Matrix Solvers
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Lecture – 10
Representation of Physical Systems as Matrix Equations

Hello. So, today we will discuss a very important topic of matrix solvers, which actually gives us shows us a light why should we use matrix solvers which is how physical systems can be represented as matrix equations, and what are the errors associated with it.

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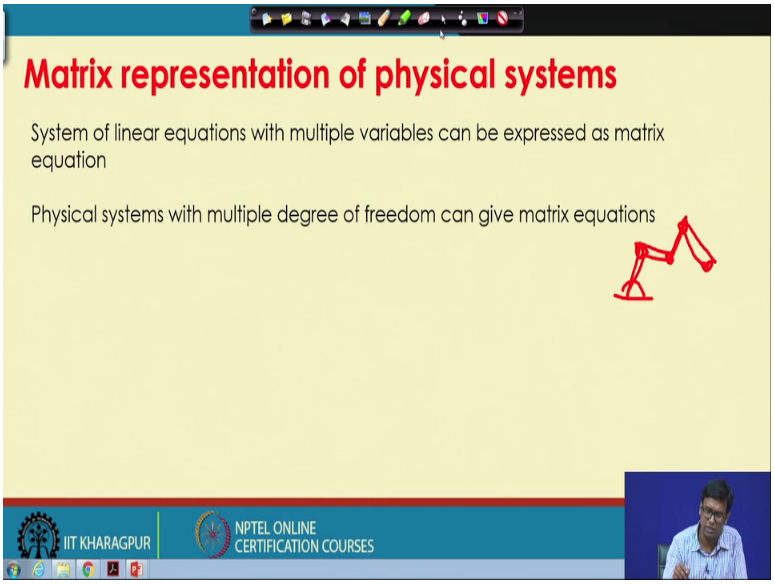

So, this is matrix representation of equations coming from physical systems. System of linear equations with multiple variables can be expressed as matrix equation; this is the basic definition we went through that in the first few classes. Physical systems with multiple degree of freedom can give matrix equation.

For example, if we think of a linkage per mechanism, where something like mechanism with many links with each link has its own degree of freedom; each hinge has its own degree of freedom; and then we can get a matrix equation defining the motion of all the links. And this motion we will get a matrix equation, when there is some interdependence among the motion of different degrees of motion associated with different degrees of freedom.

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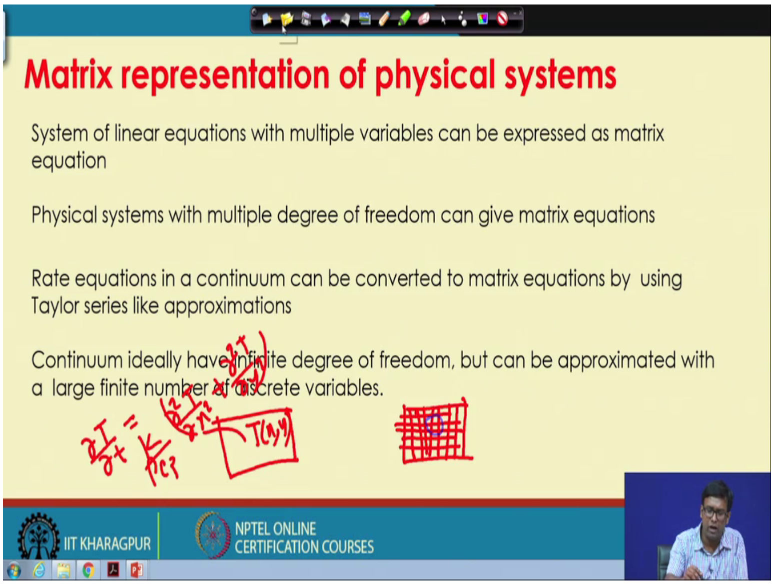

Now, there also can be a what is called a continuum, where it is not discrete bodies or it is not collection of discrete bodies, rather it is a continuous medium like air or like an iron bar, we cannot really identify each discrete molecule, here we think it is it is to be an continuous space where we can get rate equations. And this rate equations can also be converted to matrix equations by using what is called Taylor series approximation, and using some other methods. And we will look into some of these methods in today's class.

But the continuum we will have infinite degrees of freedom. For example, if we think of a continuum space, and we are like this is a metal metallic strip, here we are solving heat conduction equation, which is like del T del t is equal to K by rho c p del 2 T del x square plus del 2 T del y square an equation like this. So, there are anywhere in this point temperature has a variation T x, y and there should be therefore, there should be infinite values of T x, y. For any x y; x y can it is a continuous space can have infinite values for any x y there can be one particular T x, y.

