Design and Optimization of Energy Systems

Prof. C. Balaji
Department of Mechanical Engineering
Indian Institute of Science, Madras

Lecture No. # 15
Lagrange Interpolation Contd…

Let us consider a Lagrange interpolation formula. I am looking at higher order derivatives. So, we used the Lagrange interpolating polynomial to find out the intermediate values in the last class.

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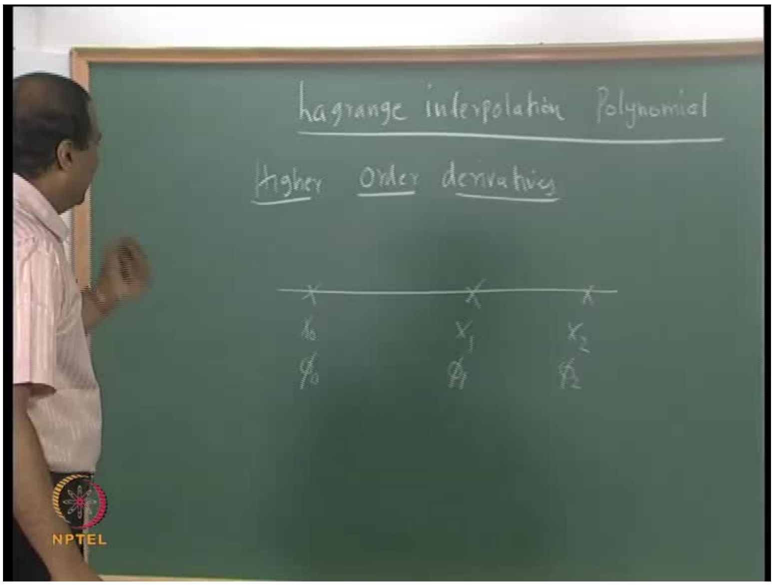

I quickly went on to getting the first derivative, second derivative, and then I went to Laplace equation. I did so many things very fast; so, now I will try to slow down, and let us go through whole thing again.

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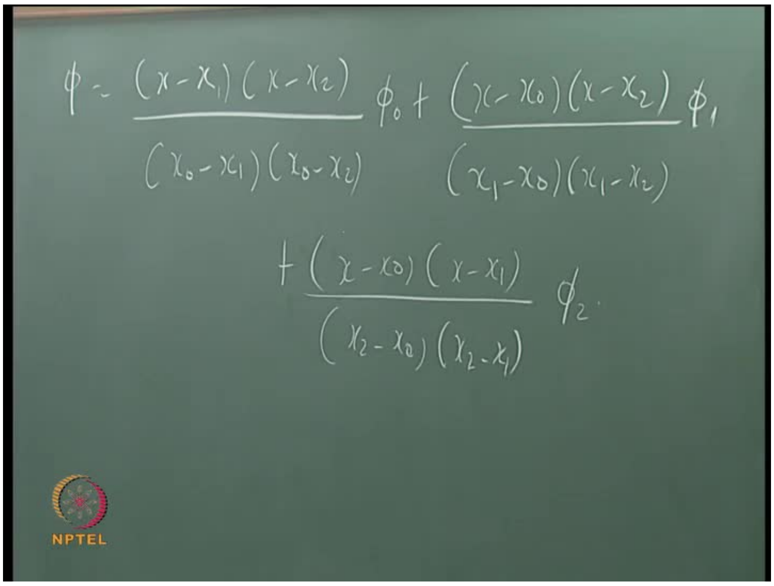

So, the phi given by… so far so good; so, the beauty of this is, at exactly x naught x 1 and x 2, at x naught x 1 and x 2, this will be exactly satisfied; there will be no error, but it does not mean that all intermediate points, it will satisfy because using three points we are approximating it by quadratic. So, there will be error when interpolate between these thing; interpolating in between x naught and x 1 or x 1 and x 2, but given that you have only three points, and you want to have a polynomial which passes through all the points, the best is the polynomial of order two; this is the best you could get. Locally, you can have a linear interpolation between x naught and x 1, and x 1 and x 2; this is what you did in your using steam table.

But if the function is non-linear, this is the much better approximation compared to linear interpolation, though linear interpolation can be quickly done on a calculator. This will take a little longer time, but this will be more accurate. I also told you that it has wider amplification. You can take the derivative at dT by dx x equal to 0 multiplied by k and use the energy balance equation; get the heat transfer coefficient, skin friction coefficient, and so on.

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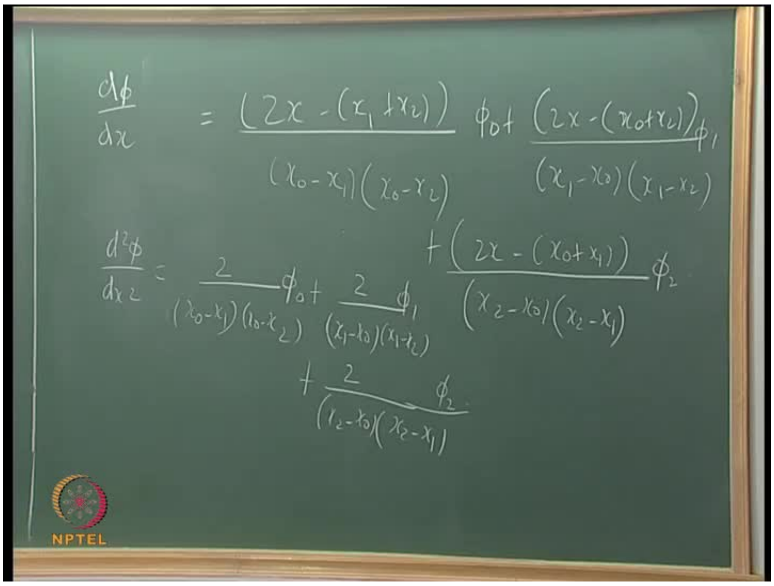

Now, let us try to get d phi by dx. This will be… is it correct?

No?

Let us let us first get the general expression. Any problem?

Now, what will this become? Can you simplify?

Not 2 phi that is d square or you want to take d square, go ahead; no problem.

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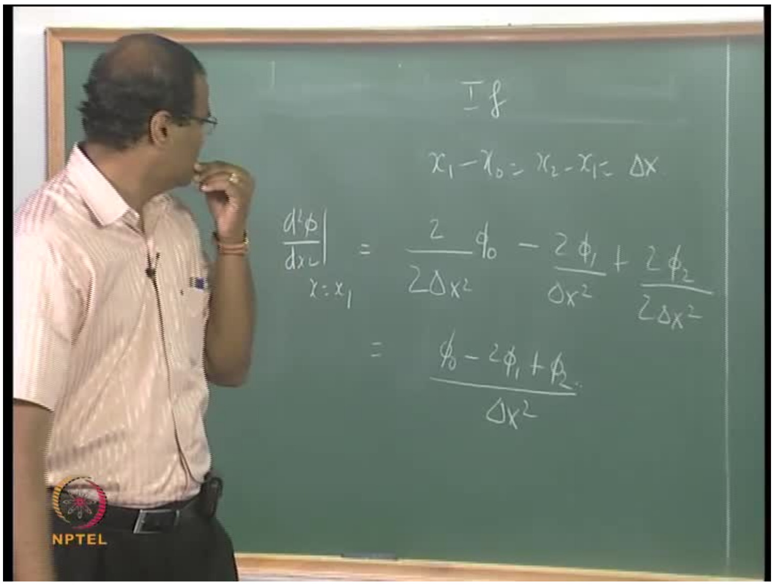

Let us take phi. If that is you got a equal spacing or equispace, we call them as equispace intervals; then d square phi by dx square; it is the same everywhere. Senthil, you had a doubt - d square phi by dx square is same whether it is evaluated x naught, x 1 and x 2 because you are having only a second order polynomial, correct? So, d square phi by d x square 2 by….

Student: Delta x square.

2 deltas x square correct, minus….

By delta x square.

Plus actually equal to

Is that correct?

