Modeling Transport Phenomena of Microparticles
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Lecture - 32
Numerical Methods for Boundary Value Problems (BVP)

So, we have derived several non-linear boundary value problem and initial boundary value problem. To the model of transport phenomena in microfluidics and hydrodynamics. Now coming few lectures will talk about some outline on numerical treatment of that kind of situations. That means the non-linear boundary value problems and partial differential equations and so on.

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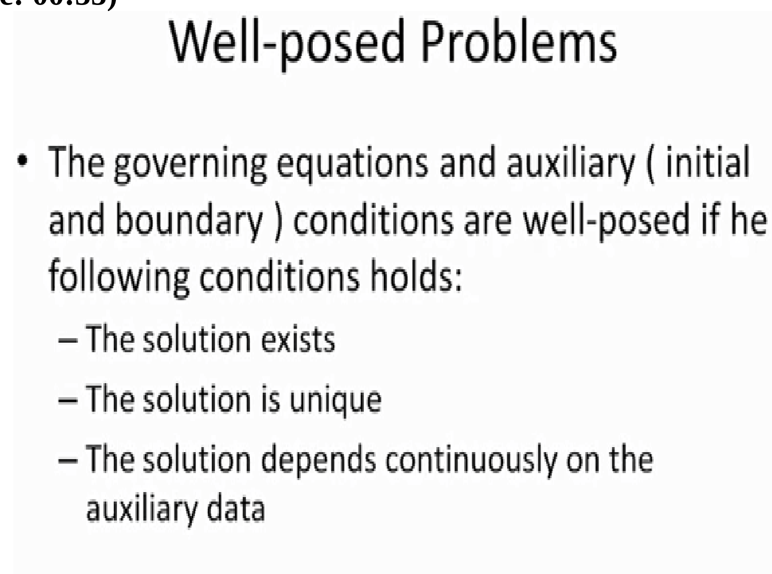

Now first of all, whatever the problem will be looking for the solution numerical solutions is assumed to be well-posed. Now what is the well-posed can be said in a very brief manner. In mathematical problem can be said in this way that the solution exists; solution is a unique and in continuously depends on the auxiliary data.

That is the initial conditions, boundary conditions, and so on. Now we will be interested in numerical methods for boundary value problem. So, what is boundary value problem?

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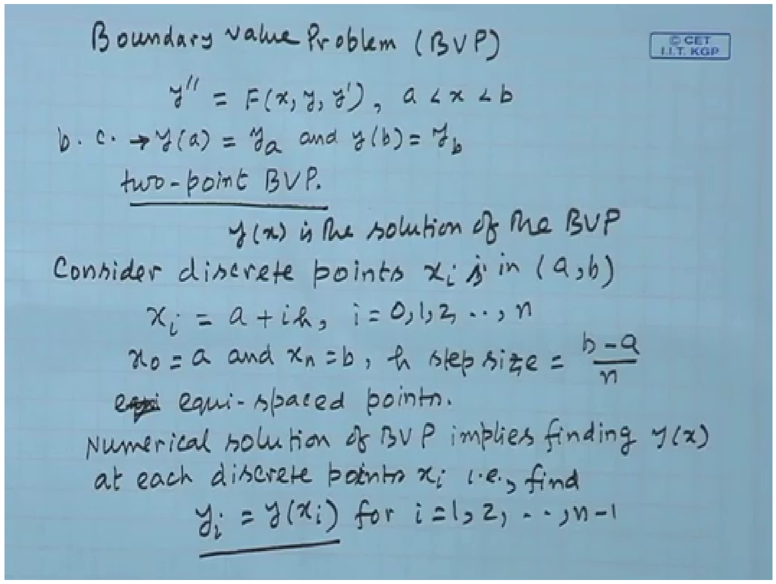

So, in short boundary value problem which is referred as (BVP). Now (BVP) is where the conditions are given at two different from points. So, you have a differential equation Y = F (x, y) y dash. Where is any function of this Y and Y dash. Where Y is a variable depends on X and say X is the independent variable defined between a to b. And this is the boundary conditions Y = ya and y b = yb.

This kind of problems is called the two-point boundary value problem two point (BVP). At least we will be second order differential equations because there will be two conditions. So obviously the order of the differential equation will be at least two, it can go beyond that and consequently the number of boundary conditions also will be moved. So, this is the conditions we call as boundary condition in short form in BC.

So the solution is Y(X) is the solution of the BVP. So what does it means is BVP. So if yx is the solution means it satisfies the given differential equation and as well as the boundary conditions this is the requirement for YX to be a solution of the given boundary value problem. Now we are looking for numerical solution, so numerical solution we cannot get a solution in analytic form that is a function form of YX.

