Modeling Transport Phenomena of Microparticles
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Lecture - 35
Numerical Methods for PDEs

So we were discussing about the higher order differential equations boundary value problems of more than two orders in that case it leads to a system up block tri-diagonal matrix so that means we get a system in which every entry of the matrix is square Matrix..

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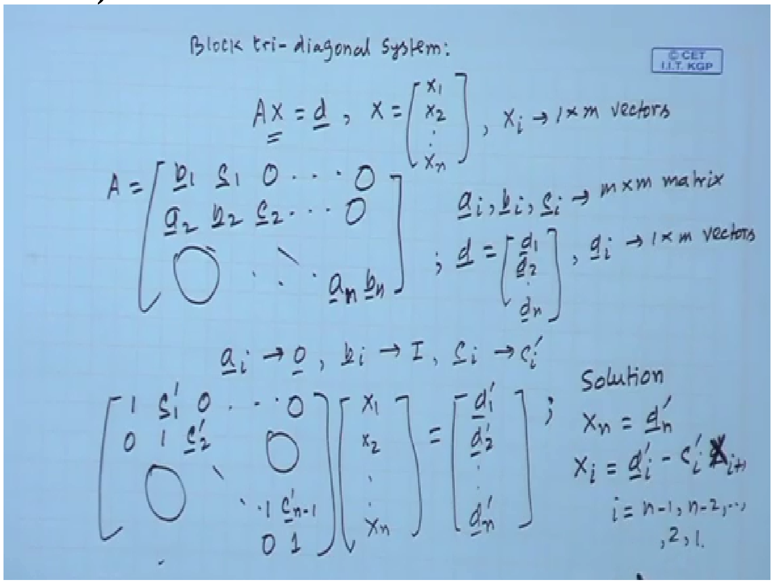

So basically what we found is that a AX equal to let us call D where is the component of X itself is have some vectors. So x1 x2 xn which are each of xi say 1 cross M vectors and the matrix A is something like b1, c1, 0, 0, 0, a2, b2, c2, 0, so remaining all are zero, so you can put a 0 over here and the last one say let us call this is An, bn so this is the situation. So where each of these ai bi ci are say let us called M cross M matrix.

And the known vector the D is say let us called this is the form d1, d2, dn, so his are the vectors so these are also this is Di are 1 cross M in vector, so what we need is to solve this for x where that is satisfied is Block tri-diagonal system. So the similar procedure has adopted in Thomas algorithm so that means reducing it to a triangular form this matrixes. The Block tri-diagonal form by block elimination.

So what you need to do is that we will bring 0 at this Ai positions so Ai should be transferred to a null matrix and Bi should be transferred to identity Matrix and obviously Ci will not keep quiet it will transfer to some other Ci dash. So the resulting situation will be a form like this 1 c1 dash 0 1 C2 dash 0 0 0 all are ze0ro over here and the last but 1 Cn-1 dash and this is 1 so this is the situation into x1x2 xn this is equal to the transformed vector.

Which we call as d1 dash d2 dash dn dash, so once I get a system like this then the solution is very easy solution we can write as from here its Xn = dn dash and generally X i = Di dash - Ci dash Xi + 1 is vector, where are i = n - 1 and n - 2 to 2 etc., by back substitution one can obtain the solution. So this last one like the Thomas algorithm so the last one prefer to get it then subsequently all this all the vectors of unknown.

So each of Xi vector one cross n so what is remaining is how to get Di dash and Ci dash so the algorithm gives us the way of finding this is so this Di dash and Ci dash.

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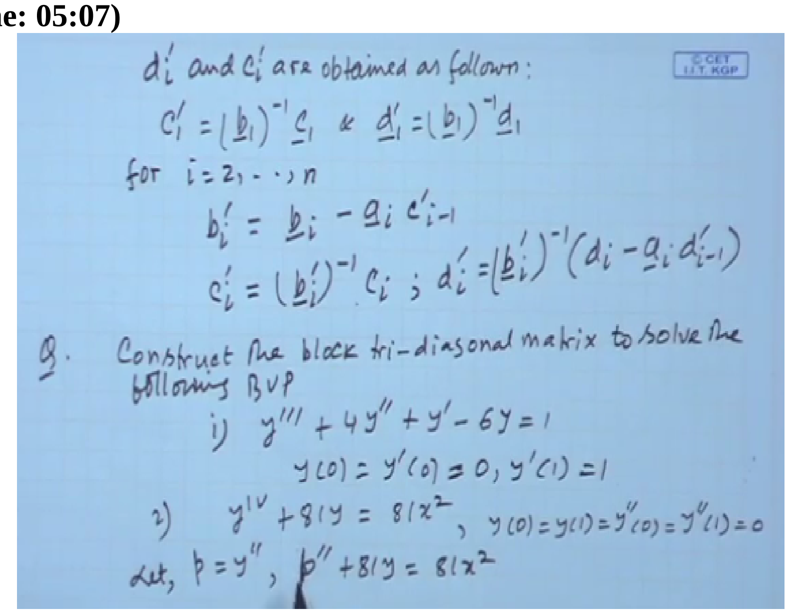