So, we will have a infinite degree of freedom space, but it can be approximated to a discrete finite number of freedom space in state having a continuous space, we can have many small control volume like of things or many small node points inside the domain, and we can try to see what is the rate equation or the matrix form of the rate equation at that particular point. And we can have though continuum ideally have infinite degree of freedom, but it can be approximated with large number of discrete variables. So, we will see it through an example.

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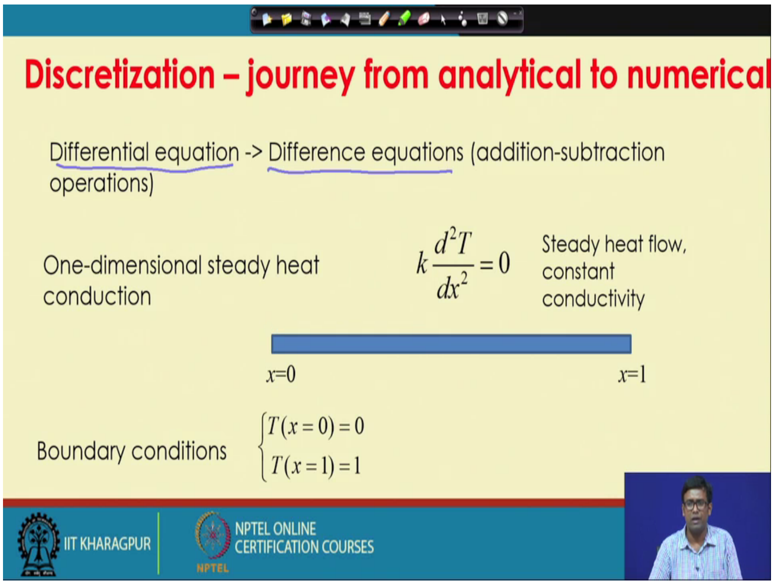

And this is this method is called discretization or continuous space is discretized to a finite degree of freedom space. It is a journey from which analytical methods brings a numerical method. We have a differential equation, here are all rate equation del t del t like del capital T del T is equal to something, this is rate of change of temperature or del 2 T del x square plus del 2 T del y square is equal to 0, which is state conduction equation is also rate of heat flux, how heat flux are related.

So, these rate equations are differential equations. And if we use a any computer program, computer does not understand about the differential equation; it does not have any idea, what a limit is, how to make take derivatives, what is continuity of a function, computer cannot work on differential equation. What computer can do it has some electronic components, which can operate logical gates and through which it can handle addition, subtractions.

Therefore differential equations are to be transformed to difference equations for computer programming. And we can see an example here that one-dimensional steady heat conduction equation, which is k d 2 T d x square is equal to 0. So, this steady heat flow for constant conductivity. We considered a straight rod with length x is equal to length unit length x is equal to 0 to x is equal to 1. It is given with boundary condition, temperature is 0 at x is equal to 0; temperature is 1 at x is equal to 1; and the equation governing equation is steady heat conduction equation, which is k d 2 T d x square, which is equal to 0. Now, I know analytical solution is trivial in this case, it is very easy in this case. But if I try to solve it using a computer program, computer will not understand what is d 2 T d x square.

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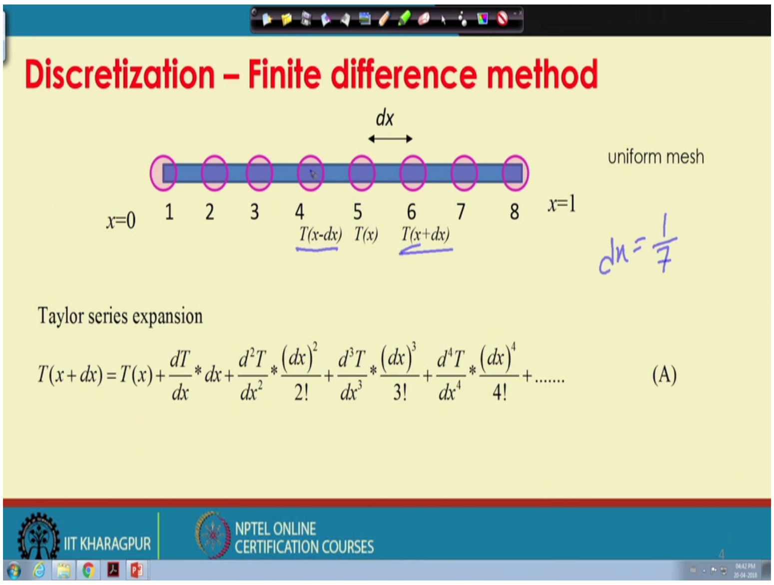

So, what we have to do we have to transfer transform this into a difference equation. In a sense I said infinite degree of freedom represents a continuum space a long rod every point inside the rod is a member of the continuum, and there are infinite points inside the rod. A line has is a collection of infinite points. However, when we try to do a computer programming to solve this, we have to discretize into number of finite number of points, and this is called discretization. So, instead of solving the equation at all the points along the rod, we solve the equations at finite points, which are shown as certain points.

