Modeling Transport Phenomena of Microparticles

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Lecture - 33
Numerical Methods for nonlinear BVP

So the truncation error arise when we have we can write a very short form truncation error.

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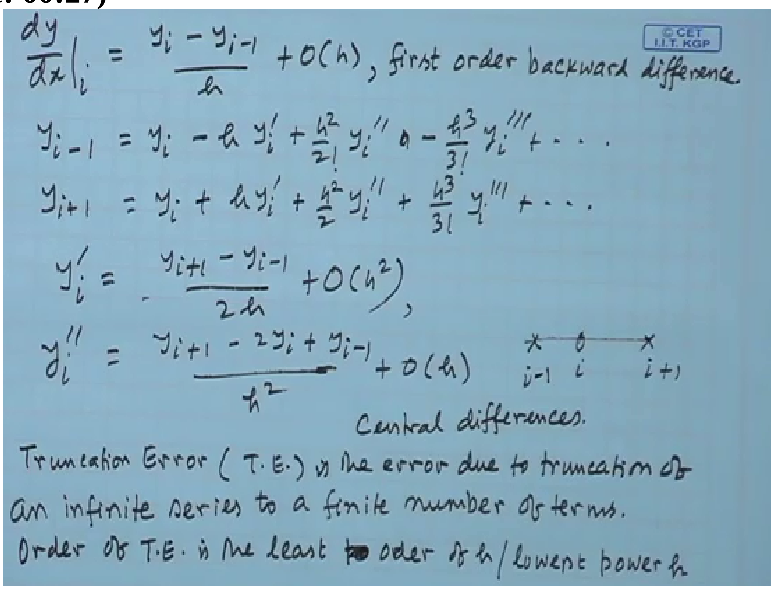

So in short way I have written error due to truncation of an infinite series to a finite number of terms and we define the order of truncation error, order of t is the least power of or least order of lowest power of h, least order of h, lowest power h because this is a series in power series of h step site so this becomes the lowest order or lowest power of h, so now this formula gives us the way the derivatives can be approximated now let us substitute.

The approximation to the given boundary value problem.

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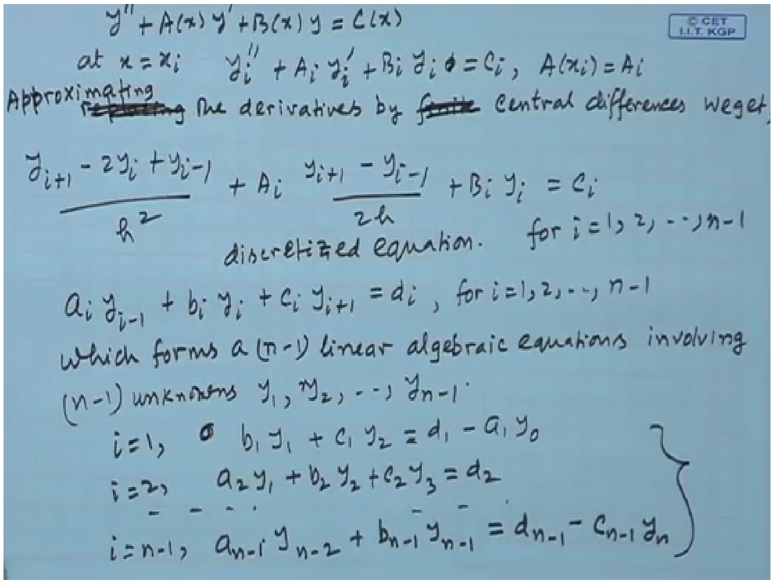

So we have the boundary value problem if I recall y double dash + xy dash + b x y = C(x) at x = xi, any grid point, we have yi double dash + Ai yi dash = ci, her we denote A(xi) = Ai in short now replacing the or approximating I think that will be the better term approximating better term and the approximating the derivatives bye finite differences by central differences we get if I know approximate the derivative by central difference formula so here we get, yi + 1 – 2yi + yi – 1 by h square + Ai yi + 1 – yi – 1 by 2h + Bi yi = Ci.

So this is the one is quality discretized equation which is referred as the discretize equation, now at each grid point, so this for i = 1, 2, n – 1, now we are looking for the values of y0, y0 yn is given so I want to yn - 1 so if I put together we collect that like omissions and put in this manner ai yi - 1 + bi yi + ci yi + 1 = di for I = 1, 2, n - 1 which forms a n - 1 linear algebraic equations involving n - 1 unknowns what are the n – 1 are y1, y2, yn-1 because y0, yn are appearing but they have given values are prescribed so that can be transferred to the right side.