So what we do is we consider some discrete points Xi, in number of discrete points in the interval (a, b) that means. We choose if this points are equiv spaced we can choose Xi = a + ih, i

= 0, 1, 2 up to n. So in our notation X_0 is a and X_n is b. action equal to b and H is the step size which is equal to it becomes b - a by n, n is the number of discrete points so these are called the equi-spaced point.

So our intention is to get so numerical solution of BVP implies finding y x at each discrete points at each of these discrete points xi. That is we need to get find yi which we denote which is the Y at xi for equal to 1, 2 n-1. Because y at zero and y at n are given. So numerical solution means we need to find out what are the yi at this discreet points i equal to 1 to N -1 no the points may be discrete for simplicity. We have considered discrete simplicity.

Discrete points are considered equi-spaced. Because it has an equal interval, now, what are the methods so this is our objective now one of the methods is the very simple one which is referred as the shooting method?

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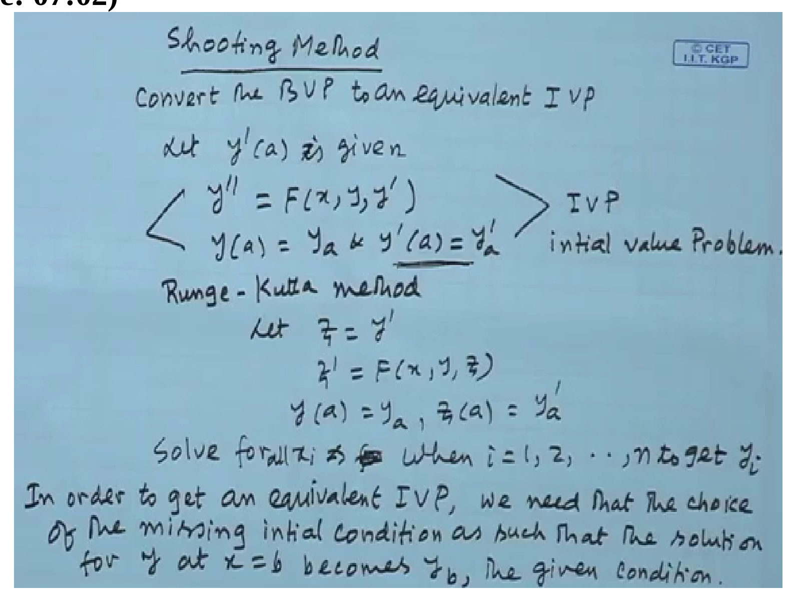

In shooting method what we do is convert the (BVP) to an equivalent IVP now in this boundary value problem what is the difficulty is that we have the conditions at two different points. Now, let y dash (a) is given why does he is given in that case the problem becomes y double dash = F(x, y, y dash), y(a) = y a and y dash (a) = y dash a , Okay.

So this we can treat it as a initial value problem IVP is Initial Value Problem. Now this solution can be obtained by any method say Runge – Kutta method for example, now I am not going to talk about Kutta method, now what you can do is to solve this say let z = y dash and z dash = f (x, y, z) so you get y (a) = ya and z(a) = ya dash so solve for xi for I equal to xi where is wearing from 1, 2 up to n. So in that process because our task is to suffer for all xi when I equal to 1 to n to get yi so our task is to get yi, this is one among the method.

Where we assume the if you have supplied the missing the initial condition corresponding initial condition y(a) = y dash a, so I can convert the given boundary value problem to initial value problem and solve step by step starting from x = a, then we go much for what and get the solution of to n. These two solutions will be equivalent, provided we get the ya, we get the solution by this manner, x = b and at y b, so that correspondence has to be satisfied.

So in order to get an equivalent IVP we need that the choice of the missing initial condition search that y whatever but at X equal to that the solution for y at X =b becomes yb the given condition obviously we do not have the idea that y, what the y dash a should be so we go in a iterative fashion so at each iteration.