Those are obtained as follow, so first one can obtain the C1 dash which is quite evident B1 inverse C1 and D1 dash = B1 inverse D1. So this is the two elements for i = 2 to 2 - n in here, so this is Bi dash it is the in between matrix which we do not required to store once, we get this other co-efficient Ci dash is = Bi dash inverse Ci and Di dash = Bi dash inverse Di - Ai Di dash - 1, so this is i = 1 to n.

So once we complete this we get the whole reduced coefficients or reduced form of the block tri-diagonal Matrix. So this gives us the complete algorithm so that means what we need to do is we fit the coefficients disgraced equation the corresponding coefficients Bi Ci etc., from there we construct Ci dash and Di dash and so one can obtained the block tri-diagonal also construct the block tri-diagonal matrix to solve the following BVP once Y triple dash + 4 Y double dash + Y dash - 6 Y = 1, Y0 = Y dash 0 = 0 and Y dash 1 = 1.

The question to we can have 4th order it 81Y = 81 x square and you are given the condition Y0 = Y1 = Y double dash 0 = Y + 1 = 0, now in many cases as we have started with that we can directly solved by this 4th order or third order we can reduce to a we can use 5 point formula and get a system of equations but the thing is that we would not get a tri-diagonal form because there will be 5 variable unknown.

But your 5 girds are involved at each location at h, xi grid points is associated with i – 2 to i + 2 so which rules out the consideration of tri-diagonal system now if you do not have a tri-diagonal we want all the thing is we all get a direct method to solve this but if I go by this manner, say let p = y double dash and p double dash = 81y = 81 x square, so this is a system of two second order equation with boundary conditions are y0 = P0 = 0.

And y1 = p1 = 0, so any number of grid points one can obtain a block structure corresponding to this and can apply the block tri-diagonal algorithm what we just described and get the solution for any choice off the grid points. So this is about the linear situation of when we have a nonlinear situation so things become quite complicated because if we have a nonlinear differential equations.

Now if we apply the finite difference scheme central difference or whatever scheme so it will lead to a system of nonlinear equation so it is expected.

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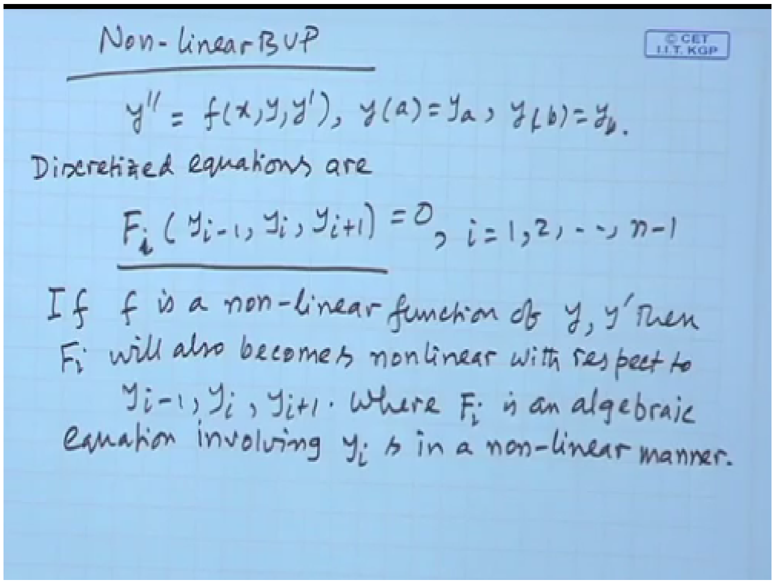

So go for nonlinear BVP so to solve this nonlinear BVP so nonlinear BVP means it will be of any form xy y dash y(a) = ya and y(b) = yb so we need to solve this for a less than x, less than b so if discretize equation looks like will be of this form equation for if I say the discretize equation at this point Fi(yi - 1, yi, yi + 1) = 0 this kind of equations, we can get for i = 1, 2, to n – 1 to our notations whatever notations we have used.