So one example if I put i = 1 so which looks like a bee b1 y1 + c1 y2 = d1 – a1 y0 which is given the next is this is for i = 1, i = 2, if I substitute so I get a a2 y1 +b2 y2 + c2 y3 = d2 and so on i = n – 1, to last one is given an-1 yn - 2 + bn - 1 yn-1 = dn - 1 – cn – 1 yn because this is known sure this is why and we can transfer to the right side the known site so this other system of linear algebra equations right side is the known vector.

Now if I put in a matrix form so writing let us call this is the system of equation has one, so if I know introduce a vector.

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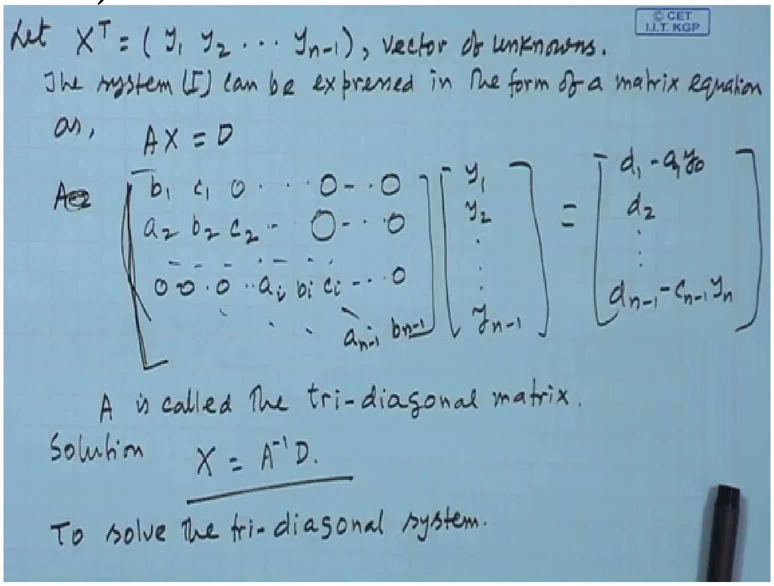

Let X transpose is this vector y1 y2 y n -1 vector of unknowns, so star can be the system 1 notes till one can be expressed in a matrix equation as AX = D or par ability, where A how it looks like A or this Matrix say if I write the first row it will we b1 c1 all the elements that you are next row a2 b2 c2 all the remaining elements are 0, and like this way any ith row what you find that these are all 0 and except ai bi ci okay so let us call this 0's so these are all zero elements.

And finally the last row will be a two elements a - 1 bn - 1 and here it is multiplied with the vector y1 y2 yin - 1 equal to this is d1- a1y0, d2 and dn - 1 – cn- 1 yn, so the matrix equation looks like this for this kind a matrix A is called a tri-diagonal matrix so solution will be basically what we are looking for the solution X = A inverse D, now our task is to solve the tri-diagonal system.

So if the matrix is a trade I want to so it is very little easier compared to other situation because it a diagonal tri-diagonal matrix can be very easily convert it to a lower triangular matrix or upper triangular matrix before that let us consider a simple situation consider this linear boundary value problem.

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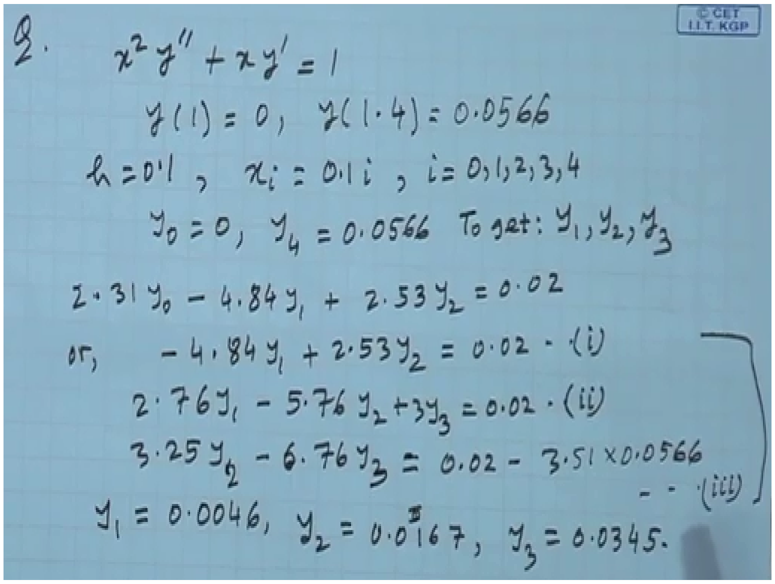