This is purely from getting an interpolating polynomial by using the concept of interpolating polynomial, using a second order accurate interpolating polynomial, we are able to get the second derivative of a variable phi; that variable phi could be anything; it could be temperature; it could be stream function; it could be potential difference whatever depending upon electrical engineer or civil engineer or ground water potential. There are so many; phi can take on any value; phi can assume any form. Now, this this basically is called the central difference approximation in finite difference. What is the central difference approximation? What do you want to call it as? Similarity to…

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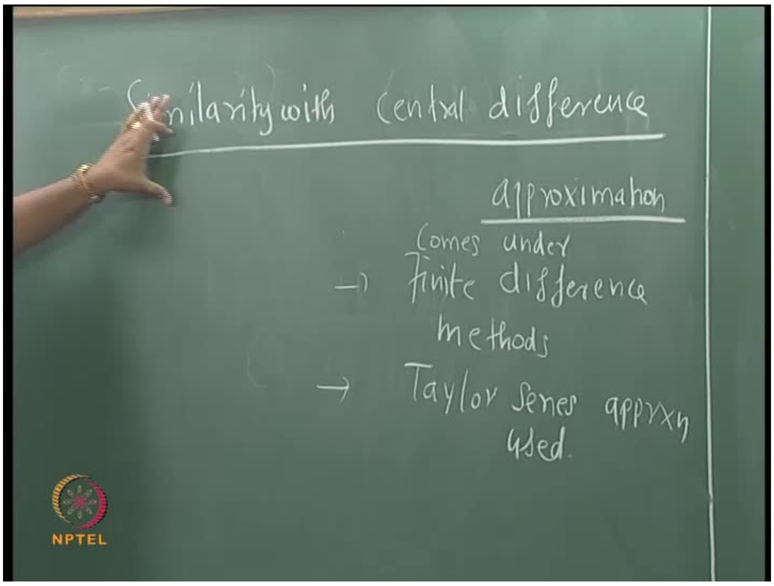

The central difference is basically one way of giving a discrete form for derivatives and so on. So, it comes under general concept of finite difference method. So, in finite difference method, where you do is, what we do is basically use a Taylor series approximation. What is the connection here?

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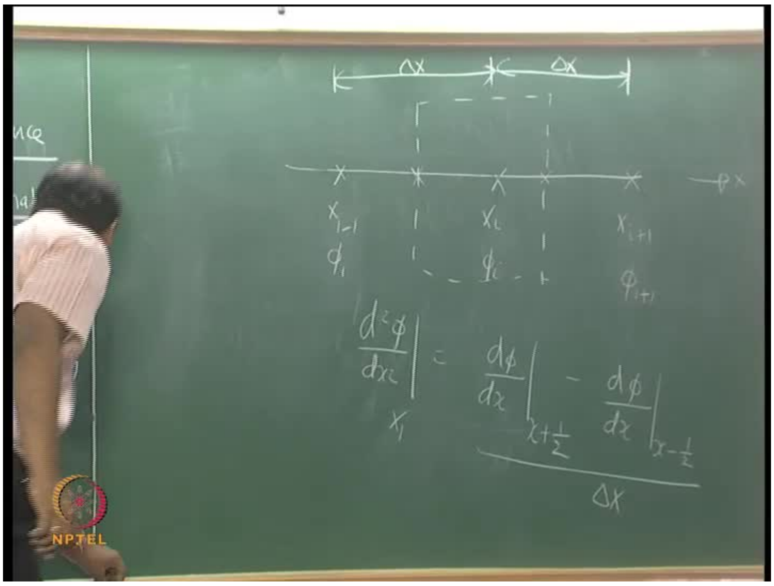

So, this x naught…, so you can draw something like this; now, I can actually replace it by to be consistent with terminology using finite differences. In a one-dimensional representation, this will be this will be X I; so, this will be phi I. In a two-dimensional representation this will become phi i j, where j is along the y direction; this is x direction.

Now, I can say that at X i, I am assuming that this is delta X; this also delta X. It is perfectly for me to say to say that the d square phi by dx square at this point will be equal to d phi by dx ahead minus d phi by dx behind divided by the same delta X. I have taken this to be at the by section of these two; this to be at the by section of these two. Therefore, this is delta X and this is delta X; this is also delta X; what is the finite difference representation for d phi by dx?

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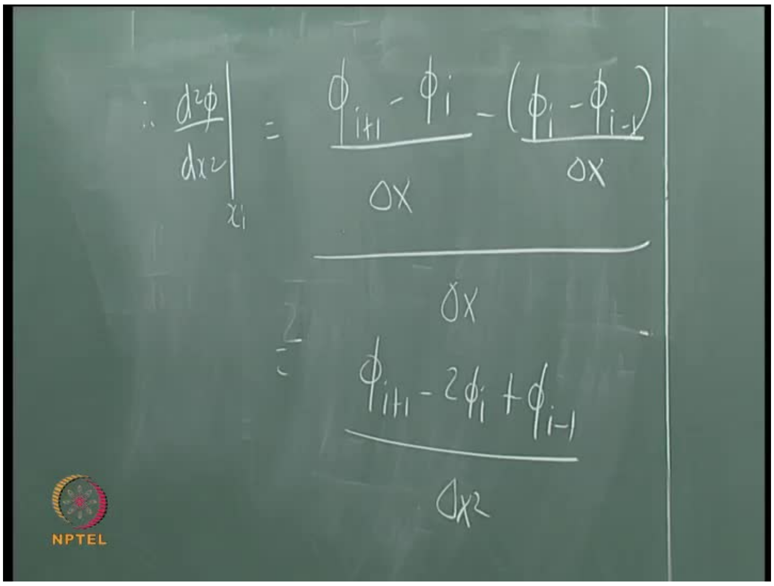

Therefore, this is the way central difference is worked out in when somebody teaches you finite difference methods. Now, you can see that the result you obtain using finite difference is very similar to what you obtain using Lagrange’s interpolating polynomial; is that clear? This was not very clear in the last class; now, it should become very clear to you.

Now, I can use a Lagrange polynomial of order three and four; so, this equivalently in finite difference, this will need to what is known as high order schemes. Mathematicians are always constantly trying to develop high order schemes in order to improve the accuracy, convergence of various types of partial differential equations.

Engineers, we want to get a quick solution, we want to get an engineering solution, a solution that was with which we can design shapes airplane and so on. Mathematicians are always interested in convergence, existence, uniqueness; they want to clean up the mess left by engineers. We do something and then we do not… any engineer we ask what is the order of the scheme? What is the order of the error? And all that, what is the order of the accuracy? We say no no no it works; I have done grid independence; that is all, but those fellows want to clean up. Suppose, you have a Taylor series expansion, they will take the un-truncated series minus truncated series, what is the order of the error? How we proceed with iteration? So, they will…, so what they want is paper, pencil, and dustbin.

Now, even now, today if you go to TIFR, for example, you visit TIFR either in Bangalore or Bombay, so there is a group of Professors on partial differential; I have talked to many. Morning they will come; they do not have lectures also; they do not have BTech or this thing; they have, they teach one course year; they will take the paper and pencil, they will keep on solving some partial differential equation. They will try to integrate this thing and they will find error in this thing. So, they will say that we are cleaning up whatever engineers have left. So, that is what they try to do; higher order schemes and all.

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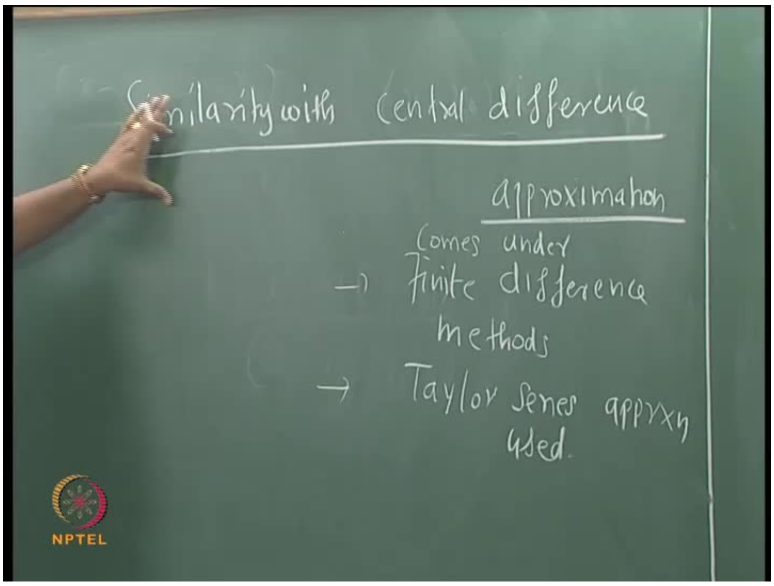

So, in this class, I will simply demonstrate, I have just given a simple demonstration that a Lagrange interpolation formula if you get the second order, it is the second derivative, is it is same as what you would have got using a Taylor series approximation with central difference.