And we assume that all these points are equi spaced, so we will call it an uniform mesh. A mesh is basically arrangement of the points in which we are trying to solve the equation. And the discretized geometry has 8 this finite points, and the difference between them is d x. This method which we will use here is called the finite difference method. So, now, at any point say point number 5, it is a temperature is a function of space we assume, temperature is given as d x. At a point d x away from 5, which is point

6 temperature is T x plus d x. And a point d x in the backward side of the d x, d x away from the T x from point 5, which is point 4 temperature is T x minus d x.

Now, if I use Taylor series expansion, T x plus d x can be expanded as T x plus d T d x into d x plus d 2 T d x square into d x whole square by factorial 2 plus d 3 T d x cube into d x whole cube by factorial 3, where d 4 T d x 4 d x whole 4 whole to the power 4 by factorial 4, and it goes on up to infinite points. Interestingly you see, d x the total length is 1, so d x is less than 1; d x is equal to basically 1 by 7 here. So, d x to the power 4 is 1 by 7 to the power 4, which is a small number, which is less than point less than 0.01 even, d x cube is also a small number.

So, if we increase the if we go for the higher order terms, it is d x to the power 8; d x to the power 10; d x to the power 11; which is a very small number. And in practical cases, we can eliminate those numbers, because the difference in temperature due to those small variation is probably non even non measurable by any standard measurement techniques. So, you can easily discard the higher order term. So, however, we are not discarding it at this stage.

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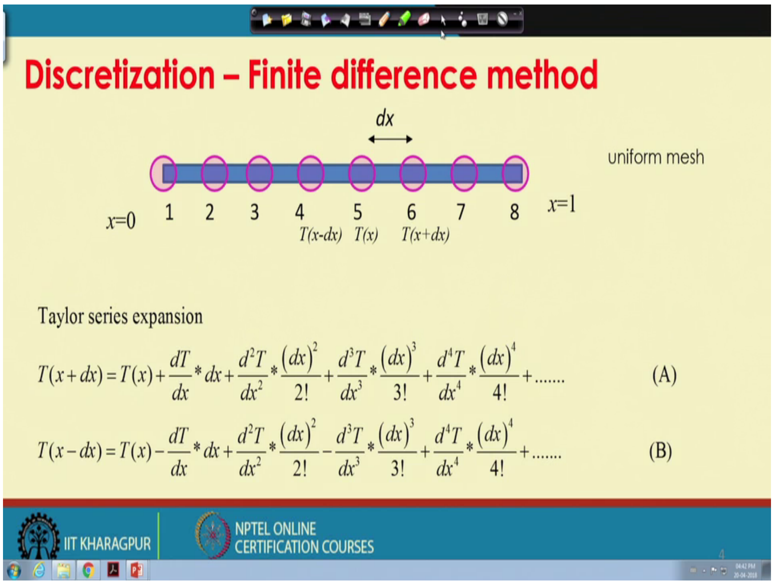

What you see, we can similarly do a Taylor series expansion for the next term, which is T x minus d x is T x minus d T d x only, because d x is negative here, so only the even odd terms; odd power terms will have a negative coefficient.

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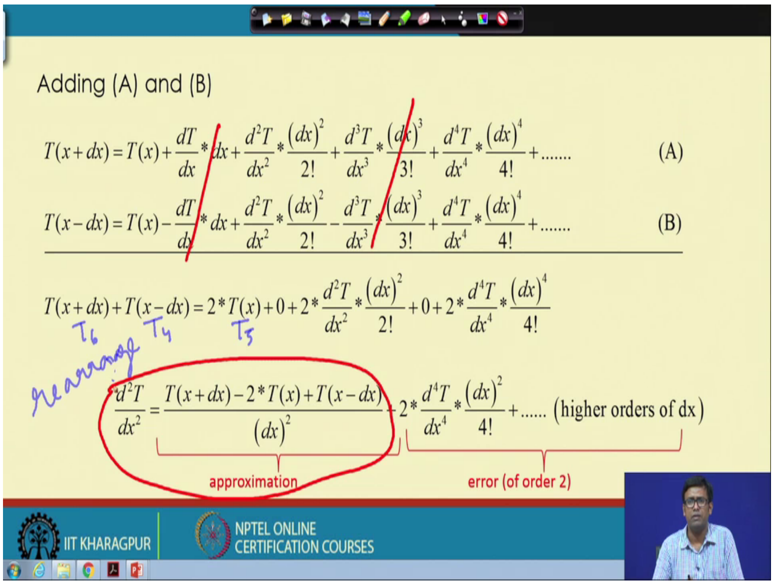