We have taken the grids as xi and we need to find out the yi from equal to 1 to n - 1 discretize it is grid we use central difference scheme for y double dash y there is so I get it now if f is a nonlinear function formation of y, y dash then fi will also become nonlinear becomes nonlinear combination also becomes nonlinear with respect to y i – 1, yi, y + 1.

So now that algebraic equation whatever they will also in aware if fi is a say and algebraic equation, equation involving yi s in a nonlinear fashion thus reducing it to a matrix form is not going is ruled out is not going to be possible for this nonlinear set of equation so if we have grid say n, now we get n - 1 of grid points, and for each you have equation given by this way. So do that we use the Newton Raphson method.

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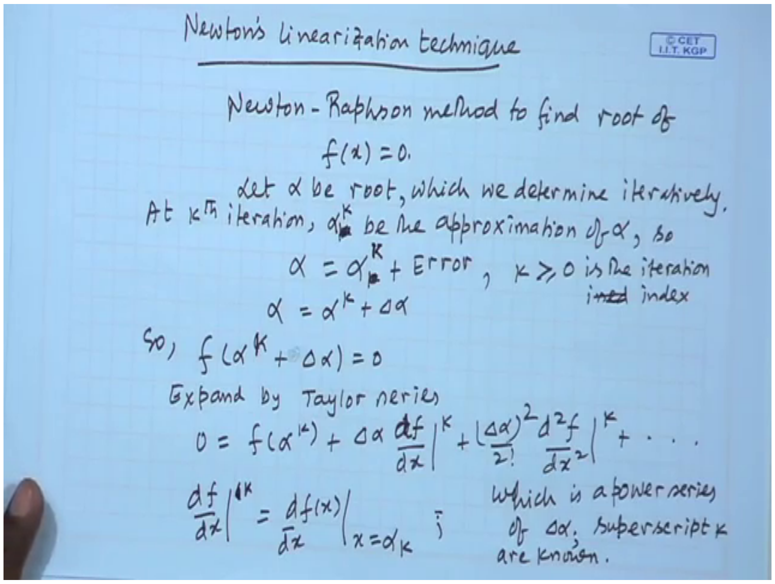

To say in Linearization technique it is an iterative procedure before I talk about the Newton technique with respect to the knowledge about your problem. So first recall what is that Newton Raphson method for finding root now Newton Raphson method to find root what I do to find root of se F(x) = 0 and algebraic equation some equation text or algebra. Whatever so what do you do is let Alpha be the root which we determined iteratively at k + kth iteration Alpha K be approximation of Alpha so we can write Alpha = Alpha k + some error.

Because obviously this is not the same as the root case let us put here as k as superscript because so that we can distinguish it with the iteration index where k is greater than equal to zero is the iteration index. So let us call this is Alpha = Alpha k + Delta Alpha obviously f (Alpha k) + Delta Alpha = 0, because it is the exact solution of the route we expand by Taylor series so what I get is 0 = f(Alpha K) + Delta Alpha into df.

Because it is only single variable should dx this is approximate value kY that needs access replaced by Alpha k then Delta Alpha whole square by two factorial d2f by dx 2 k, k means Alpha = Alpha k + etc., okay, now where notation denotes that this is ddx of F(X) at X = Alpha k this is not a ship we have used similarly second order and all defined that this is a which is a power series of Delta Alpha so all this with superscript k variable superscript unknown.

So basically this is an equation for Delta Alpha to solve the infinite degree polynomial and get Delta Alpha you get the exact solution which is not possible. So I do is we can solve easily up to the linear order terms, so I retain after the linear order at drop all these terms beyond this if we do that so what I get a approximation.