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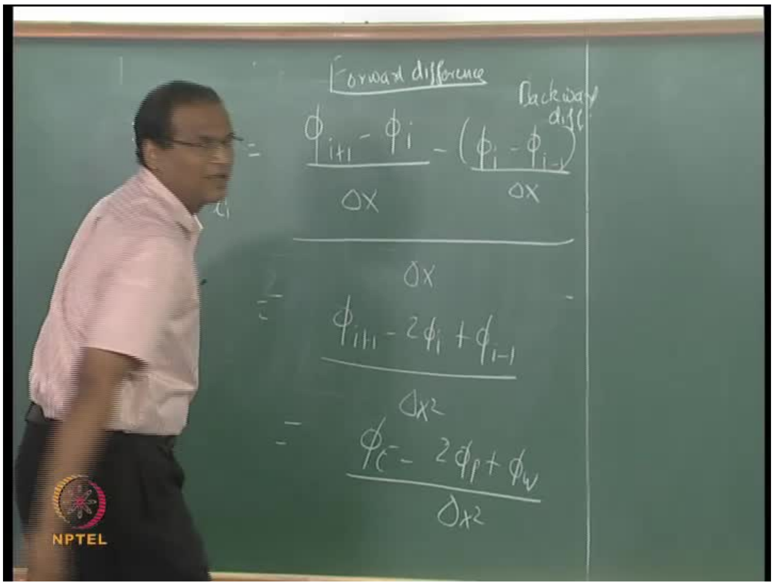

So, what is this? This called a forward difference; this is the backward difference.

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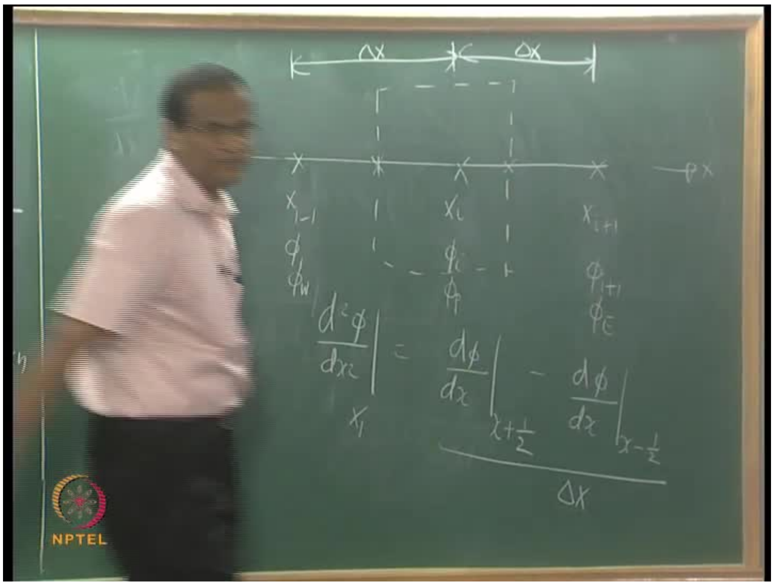

We can also write it as phi east minus 2 times phi correct, where this is phi of P phi or phi whatever.

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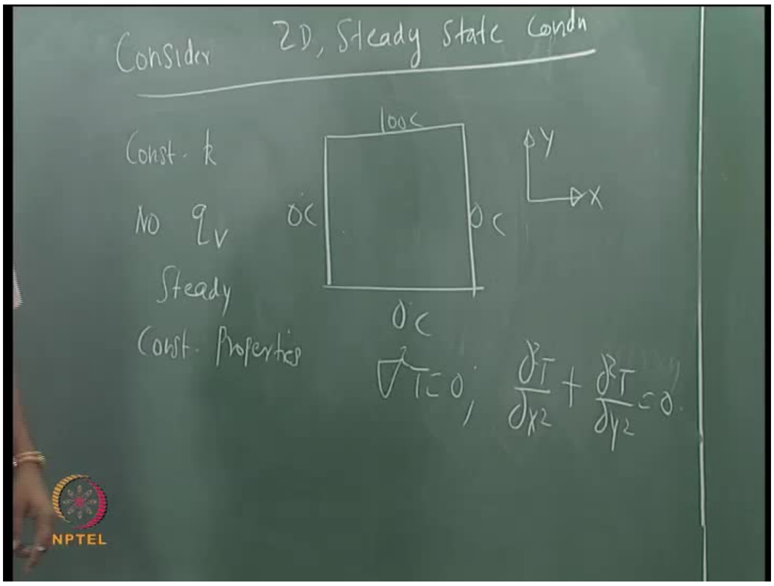

Now, consider, I am teaching simulation for you; how to simulate 2D steady state conduction; you can simulate it using, I mean you can get it analytically, you can go to mat lab or you can use fluent and do it, but of course, it is not system simulation because its only one system; but if we when we are considering a couple system, when we are considering several system in series or parallel, then it becomes a system simulation. For example, let us take a slab like this, so this is x, this is y; let say it is maintained at 100 degree centigrade. So, let us say constant k; no heat generation; steady and constant properties.

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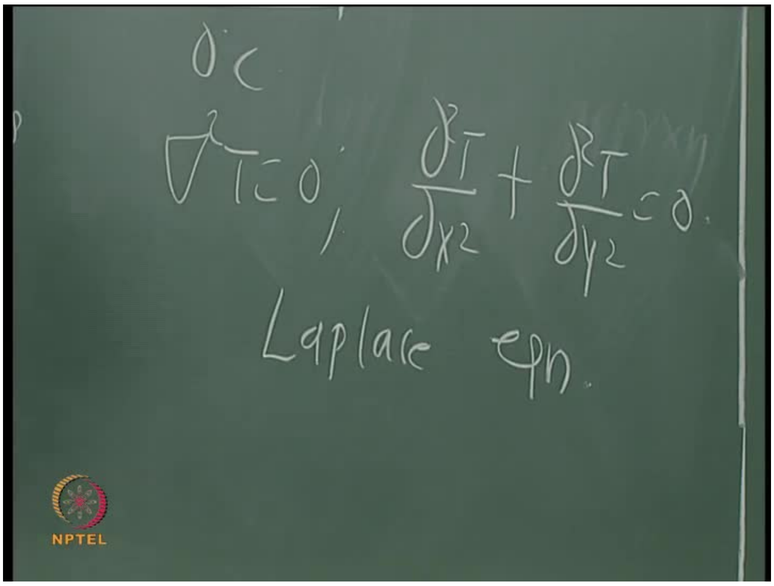

So, the governing equation is delta square T is equal to 0. Correct? This is called the Laplace equation.

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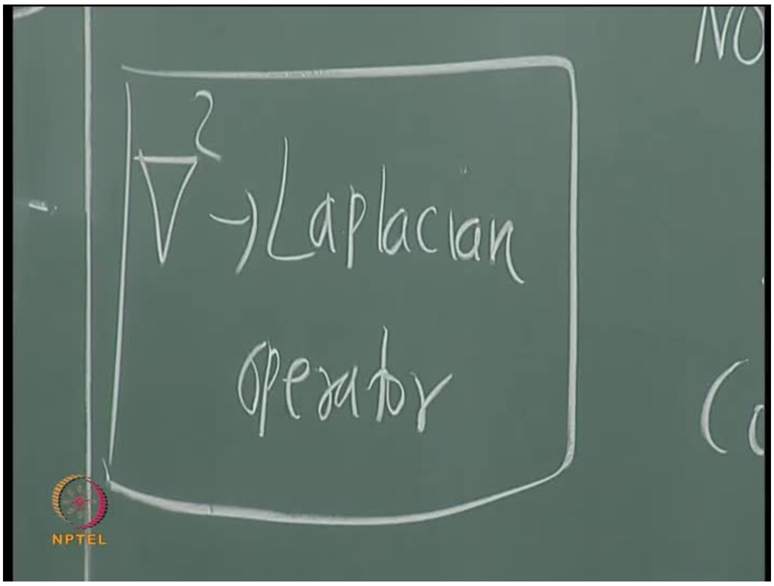

Delta square is called a Laplacian operator. We can solve it by using the method of separation variables; we can solve it by using the method of separation variables. How do you do that?