So x square y double dash + xy dash = 1, y(1) = 0, y(1.4) = 0.566, if I choose h = 0.1 and xi = 0.1i, i = 0, 1, 2, 3, 4, 0 and 4 are the y0 = 0, y4 = 0.0566 and write the boundary conditions and all. So, what I find that this equation becomes 2.310 y0 - 4.84y1 + 2.53y2 = 0.02 in other words I can write this is -4.4 or this is y0 is given transferred to the other side -4.84y1 + 2.53y2 = 0.02 equation 1.

So this are given to get y1, y2, y3 so this is the first equation next equation then next equation is 2.76y1 – 5.76y2 + 3y3 = 0.02, this is equation number 2, then next equation 3.25y2 – 6.76y3 = 0.02 – 3 because it will y2 y3 y4 so y4 is 3.51 into 0.0566 so this is y4 so this is the constitution the equation third, so we have now three linear algebraic equation which can be solved and that looks like it will be a solution has 46, y2 = 0.0167, y3 = 0.0345.

Now we are lucky because we have a 3 by 3 matrix equation or 3 by 3 systems of equations which can be solved quite easily by this matter. But if we have a large number of systems so in that case we may not be that lucky to solve by a manual procedure so that required a algorithm which will discuss now.

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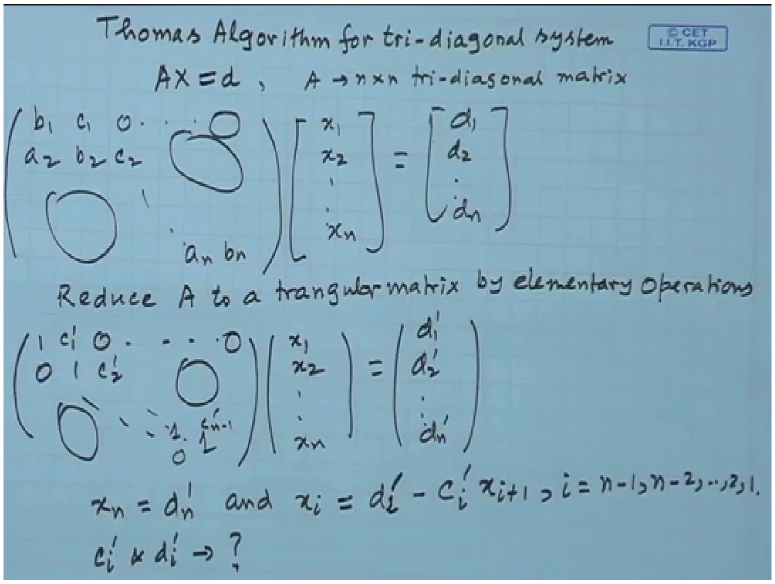

So this is called the Thomas algorithm for tri-diagonal system Ax equal to say D, so we have a tri-diagonal A is a n by n tri-diagonal matrix, this is the b1 c1 0 0 0, a2, b2 c2 so let us put a big zero over here and the last one an bn and this is a x1 x2 xn this is a vector of unknown and d1 d2 dn, so in this what we will do is reduced A to a triangular matrix, by elementary operations so that means what I do is before the diagonal elements.

All the Ai position we bring 0, diagonal positions we bring to 1, for example and so the reduced form is 1 c1 dash 0 0 0, 0 1 c2 dash and the last one is 1 and this is 1, so this is x1 x2 xn, so obliviously these positions also get changed because we are doing the elementary transformation so the coefficients are alter. Now we get a triangular system where all the elements are 0 at the one so this is the 1 and then next one is 0, so next one if I write this is cn -1 dash.

And this is also so this is 0, now once I have a system like this way I can very easily write the solution has xn = 0n dash and xi = to if I go by back substitution xi = di dash minus ci dash xi +1 i = n – 1, n – 2, etc., 2, 1. So first one I get the last variable from the last equation that is we get the first then subsequently us part 1 and so now we need a algorithm.

So what is ci dash, and di dash are what? if I know how to relate this ci dash and di dash with the given a1 b1 c1, ai, bi, ci, etc., so then we are through so at this stage we get the solutions which is required to be opted so Thomas algorithm and also one can also derive that is if you do this step by step procedure.