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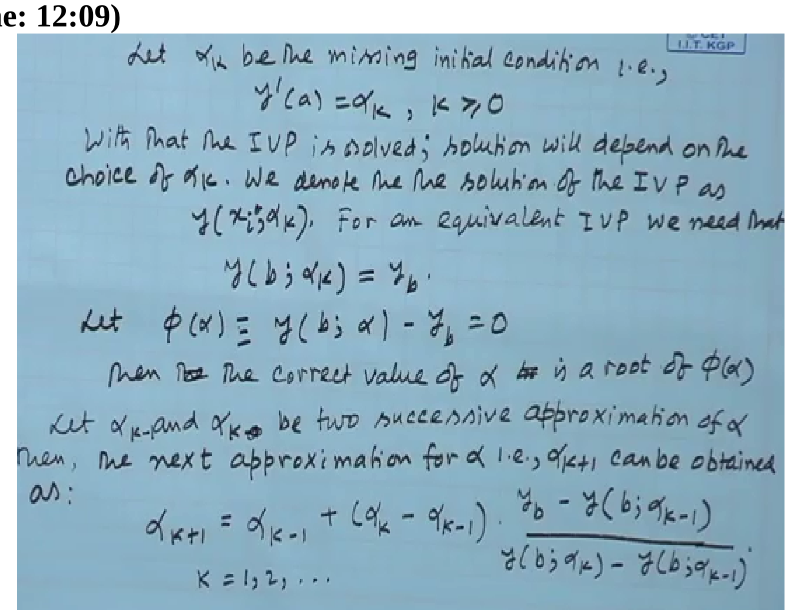

Let Alpha k be the missing initial condition that is y dash (a) = Alpha k, k is some number, greater than equal to zero, we define what k is, Now with that the IVP is solved obviously this IVP the solution will depend on the choice of Alpha k so we denote the solution, to do that with denote the solution of the IVP as y(xi, Alpha k).

Because this why y(xi, Alpha k) will vary on the choice of a Alpha k, to make a correspondence we have written this as a function of Alpha k , now for an equivalent IVP, we need that y at b Alpha k should be equal to yb, so that need to be satisfied. So this gives a guideline to find the Alpha k the missing initial condition so let if we define a function that Phi Alpha is a function which is yb Alpha - yb = 0.

Then the proper choice the correct choice Alpha is a root of this above equation, root of Phi Alpha convince that particular Alpha who is satisfied this equation will be the correct choice for the missing initial condition because for that only we get this. Now what we do so this gives a way how to find this Alpha so far we have not talked about Alpha what we talked that you choose some assume some value for the missing initial condition solve the IVPS.

Equivalent IVP and get the solution y(xi, Alpha k) for all this i get points and get why yb Alpha k. Now that Alpha k which is the missing initial condition will be correct provided we get this relation this will give you. So we know construct a equation for Phi Alpha = 0, Defined. By this way so this gives the clue and how to find this Alpha Q, now let Alpha k and Alpha k - 1 be rather Alpha k – 1 and Alpha k be two successive approximation of Alpha.

Then we can determine the next approximation for Alpha let us called that is an Alpha K + 1 can be obtained as so here we apply the second method for finding the roots that means we join the two points by a straight line and the point where it meets the x-axis is taken to be the next approximate value for the root, so y b – y(b, Alpha k – 1) by y(b, Alpha k) – y (b, Alpha k -1,so k is 1, 2, etc.

Now we get a idea or get a guideline that, how to get the missing initial condition which should be the proper one in order to replace that IVP, in order to replace the boundary value problem BVP 2a IVP so what do you do that we choose two successive approximation so if I start the iteration so k = 1 so you get 0 at 1. So Alpha 0, Alpha 1, so the iteration process goes like this way.

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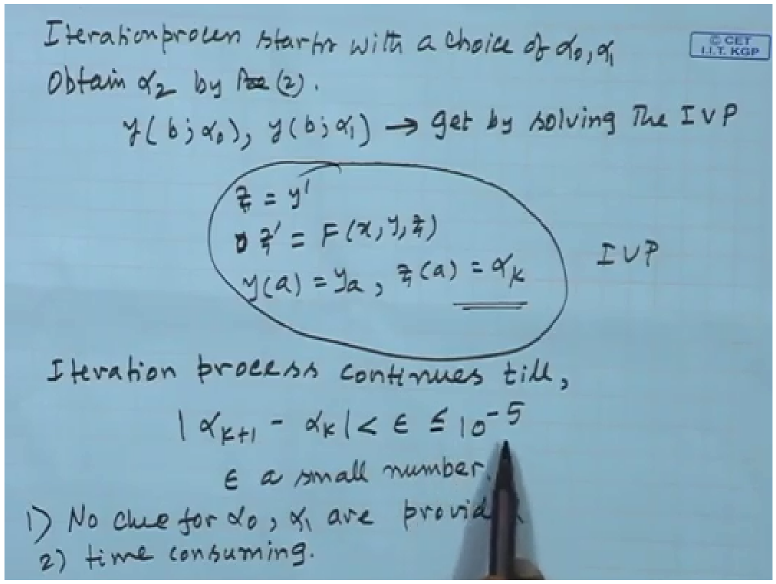

So the iteration process starts with a choice of Alpha 0 Alpha 1 then obtain Alpha 2 by the previous relation solved solution as equation 2 and the IVP we call as equation one so by two, to get that Alpha 2 what I need is we need to find out the y b Alpha 0 and y b Alpha 1. So for that get by solving the IVP okay, so once I get the Alpha 2 so again I go back and solve this IVP.