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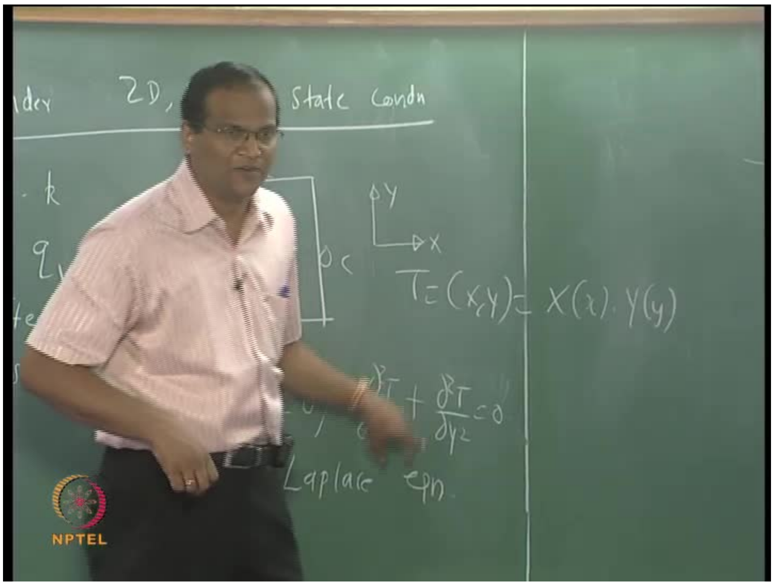

Assume that temperature T is the function of x y. Now, assume that this is the function of X into…, that is assumed to be a product of two solutions X of x and Y of y, where X is just a function of x and Y is just a function of y. When you substitute this, this partial differential equation is broken down into two ordinary differential equations. So, the left hand side will be a function of x; right hand side will be a function of y. There is no reason, when the left hand side it is the function of y, and right hand side it is a function of x or whatever; why they should be a function of x or y either; they have to be equal to the constant. If this that constant is proportional to lambda square or something, then you will get two ordinary differential equations. If you solve, you will get separately the solution to X and Y, and then using the boundary conditions you can get all the constants a, b, c, d. That is how you close the problem.

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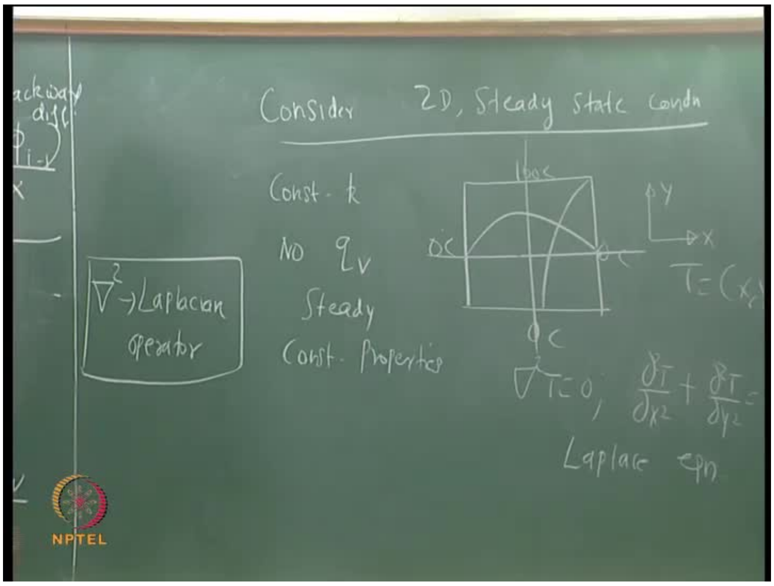

Now, you have to see what are the possible forms for x and y for this problem. In this case, you can see that since left side is 0 degree centigrade and right side is 0 degree centigrade, the temperature is expected to be symmetric about x. So, you will have a sinusoidal variation x. So, you can chose a sine form for x, whereas a temperature is decreasing monotonically from 100 degrees to 0 degrees along y. So, the temperature will go like this; so, you can have…. So, you will have e to the power of minus or you can have, e to the power of is also similar to sine h m l and cos h m l. This is what we got in your fin equation also; the fin temperature distribution exponentially is very similar to hyperbolic function. So, you get a composite function where one is a sinusoidal and one is exponential. If we combine it, so this is what is called the elliptic equation because information on all the four boundaries is required to solve this problem.

So, 100 degrees, 0, 0, 0, I got four boundary condition, so it is second order in x it supports two boundary condition, it second order in y its supports two boundary condition; if I use all the boundary condition I can get a, b, c, d, and solve the problem; fine. Now, how do you solve it using finite differences? If you want to solve it using finite differences, we already have a representation for this. This is for d square phi by dx square. Now, I can call it as dou square phi by dou x square where phi is a temperature in question; similarly, you can write out an expression for dou square phi by dou y square and then you will get a expression relating the temperature at particular node in consideration in relation to the neighboring at its in relation to the temperature at its surrounding nodes.

You will get a relationship for every such node, every such phi of P; then, you get a simultaneously so you get a set of simultaneous equations; go ahead and use the Gauss Seidel method, and simultaneously solve it; that is the story. So, this is basically 2D steady conduction. So, it is called a principle of super position. It is valid only for a linear partial differential equation; it cannot be done for a Navier-Stokes equation is non-linear.

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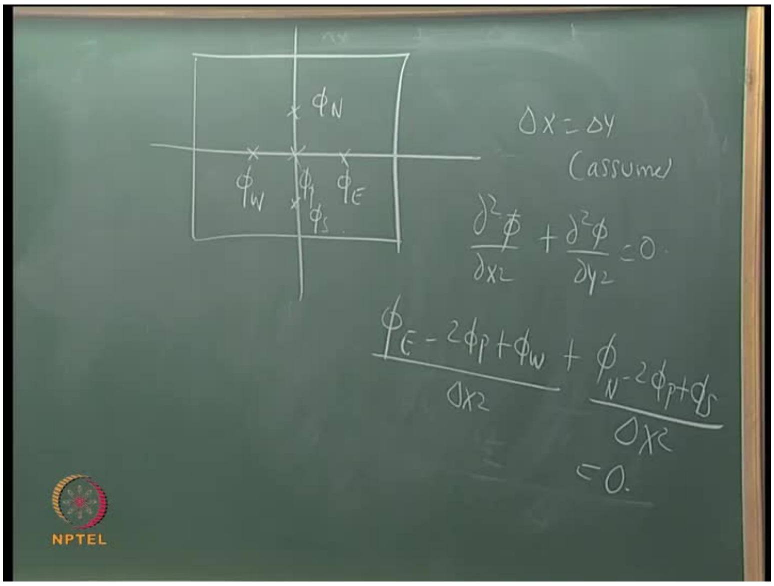

Consider the same problem. Now, so, this is phi of P, now delta X equal to delta Y. Assume, so d square phi, phi is a temperature for example; so for this, using this, you can write that please note that I am writing again delta X square because delta X equal to delta Y equal to 0.