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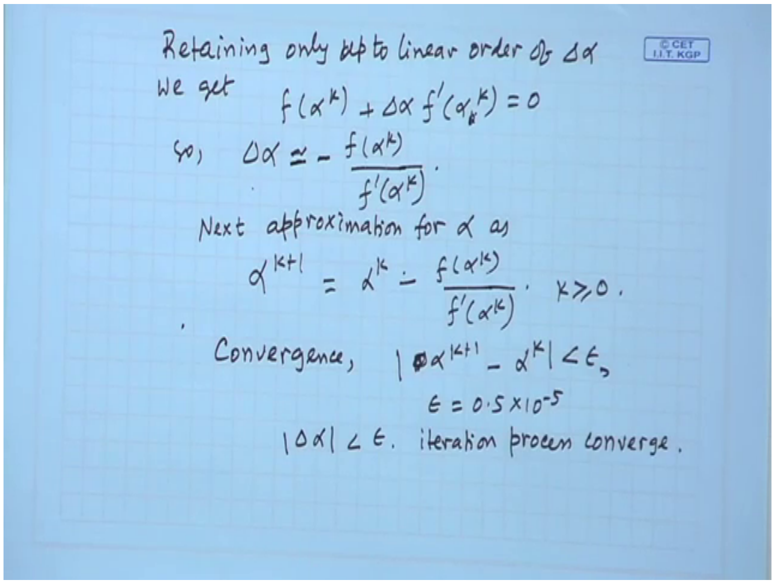

So retaining only have two linear order of Delta Alpha we get f (Alpha k) + Delta Alpha f dash Alpha k = 0 this is also we can write this way equal to see. So this gives you Delta Alpha which is the error at the kth iteration as f (Alpha k) by f dash (Alpha k) so obviously this error is not the exactly the same as the error we are looking for. So we call the next approximation for Alpha K + 1 = Alpha k - f (Alpha k) by f dash (Alpha k).

So basically what you are doing his k greater than equal to 0, tell you what you are doing is getting an approximate value of the error at the kth iteration by this manner. And then we are heading to the existing value Alpha k find a to get a modified and Alpha k + 1, so this is the way subsequent iteration proceeds so for convergence of the iteration we need that Delta Alpha, so what I need is convergence that two successive iterated values should be very small and Epsilon e is a say something like 0.5 into 10 power – 5.

So very small quantity so in other words if I Delta Alpha there is an Epsilon so iteration can watch, so this is how the Newton Raphson method for finding root of a non-linear equation is same procedure will adopt here for the case of a nonlinear boundary value problem so the nonlinear boundary value problem what do you do is for we go back to our nonlinear cases.

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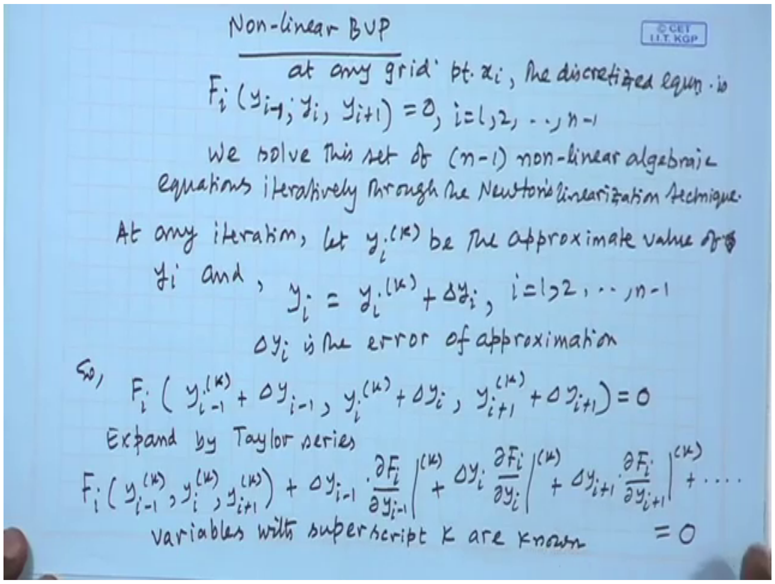

Non linear BVB so we have fi at any grid xi the discretize coefficient is fi y - 1 yi yi + 1 = 0, we substitute solve this equation this is what i = 1, 2, n - 1. So we solve this set of n -1 nonlinear, here it is algebraic equations iteratively through the Newton's lineation technique for that what I do at any iteration let yi (k) be the approximate value of yi and we can write this yi = yi (k) + some error + Delta yi, where Delta yi is the error of approximation at the kth iteration i = 1, 2, n – 1, at the 2n, i = 0n,we have given the yi.

