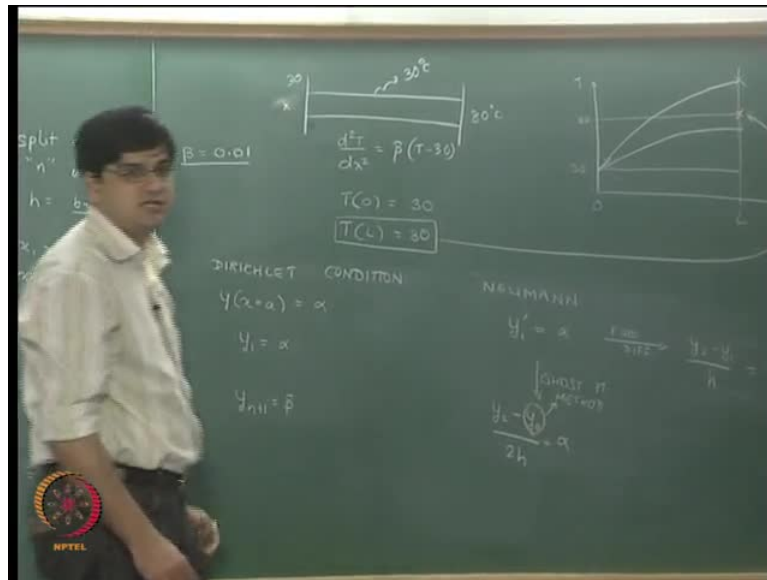
I will talk about the forward difference formula first, because it is more straight forward. In forward difference formula, we use a forward difference Δ at this particular location to express y_1 dash, and y_1 dash is nothing but y_2 minus y_1 divided by h .

(Refer Slide Time: 47:54)



So that is the y_1 dash using the forward difference formula that is going to be equal to α . Now, the problem with using the forward difference formula is **this is** the order of accuracy of this formula is h to the power 1, whereas the order of accuracy for our central difference formula, for the formula that you have used to expand this particular model, the order of accuracy for this particular formula is going to be h squared. So, we **have the** Δ in the entire domain, we have a formula that is h square accurate, but at the end of the domain, we have the formula that is order of h accurate.

(Refer Slide Time: 48:10)

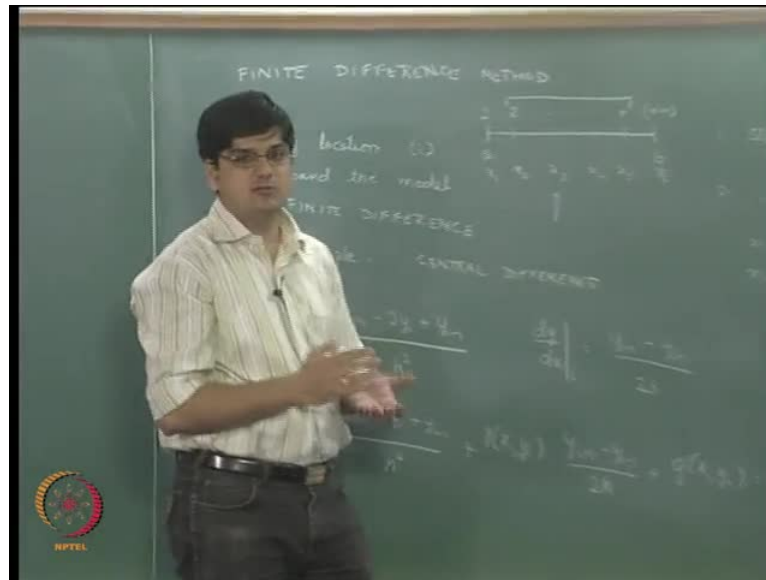


The largest error is going to govern the overall error in this **in of in the** solution. Since the largest error is h the one order error, the overall solution is going to be h to the power one accurate, in spite of us spending a fair amount of effort in getting h to the power 2 accurate solution in the domain using a central difference formula.

So, that is why this method may not be a preferred method. So, instead **we will** we will have to use an h square accurate formula, and h square accurate formula is going to be basically $y_2 - y_0$ divided by $2h$ is going to be equal to alpha.

Now, the problem is that, this particular guy is a ghost point; this point does not really exist; so this point is a point that we have concocted. We have concocted **to the left** to the left, in this particular case to the left of our initial point.

(Refer Slide Time: 49:47)



So, now, instead of having $n + 1$ unknowns, now we have $n + 2$ unknowns, because we have added this also in as an unknown. So, what we do in this particular case is that we add this particular equation, addition of this equation, add one more variable. As a result, the domain equation that is this model equation is going to be solved not from two to n , but instead it will be solved from one to n .

So, if we are going to use ghost point, then at location 1, we are going to specify the boundary condition as well as the domain equation. From location 2 to n , we will specify the domain equation and at location $n + 1$, we will specify the boundary condition, if it is a Dirichlet boundary condition; if it is either a Neumann or mixed boundary condition again, we will use a ghost point approach at this point in which case we will have $n + 1$ governing equations and two boundary conditions for $n + 1$ points in the domain and two ghost points.

So, with this I come to the end of this particular lecture of this module. What we have covered over here so far is to give an over view to boundary value problems and discuss two methods to solve the boundary ODE boundary value problems - the first one is the shooting method and the second one is the finite difference method. What I am going to do in the second lecture is take up the shooting method and show a numerical problem in Microsoft excel and discuss a few things about the shooting method. And in the lecture 3, I am going to consider **the fixed point** Sorry the finite difference method and look at

another another example and solve that using the finite difference method and also discuss about some of the issues with finite difference method.

Thank you and I see you in the next lecture.