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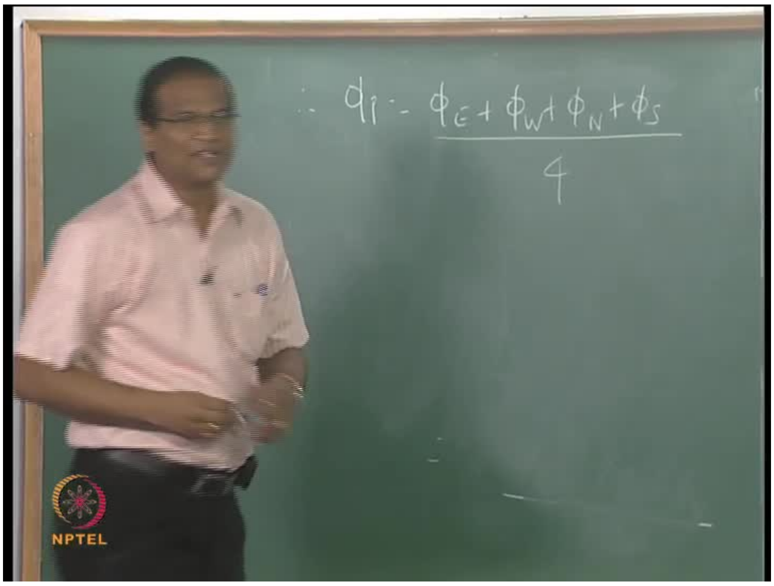

So, if we simplify, it is as simple as that. So, the value of the temperature at a particular node is algebraic average of the temperature at its surrounding nodes; looks reasonable, provided delta X equal to delta Y. So, this is also the common sense answer you could have obtained.

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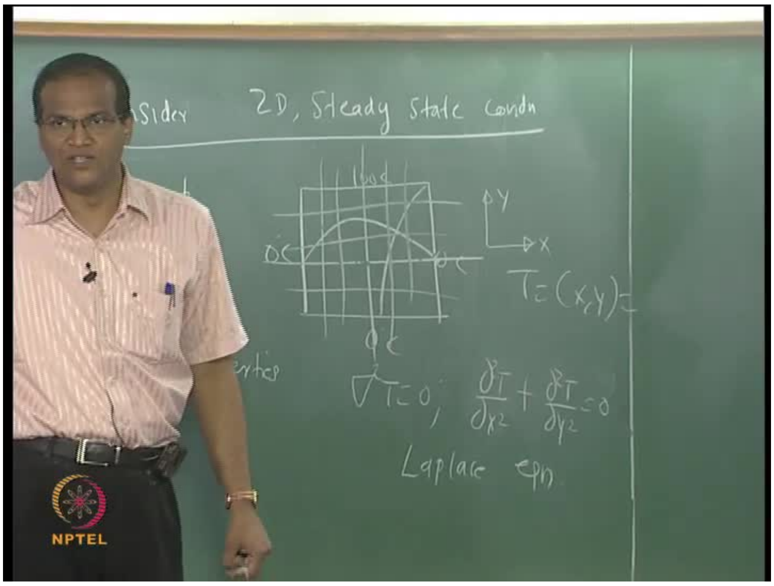

So, for the problem and question: If this is the problem I had given you 100, 0, 0, 0, if the whole thing are considered to be, if this is considered to be delta X, for example, then this temperature will be 100 plus 0 plus 0 plus 0 by 4, it will be 25 degree centigrade; whatever sophisticated mathematical technique you use, the center temperature must be 25 degree centigrade; it will be equal 25 degree centigrade; so, this is the first exercise I give to my students doing project with me either B Tech, M Tech, M S or up to PhD. I will ask them to write a code and then keep on changing the number of elements, keep on changing delta X delta Y. You can use the 4 by 4 grade, 7 by 7, 9 by 9, 11 by 11; use a central difference approximation; use uniform grid non-uniform grid and prove the center temperature is very close to 25.

Once you get results where the center temperature is close to 25, then your results are insensitive to the grid and they are also validated because there is an analytical solution which is possible. This is the trivial problem for which an analytical solution is possible. In those cases where an analytical solution is not possible, you have to turn around, go back to literature, and find out how other people have done experiment and got this solution. So, if your numerical solution agrees with those experimental results, then you have a scheme which is grid independent, which is also validated.

Now, you will say that these are certain features which I have masked in order that I compare my numerical procedures with those experiments. Now, these experiments these features have not been considered. I will turn all these features on and I will get new physics, and since by solution is already validated and grid independent, there is no reason why this solution should misbehave if you turn on the additional feature. This is the research. Find out what other people have done; first find out what other people have done; find out some mistakes or some critical gaps which they have not filled. So, once your literature survey is thorough, get armed with your arsenal ammunitions and weapons; you learn numerical techniques or do experiments; then when you are doing a numerical analysis, you go through all this grid independent validation, write your own code, use mat lab, use whatever.

And once you are clean, then you then you start doing a parametric study, you obtain Nusselt’s number the is function of Reynolds number, Prandtl number, whatever, and then using your knowledge of regression get a correlation for Nusselt numbers and say that it can be used in situations which is of engineering significance. Try your luck.

Along with a guide write a paper send it to journal and see how for this flies. Research is so simple, but you should come and work; that is thing; so, is this clear?

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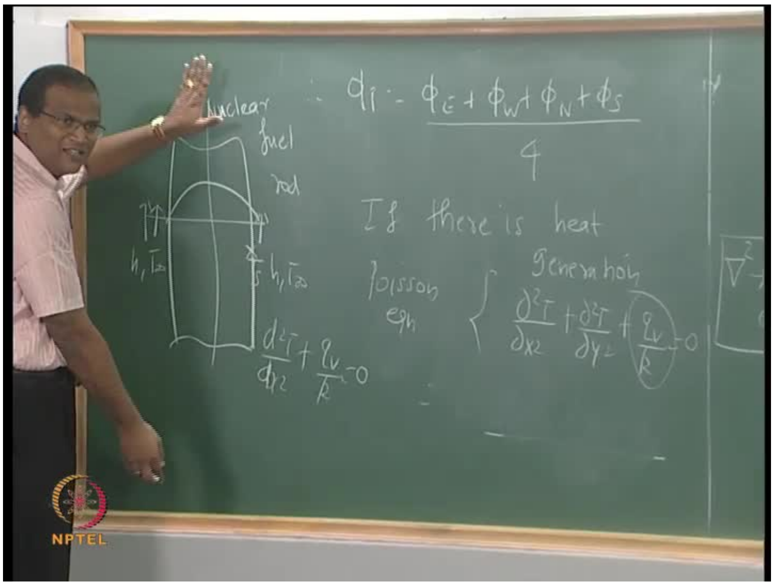

Now, so, we got this east, west, north, and south, divided by 4; suppose there is heat generation in this, what happens? Correct. These you must have learned in your heat transfer course, what is the equation known as?

So, what will happen is, look at this; these two terms will give phi east plus west plus north plus south minus 4 times, correct, minus 4 times phi of T divided by if you have delta X equal to delta Y divided by delta X square plus q v by k equal to 0. Then you can rewrite this in terms of phi of P, and then you along additional term which is the consequence of this. Why does this term arise? For example, if there is a nuclear fuel rod, it is generating there nuclear fission which is taking place here; the heat is taken away by the sodium; for argument sake, we assume that there is a temperature; heat transfer coefficient is so high so that the T s must be equal to T infinity. Now, the temperature distribution will be like this.

For this, the governing equation will be d square T by dx square plus q v by k is equal to 0 because you assume that the temperature is a function of only of s; temperature is not a function of y because it is infinite in the other direction. If we if this have to be a slab, this heat generation could be either because the chemical reaction or a nuclear reaction and so on, so you get the Poisson equation. You can still apply the Lagrange interpolation formula and finally relate the value of the node at point P to its neighbors east, west, north, south, divided by 4 plus q v by k, and you can develop a numerical scheme and use a Gauss Seidel method.