So I did not have to find out the value of yi, so we can take Delta yi – 0, if I substitute so I must have this yi (k) + Delta y - 1 this is not over here - 1 + Delta yi , yi + 1 (k) + Delta yi +1, so basically what I need is we need to find out this errors, to do that we expand by Taylor series as we did for Newton Raphson method so what I get is here fi (y - 1 k, yi k, yi + 1 k + Delta) there are three variable yi – 1.

So we take a partial derivative Delta yi - 1 this is that all the variables are evaluated it kth direction, so this is known this position is know, so this is Delta fi by Delta yi k + Delta yi + 1 Del fi Del yi (k) + all the higher orders so this is = 0 so here always superscript one things need to be known variables with superscript k are known, only up to the linear orders of Delta yi.

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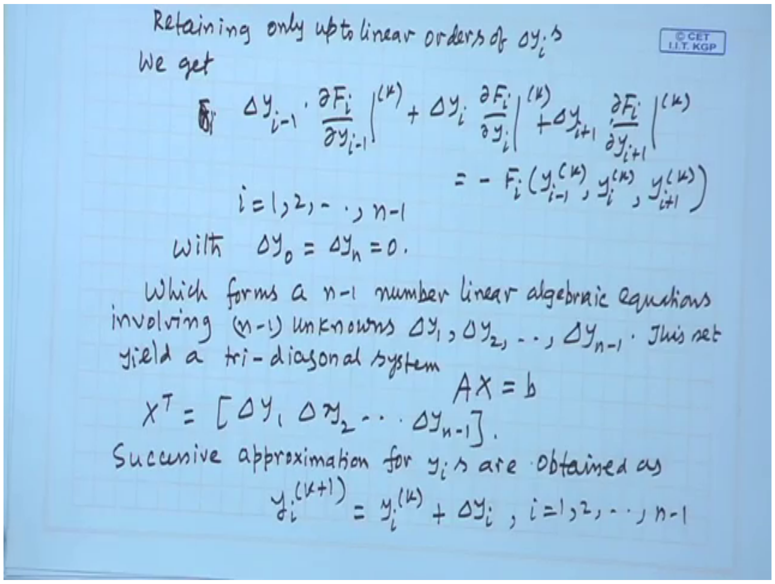

Retaining only up to linear order, orders of the Delta yi s we get fi so we get a equation is linear in Delta fi Delta yi - 1 k + Delta yi Delta fi Delta yi k + Delta yi + 1 Delta fi by Delta y + 1 k = this is known so I transferred to the other side – fi (yi – 1 k, yi (k), yi + 1 (k)), so this is for i = 1, 2, n – 1, so that means with Delta y0 = Delta yn = 0, because we are not doing any iteration, at the two boundary points are given.

So which forms a n -1 number of linear algebraic equation, equations involving n - 1 unknowns Delta y1, Delta y2, up to Delta yn -1 this set it is a tri-diagonal system one can very easily see that this is for tri-diagonal system Ax = b, where X transpose is vector Delta y1, Delta y2, Delta yn – 1 so solution of which will give you the X. So once I obtained the solution the successive approximation for yi ‘s are obtained as yi k + 1 this is our next approximate value.

This was the old one plus whatever the value obtained now for i = 1, 2, n -1, so this is iteration procedure as to use it like this way so that means every iteration, we are basically solving a tri-diagonal system given by this is Ax = b, once I solved I get the error vector, Delta y1 Delta y2, Delta yn -1 at the kth iteration.

And K is greater than = 0 so once I get this Delta yi's I add to the previous iterated value, yi k and get the updated value yi k + 1, so iteration value should go on till we get, so iteration procedure converges.

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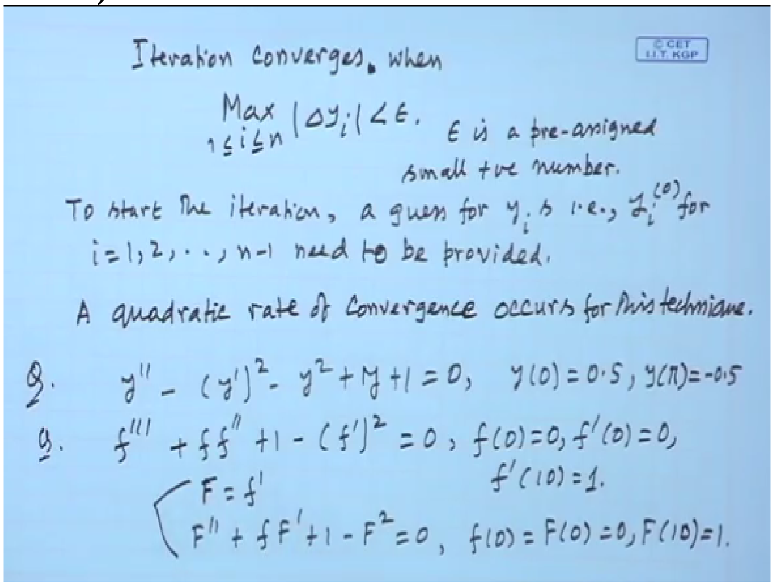