Which is again if I repeat can be written as a z = y dash, z dash = f(x, y, z), y (a) = ya and z (a) = Alpha k. So Every time we solve this one IVP this is the equivalent IVP to get this y Alpha k, where k is obtained go the equation two, get the next modified Alpha K + 1 and repeat the process, so iteration process continues till we find that two successive approximation are very, very small listen say like 10 to their - 5 or less, depending on your order of accuracy and this is a small number, which established the criteria for convergence.

So this is how the shooting method goes, so that means shooting method we can use for any sort of problems with it is a material of whether it is a non-linear or linear problem iteration process starts with shooting method we replace the given point value problem to equivalent initial value problem by considering a missing initial condition assume the missing initial condition with the missing initial conditions solve this problem go back to equation number two, to get the successive approximation.

What they are the modified form of the missing initial condition and so on, one of the difficulties in shooting method is how to choose these small number solutions. Alpha 0, Alpha 1 there is no clue, no problem does not no clue Alpha zero Alpha 1 are provided and also so these are the difficulty and also this is a time consuming because I say for example if I apply the fourth order Runge-Kutta method.

So we have to go from A to B with few numbers of steps and it will go for quite a reputation because depending on how many K you required to satisfy this criteria. So this will be a time consuming process now one easier method that is the most popular the finite difference method.

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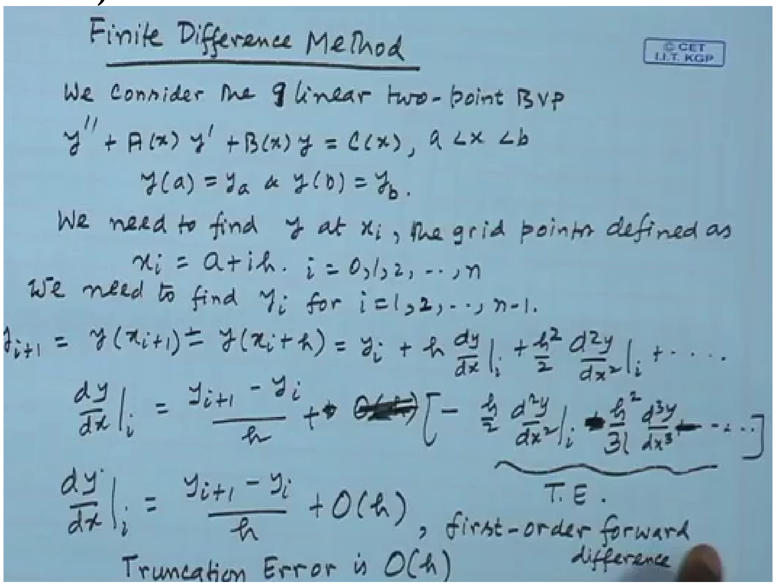

So that is our this is the straight forward way one can solve the boundary value problem at the discrete number of points again in finite difference method what do you do is approximate continuous functions at the discrete points this number of points were we need to solve the boundary value problem as that discrete points are referred as the grid points.

So if we consider Equi-space grid so we define before that so this is the way one can I would like the finite difference method.

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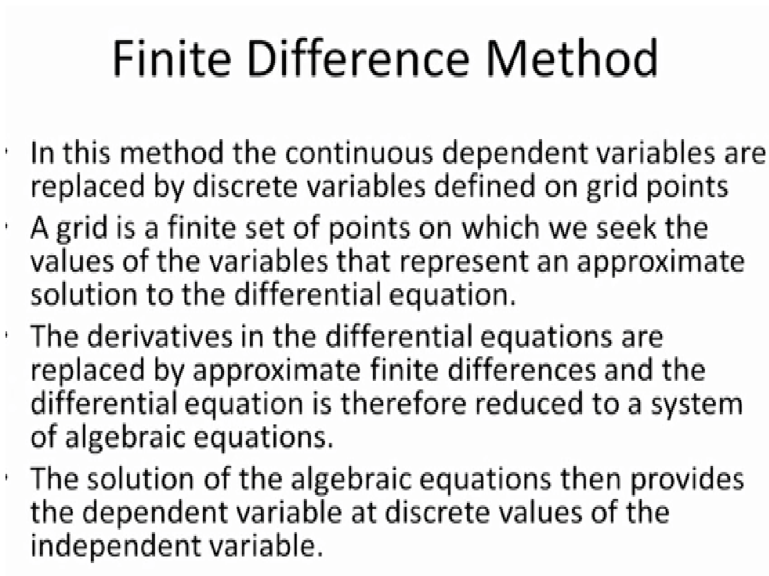

So this method the continuous dependent variables are replaced by discrete variables defined on grid points. A grid is a finite set of points on which we sit the values of the variables that represents an approximate solution to the differential equation. The derivatives in the dimensional equations replaced by approximate finite differences and the differential equation is there for reduced to a system of algebraic equation by describing the solution of the algebraic equations.