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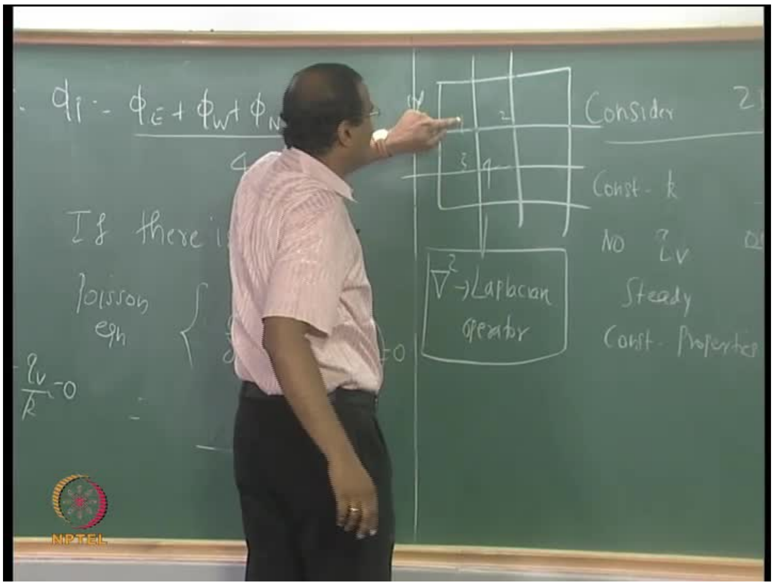

And because if you have if you have 1, 2, 3, 4, so suppose it is simple without this, which we called as a plane vanilla problem, for example q v equal to 0, then you know that this fellow will be this plus this plus this plus this divided by 4. This fellow will be this plus this plus this plus this divided by 4; this fellow will be this divided by 4, and boundary conditions are given. So, to start, you will say T 1 equal to T 2 equal to T 3 equal to 4 is 20 degrees, 30 degrees, 40 degrees to start with, and then it will eventually converge because it will diagonally dominate, and all that features will be there because you are always getting that 4; east plus west plus north plus south minus 4 times P divided by 4. So, it is at least, it is at least equal to the sum of all the coefficients. Are you getting my point? a i i is equal is equal to sigma of a i j, for all j j not equal to i. Fine. So, with this we close our discussion on Lagrange interpolation formula.

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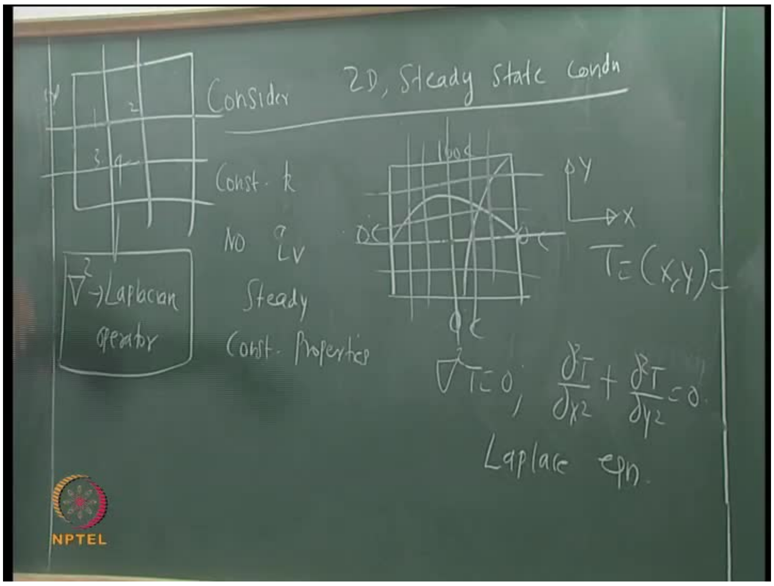

So, we if I keep on developing this, so this will be a, this will become a course on numerical analysis or numerical analysis of PDEs; it starts with ODEs, PDEs, and we can we can keep on solving various problems. Of course, if it gets tricky when there is a, when there is a, fluid motion; then it will become Navier-Stoke equation; then pressure comes; then if it is compressible, you need to have the equation of the state; you need know whether it is transonic, subsonic, supersonic, hypersonic, and so on then it becomes more and more, more and messy; shock waves will be there. See, so, of course will be there for supersonic, then supersonic compression, you have to solve Navier-Stoke equation, equation of energy, species concentration equation; where are all these used? Because you want to a fly aircraft Mach number 6.5, not aircraft, a missile, why do we want to do that? 6.5 Mach number what do you get? What is the great thing? Even supersonic flight we have discontinued, right, concord.

Why you want to build Mach number 6.5?

Student: Cannot be intersected.

Simply you want.

So, we have 20 second flight this thing and nuclear war head attached to it and you can demonstrate supersonic compression, hypersonic compression; Mach 6.5, it can be released at an altitude of 32 kilometers, and then you fire. So, this will be kerosene will be the fuel; kerosene will be the fuel, and so even if it flies only for a few minutes, it is enough; the technology is not demonstrated. NASA demonstrated it for a 20 second, 10 second; India is doing that for 20 seconds; 20 second flight we are doing. It is called HSTDV - Hypersonic technology demonstration vehicle being developed in Hyderabad.

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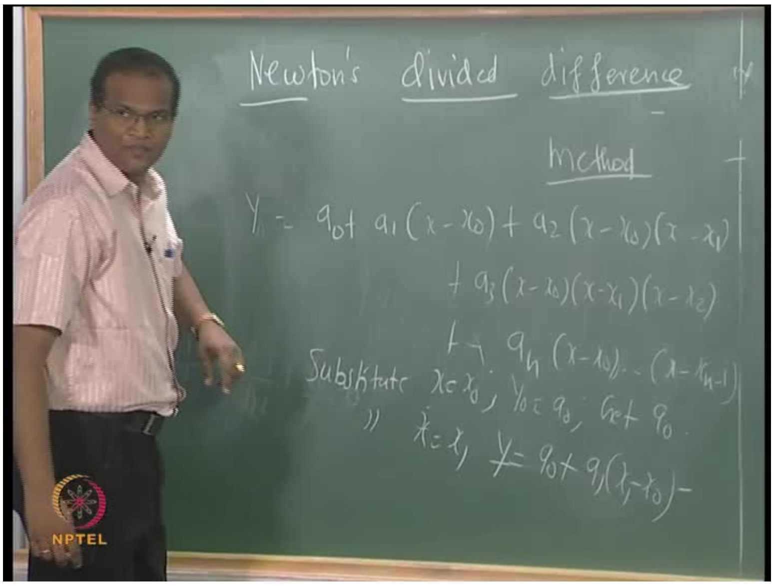

Now, Newton's… yet another way to… please remember that we are still doing exact fits, a three point we try to fit a polynomial which goes through all the point. We can have… no, so this called the Newton's divided differences method. Here, the x naught, x 1, x 2, all need not be equi space; so, substitute x equal to x naught; what do you get? Y naught equal to a naught; so, you get, what do you get? You substitute x equal to x naught; everything will become 0 expect the first term. So, the Y naught itself will become, Y naught will become.

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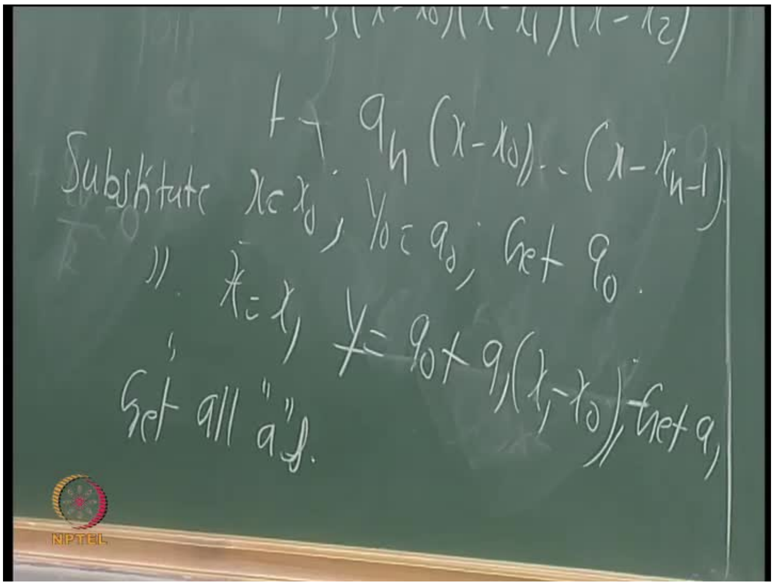

What is the problem? We are trying to fit a, we are trying to fit a polynomial for Y in terms of x. So, you get all these coefficients a naught, a 1, a 2. Now, I am giving the procedure to determine all these coefficients. So, if you substitute x equal to x naught, then all the things will vanish expect the first term. So, you will get a naught. Now, substitute for a x equal to x 1. So, Y will be equal to a naught plus x 1 minus x naught, correct? All the other terms will vanish; you already know a naught; you know this x 1 minus x naught; so, you will get a 1. So, you get all a's. What is the big deal?