When we get when Max of 1 Less than i less than equal to n, Delta yi is less than Epsilon, it is as good as saying that two successive iteration values are less than Epsilon, so in that situation Epsilon is pre-assigned small positive number, now here we can see that to start the iteration point a guess for yi s that is yi (0) for i = 1, 2, up to n -1 need to be supplied or provided or assumed.

This method does not give any clue to how to choose this yi0 but one attractive feature is that the quadratic rate of convergence occurs for this technique that means if we get convergence it converts very fast within few steps itself so this is a very biggest advantage to solve the nonlinear equation so basically what I do in the Newton Raphson and Newton lineation procedure is that we have the nonlinear quadric value problem with it is discretize through the scheme.

Whatever we fill, say central difference scheme and that will lead to a set of linear set of nonlinear algebraic equation of the group values that is grid we assume some value as yi0 and then subsequent values obtained by choosing a error yi and yi + k like yi + Delta yi Delta y's, i satisfies a linear system which for tri-diagonal one can solve this with y0 = 0.5 and y(Phi) = -0.5.

So this is a nonlinear now one thing to be remembered that here whenever we talk about the nonlinear it is, we talk about the nonlinear of y not about x, so another third order equation this is very common equation which appears in free dynamics boundary layer flow pro positive edge. So this is 0, f dash 0 is 0, f dash (10) = 1 to solving the set of equations is required the computer programming.

But one can get a better one tri-diagonal system for this case it is to be block tri-diagonal because if I substitute is f = f dash, so we f double dash + ff dash + 1 – f square = 0, so it is a nonlinear system with condition as f(0) = f(0) = 0 and f(100 = 1, so this kind of system using the Newton lineation technique one can derive the block tri-diagonal form and iteration procedure will provide the approximate solution at every iteration okay.

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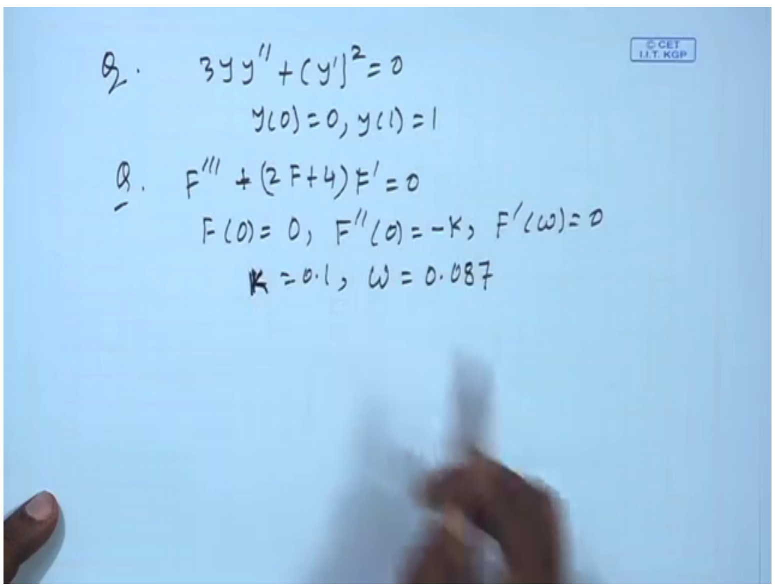

Now one more problem I can give is 3yy double dash + y dash whole square = 0, y(0) = 0, y(1) =1 and then another is this is for the thermal flow through an orifice, as a orifice free dynamics problem orifice flow post office if you have a small orifice f double dash is the flux which is given as k and f dash Omega = 0 , k is taken to be 0.1 here and Omega = 0. 087 so next will talk about that partial differential equation that is functions of which is depending on more than one variable in the next lecture thank you.