Then provides the dependent variable and discrete values of the independent variables. So consider the, first we consider the linear two point BVP, the linear two point BVP in general should be like this a less than x less than b, y(a) = ya and y(b) = yb these are the conditions are given, a b c are either constant or maybe some of them maybe 0 or functional, at the most function of x.

So we need to find out find y at xi at the grid points defined as xi = a + ih, i is 0, 1, 2… n, so basically we need to find yi for i = 1, 2….n - 1, because i = 0 and n it is given. So at every grid point we approximate the derivatives by the finite differences, how do we do that? Now y i+1 = y(xi + 1) which is nothing but y(xi +h) now if I expand by Taylor series I get, yi + h dy dx i + h square by 2 d2y by dx2 i and so on okay.

Now I can write from here where dy by dx I = yi+1 – yi by h, so the remaining terms will be of order h, because that is list order terms. So or if I write little details this will h by 2 d2y by dx2 at I – h square 3 factorial d3y by dx3 and so on. Now suppose this is + and all this terms no this is minus, I am not taking the common things so this part is the called the truncation error, now if I truncate this, so if I now approximate dy by dx at i = yi+1 – yi by h and this is the error and this will be of order h.

Where the truncation error is of order h, truncation error, because we have truncated the infinite series to a finite number of times, so beyond this whatever infinite, there will be a infinite series, so that has been chopped out, so due to that there is truncation error and that truncation error looks like is of order h, so that is the lowest order of h. So if I now approximate dy by dx this fashion that is the difference of yi+1 to different times.

So this is called the first order forward difference, same way one can write,

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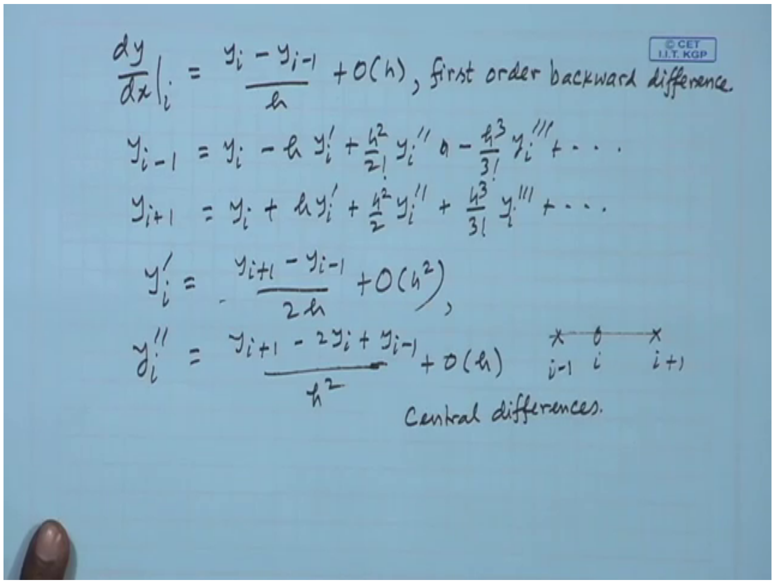

dy dx at i = yi – yi-1 by h + order h, so this is called the first order backward difference, now what I did is here yi – 1 = yi – h yi dash + h square by 2 yi double dash q – h cube by 3 factorial and this it 2 factorial yi triple dash etc., etc. And yi and just recall whatever we have done is, yi + hyi dash + h square by 2 yi double dash + h cube by 3 yi triple dash + etc., if we subtract this two, I can write yi dash = yi + 1 – yi – 1 by 2h so this becomes a order h square approximation.

Similarly yi double dash can be written if I add this two so yi double dash as can be written as yi + 1 – 2yi + yi – 1 by h square + order h so here this is the way of approximating second derivative of first derivative of higher order truncation error, now here approximating i by using i - 1 and i + 1, so that is why this differences are called Central differences, so now we got a formula that how to replace the derivative in terms of the finite differences of the function value this will use to solve the given boundary value problem in the next lecture, thank you.