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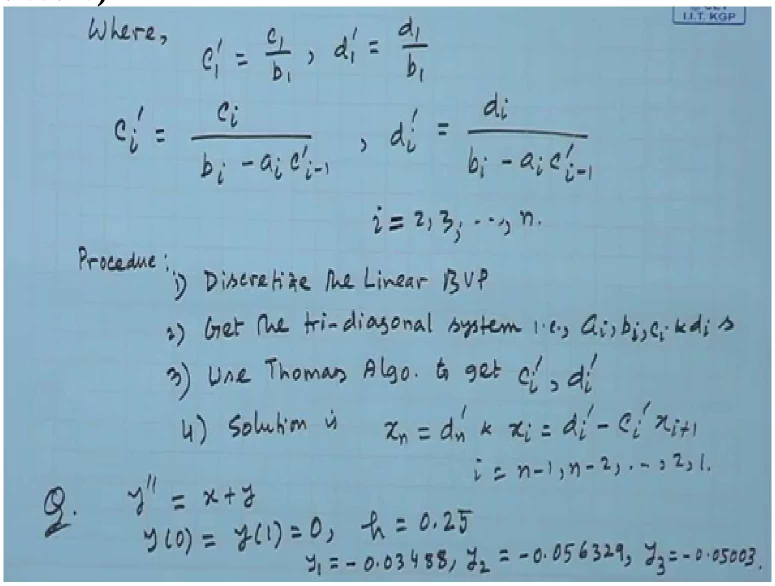

So where write this way where c1 dash = c1 by b1, I think it is very easy to say this one and d1 dash = d1 by b1 given by we were just first row c1 b1 divided b1 and we write this ci dash = ci by bi – ai c dash i – 1 and di dash = di by bi – ai c dash i – 1, this is for i = 1, 2, 3 etc., to n, so that procedure is so procedure is decretive the linear BVB, get the tri-diagonal system. that is aibi ci and di, then use Thomas algorithm to get ci dash, di dash by this manner and the solution is Zn = dn dash and xi = di dash – ci dash xi +1, i = n -1, n -2, ….. 2,1.

So this is the simple steps one need to follow to solve the linear boundary value problem. So once I derive the decretive form and then the tri-dimensional system so one can determine the ai, bi, ci are determined so through that we compute the ci dash, di dash, once those are computed the solutions are obtained. So one can solve this problem xy y0 = y(1) = 0 let us take h = 0.25 and use Thomas algorithm to obtain the solution.

So solution are so these are the solutions of the given system. So that is how the tri-diagonal system goes now here one thing to be noted is that the order of accuracy the truncation error.

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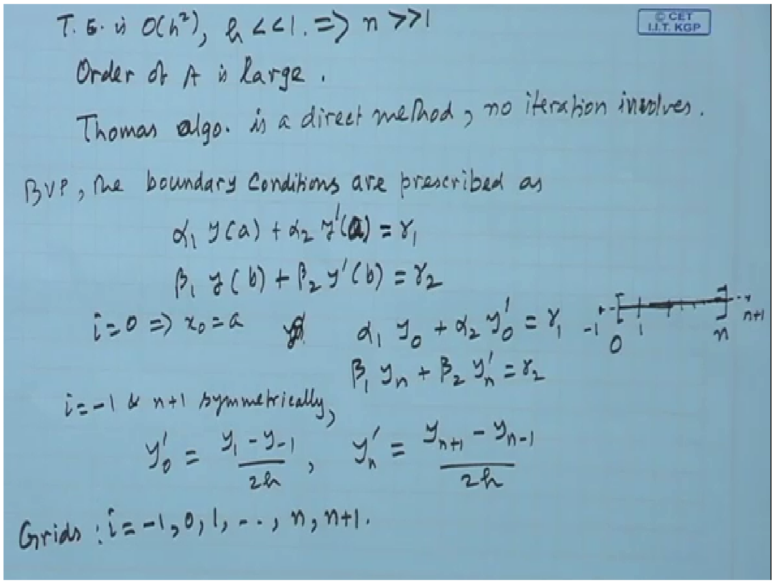

Order h square so h has to be quite small so this implies that the n number of grid is quite large so that is to say the order of A is large now because this tri-diagonal structure of the matrix A so you could get a algorithm, Thomas algorithm which is a direct algorithm without doing any iteration like Gauss IDL or Gauss Jocovis so one can obtain the solution directly so that is the advantage of having a tri-diagonal system.