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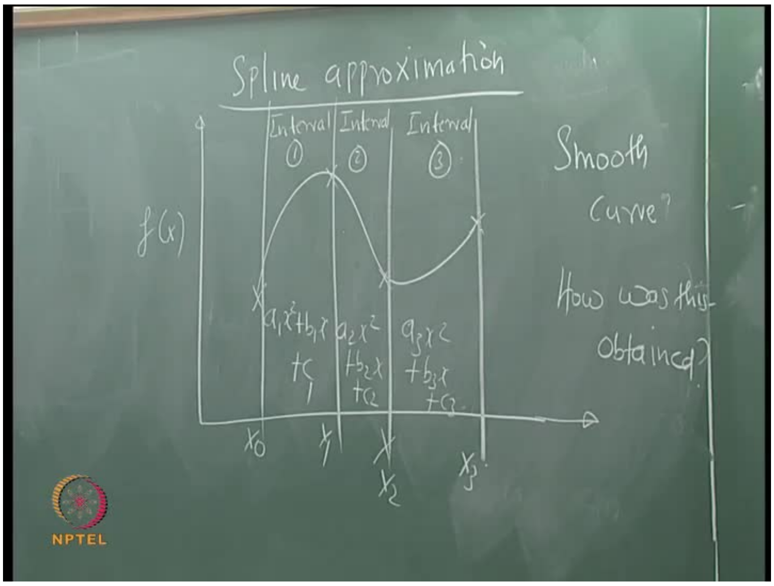

Why cannot I have a polynomial Y equal to a naught plus a 1 x square plus a 2 x 2 square plus a 3 x 3 cube and all that and get 4? Suppose it is cubic or four equation four unknowns and solve the four by four, here all the coefficients are determined sequentially and not simultaneously. So, there is no need to solve set of simultaneous equation. It is a lot simpler compared to the polynomial; even Lagrange is lot simpler compared to the first polynomial which we did because the coefficients need no have to be, need not have to be simultaneously determined. So, if that is a pain for you, then go for this, solving it simultaneously. If you have a solver, if you have a library, if you have some IMSL, we have some IMSL library, sub rooting, and if you can take the Gauss Seidel or Gauss Jordan or Gaussian elimination, you can straight away do it; otherwise, do this sequentially. The last technique which I want to teach you is a spline approximation. Suppose, if this is f of x versus x, I will join it base smooth curve, what did you do now?

It is a smooth curve right?

How obtained?

The key is fit lower order polynomial for subsets of the points and mix and match all of them to get a nice smooth curve, but all the curves do not follow one equation. Locally every three points are having drawing a parabola, or locally every four points are having a cubic, but then in order to avoid discontinuities at the intermediate point, you match the functions as well as the slopes. So, you will get again a set of simultaneous equations and if you solve for all this simultaneously, you get the various values of the coefficients and this was spline fitting is done so fit.

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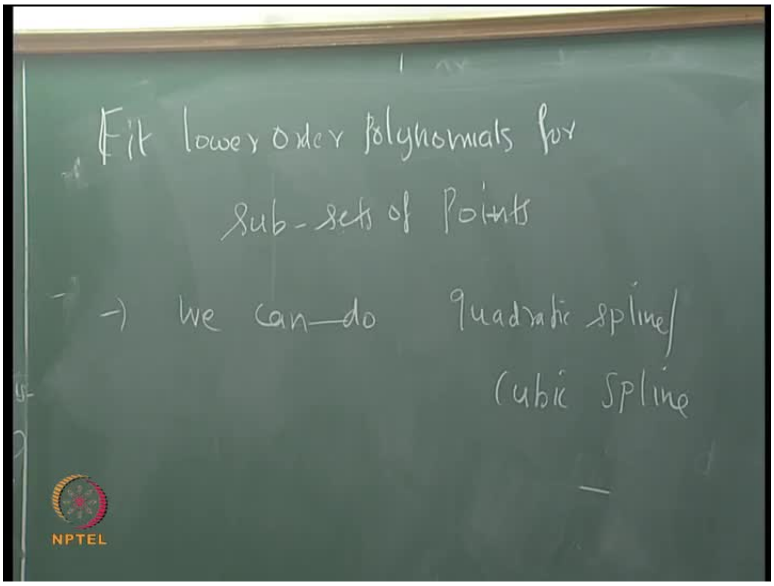

Can you start subdividing this interval and then identifying how many polynomials are required? Can you start this? If we were to do quadratic spline for this, can you do this? Meantime, I will take an attendance.

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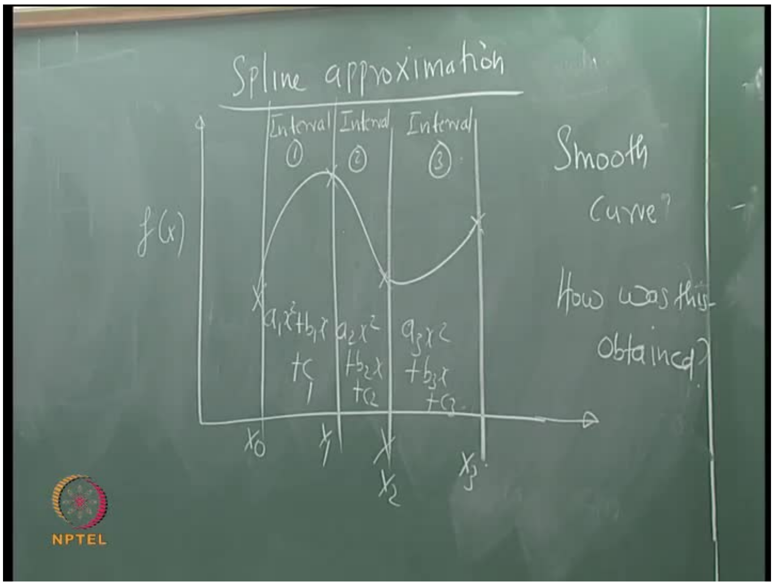

So, this interval 1, interval 2; so, here it is a 1 x square plus b 1 x plus c 1; here it is a 2 square plus b 2 x plus c 2; here it is a 3 x square plus b 3 x plus c 3. We have only the value of function at four points: x naught, x 1, x 2, x 3. How many unknowns are there to be determined?

Student: 9

9, what are they.

a 1, a 2, a 3, b 1, b 2, b 3, c 1, c 2, c 3. How many equations are required?

Student: 9 equations.

Where are the 9 equation?

4 point

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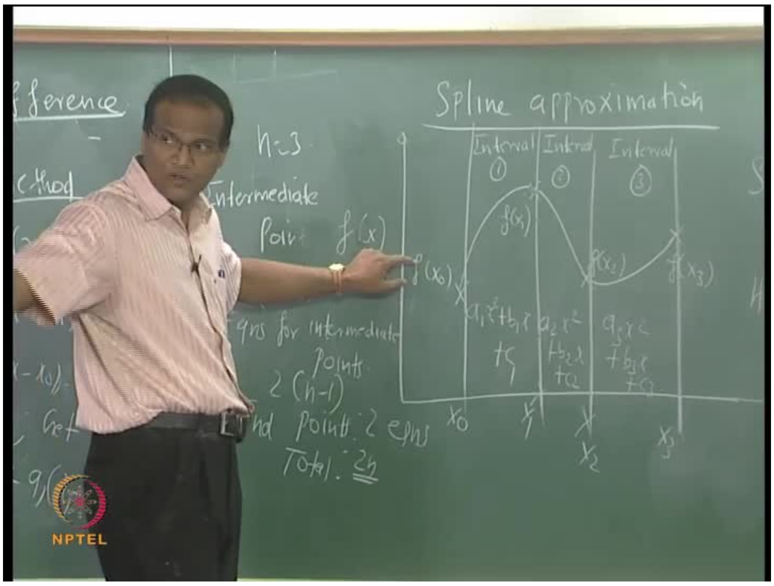

Intermediate points, so you can put it as f of x naught; at the intermediate points there is only 1 value of f of x 1 regardless of whether you use this polynomial or this polynomial. So, for every point, we will have two equations coming from the polynomial from behind or polynomial from ahead. How many intermediate points are there if n is the number of intervals? So, there are n minus 1 points. So, the total number of interval is 3. So, n is 3, intermediate points n minus 2, and so how many n minus 1.

So, how many equations for intermediate points? How many are there? Every point we have two; so, for n minus 1 points we have 2 into n minus 1, correct? Why every point is two? f of x 1 should be equal to a 1 x 1 square plus b 1 x 1 plus c 1 must also be equal to a 2 x 1 square b 2 x 1 plus c 1. So long at applying to x 1, whether you use this polynomial or this polynomial, it has only one function (Refer Slide Time: 38:51). So, every intermediate point has 2 equations. So, n minus 1 of 2 n minus 1 end points. How many equations? 2; now, total is 2n. How many constants are there? 3n.

So, what about the remaining n?

Correct.

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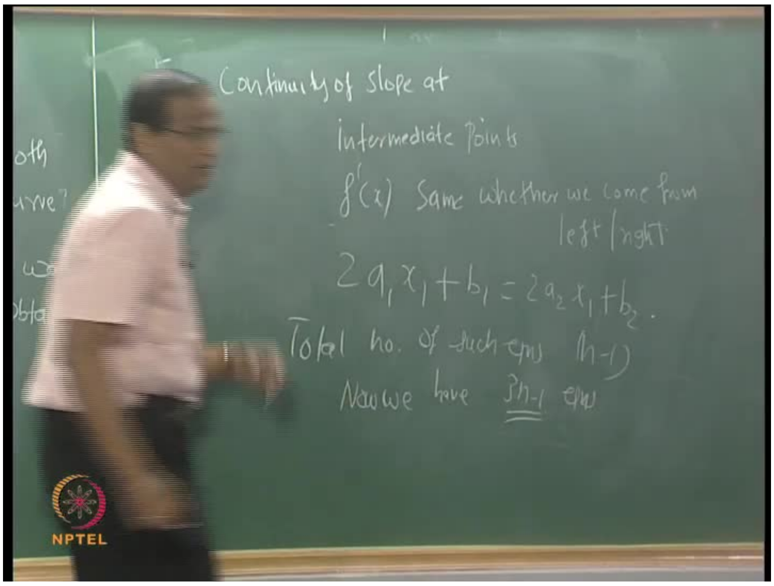

So, there should be continuity of the slope at the intermediate points; same whether we come from left or right, so, f dash of x; that means, what does it mean? 2a 1 x plus b 1 when you apply it I get x 1, therefore 2a x 1 equal to…

Student: 2a 2 x 1

Correct, good, 2a 2 x 1 plus b 2.

Correct, right, like that you can keep on generating. How many such equations you can generate? n minus 1 equation; total number of such equation. Now, we have; we are still one short. The slope at first or last find 0 something; no, no, we have to start; we have to start somewhere, but slope at first point or last point 0, that means, what are you saying? When slope at the first point is 0, what are you saying? a 1, what is slope at the first point? a 1 d square f by dx square.

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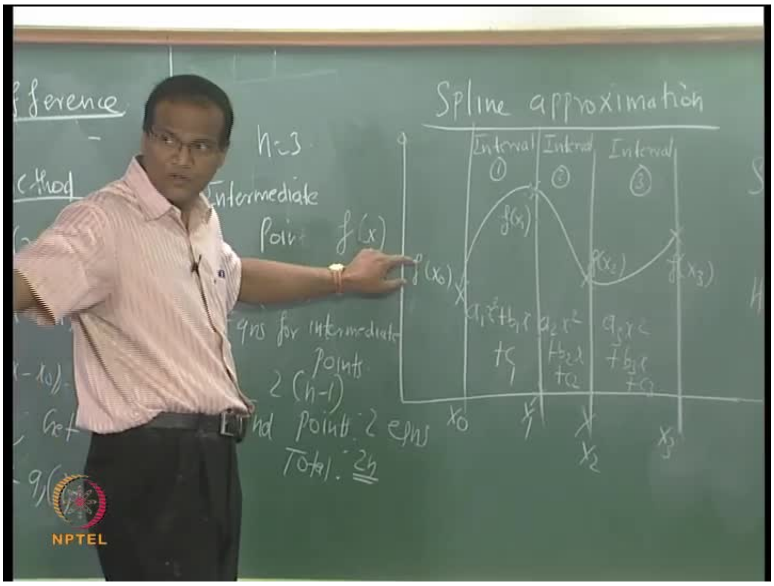

2a x, second order, I am talking about f double dash of x, second derivative sorry second derivative at 2a 1; so, when we say that second derivative vanishes at the end point, either a 1 is 0 or the a n minus 1 or in whatever 0, so arbitrarily we put one of these two things 0, if no additional information is required; is it okay? So, last condition…

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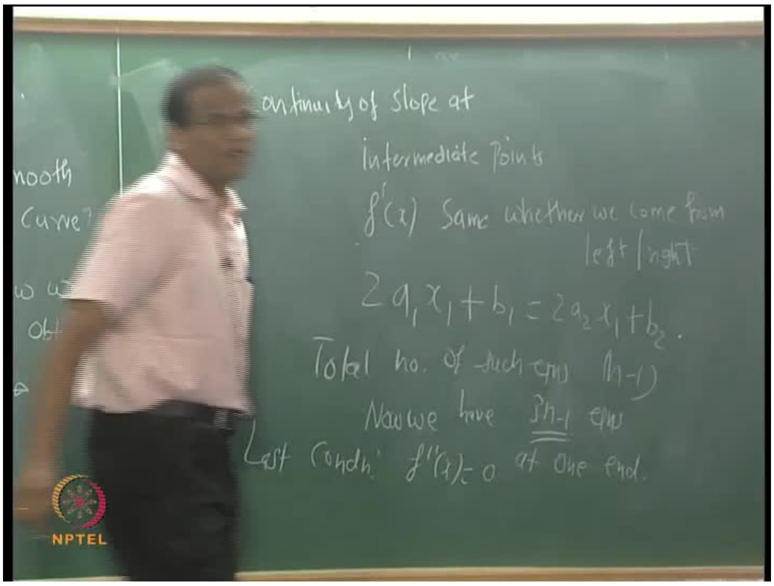

No, but some suppose, normally we use this cubic spline when there are 100s of points; when you fit cubic spline for 100 points, your eyes will not notice that you did some [FL] somewhere. So, make it at if you 100 point 34th point or 35th point you do, but there is no other way to mathematically close. This is what you are graphing software does. When you put approximating polynomial, so much of mathematics goes on in the background, you can write a program in mat lab and solve it, and then use Excel and put trend line and this thing approximating polynomial, this is what goes on. I can give you exercise; we can have a tutorial class; suppose I asking to put a cubic spline 5 points or something, you will endlessly do that. Yes, Venu.

What? You have to give me additional information. Suppose I just have five points, data points; consumption of coffee along with years, x axis years, and y axis consumption of coffee, I want smooth curve; I just do not want scatter plot. Suppose, we give additional physical conditions for some problem, as you say we can use that, but if those physical conditions are not there, we have to arbitrarily set something better to gauss the disturbance at the boundaries. So, one is linearized; I mean somewhere you have to start right, so you have to…; we cannot say it cannot be solved; I mean that is very trivial. So, you have to start somewhere; you will say that you will adjust somewhere.

So, this brings has to the end of discussion on exact fit; so, there is so much of story to be told about exact fit itself. So, these are all properly determined system where the number of point is equal to the order of the polynomial plus 1 and so on; for example, three points we have second order polynomial, but often times we have over determined system.

You do the experiment for finally heat transfer coefficient for 10 Reynolds numbers. You know that it is a Reynolds number to the power of b into Prandtl number to the power of 1; Prandtl number is fixed, right? If you have two constants, two equations are sufficient to get this, but you have 15, you have 10 of 15 total points. So, you try to get the best fit. What are your criteria for best fit? That we have to see: whether you want to minimize a difference; you want to minimize a difference in modular form or you want minimize the maximum deviation from any point, or you want to minimize the square of the error or higher order power of the error.

So, we will discuss the general philosophy of minimization and then will zero in at the least square minimization and will mathematically derive the least square equation, and I will demonstrate you it is equivalent to getting the maximum likelihood estimate if you have Gaussian distribution of errors. And then, we will do linear regression, multiple linear regression, and we will escalate and end with non-linear regression using Newton’s method.