Now so this Thomas algorithm direct method no iteration involved but the given matrix should be tri-diagonal, now one thing is that for getting tri-diagonal you have to use three points. The if I go beyond three points so that difficulties that we may not get a tri-diagonal, now some of the boundary value problem in BVP the boundary conditions can be the derivative, or prescribed as a Alpha 1 y(a) + Alpha 2 y dash (a) = Gamma 1, this is one boundary condition.

And Beta 1 y (b) + Beta 2 y dash (b) = Gamma 2, so this is the situation then there is a difficulty, now i = 0 corresponds x0 = a, so now if I have to approximate y dash 0, in terms of the that the boundary condition looks like Alpha 1 y0 + Alpha 2 y dash 0 = Gamma 1, If I want to use the central difference over here so that means but our grid starts from 0. So this is 0, 1 etc., and that is n over last point.

But the derivatives are involved at y dash 0 similarly Beta 1 yn + Beta 2 y dash n = Gamma 2, so remedy is to choose 50 CS points, say this is -1 and this is in n +1 see if I introduce i = -1 and n +

1, symmetrically, so in that case I can replace y dash 0 as y1 – y – 1 by 2h and y dash n = y n + 1 – yn – 1 by 2h so grids are now i = - 1, 0, 1, etc., n, n +1.

So we have the how many grid n + 1, - 1 so 3, 1 to n +1, 2 and 3, so this many grid points and also the equations we have this, now one can solve this for so what you can do is there by using this equations boundary conditions what you can do is we can write the y - 1 in terms of y0, y1 similarly yn, yn + 1 and so solve the discretized equation 1 for i = 0, 1, 2, ….n and replace y – 1, yn + 1 by using the boundary conditions b.c.s.

So by using the conditions y – 1, yn + 1 so the resolving system of equations will be involving n + 1 unknowns and n + 1 equations so that is a compact but the solving this is one get a again we can get a tri-diagonal because y - 1 is see this is we are replacing y0.

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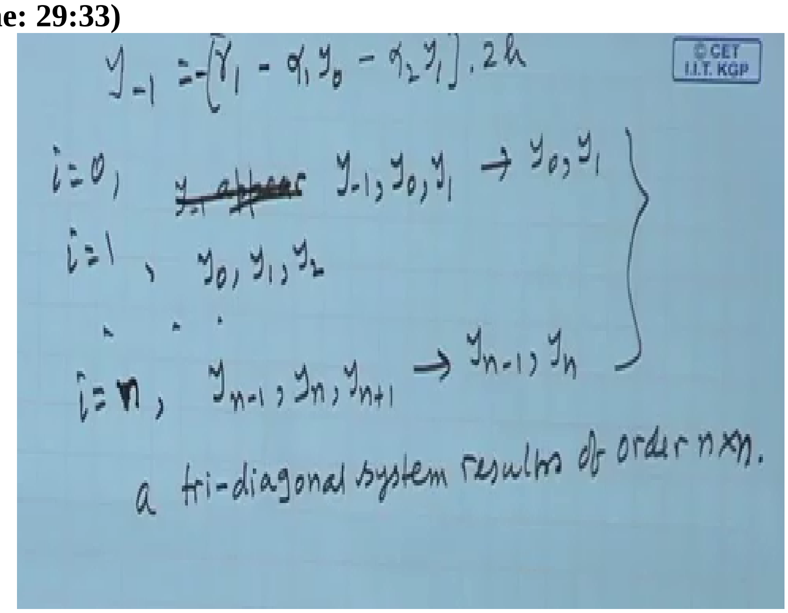

So y - 1 we are replacing by what we can write is Gamma 1 - Alpha 1 y0 and so this is -, so this is – into 2h so this is – Alpha into 2h when I write the discretize equation i = 0, so we have a y -1 appeared so i = 0, the first point so that involves y – 1, y0 and y1 so one I replace y – 1, y0, y1 so again it will involve y0, y1 and remaining i = 1 that involves y0 y dash 0 = 1, so it is tri-diagonal, so if replace i = n if I replace the grid points,.

We have yn – 1, yn, yn +1, so if I replace yn, n +1, in terms of yn and yn – 1, so again it will be reduced yn, so that means a tri-diagonal system resolves, of order n cross n, not n - 1 however this is a we can work out with that. But if it is a nonlinear equation then this is not a proper way to solve because of instability that may arise because of this fictitious point, we are considered the great beyond the domain.

To make sure that creates a non that may impose instability for nonlinear situation. So that is why we have to look for some other way to handle the derivative boundary conditions which will talk with the next lecture. Okay, thank you.