Now, what we will do, we will add these two equations. So, if we add A with B what will happen; the plus d T d x minus d T d x will cancel out plus d 3 T d x T minus d 3 T d x T will cancel out and then x terms will cancel out. So, only even powered terms will be there or powered terms will be canceled out. And if we add A and B, we will see T x plus d x T x minus d x is equal to 2 T x plus 0 plus 2 d 2 d 2 d x square d x square plus 0 plus 2 d d 4 T d x 4 d x 12 to the power 4 by 4.

So, what is T x plus d x, if we look into our previous slide T x is T 5 point 5 temperature this is T 4, and this is T 6. So, we can see the derivatives second derivative fourth order derivative are function of the discrete point temperature. So, we will do a little rearranging here.

If we rearrange this, so after rearrange, if we rearrange the equation, we can write d 2 T d x square is equal to T x plus d x minus 2 T x plus T x minus d x these are the temperatures; at those finite points divided by d x whole square plus some 4 derivate into d x square whole square divided by factorial 4 plus higher orders of d x. Right now we are not writing them, because they are even smaller numbers.

Now, if say d x we assumed 10 points, so there are 9 intervals d x is 1 by 9; d x whole square is 1 by 81 which is a small numbered x whole to the power 4, which will be the next term here, is 1 by 81 square, which is even less than 10 to the power minus 3, which is even a smaller number. So, what we will say, we will approximate this particular part as the expression for d 2 T d x square. This will be my this particular part will be my approximation for d 2 T d x square.

And the later part we will not consider here, we know it is a small number, and as we will increase the number of points as d x will be smaller, this will be further smaller. So, this will be considered as the error in our approximation, and it will be discarded in the approximation. We know that we are making an error, but we know what is the error; error is of the order of d x whole squared, because the other terms are of a much higher order, and the error is small due to the all the other terms. So, maximum error is of the order of the d x whole square.

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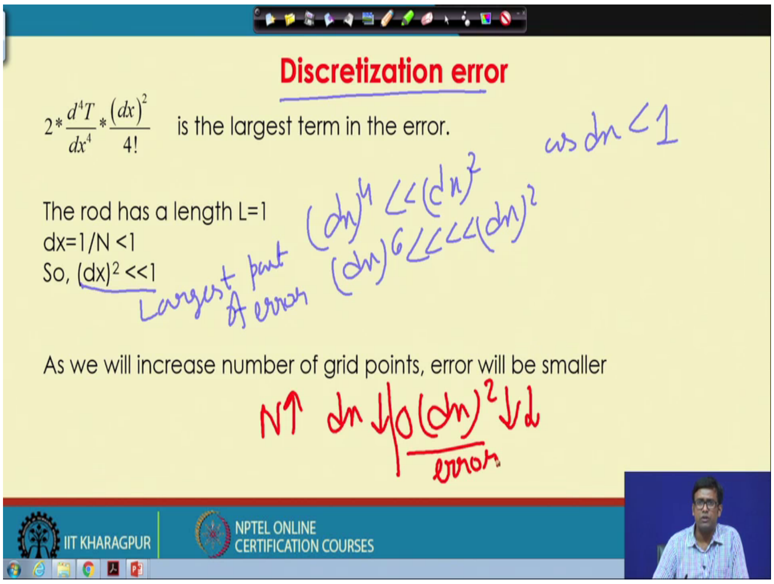

So, we call this to be discretization error. 2 d 4 T d x 4 d x whole square by factorial 4 is the largest term in the error. If the rod has length L d x is 1 by L, which is less than 1 and N is 10 d x is N is number of spacing; it is not number of points.

N is number of spacing, so d x is 1 by 10, and d x whole square is 1 by 10 to the 100 in our particular case, it is probably d x is 1 by 8. So, d x whole square is again a smaller number. And we will see that this terms d x whole to the power 4 is again much smaller than d x square, because as d x is less than 1.

So, this will be a further smaller number d x whole to the power 6 will be much much smaller than d x whole square. So, this is the large largest part of error, and this is called a discretization error. As we increase the number of grid points, N increases and therefore, d x reduces and the error will reduce. So, as we increase the number of points as N increases; d x reduces; and the error which is of the order of d x square further reduces, so this is the error further reduces. So, I will use more and more grid points the errors will be smaller.

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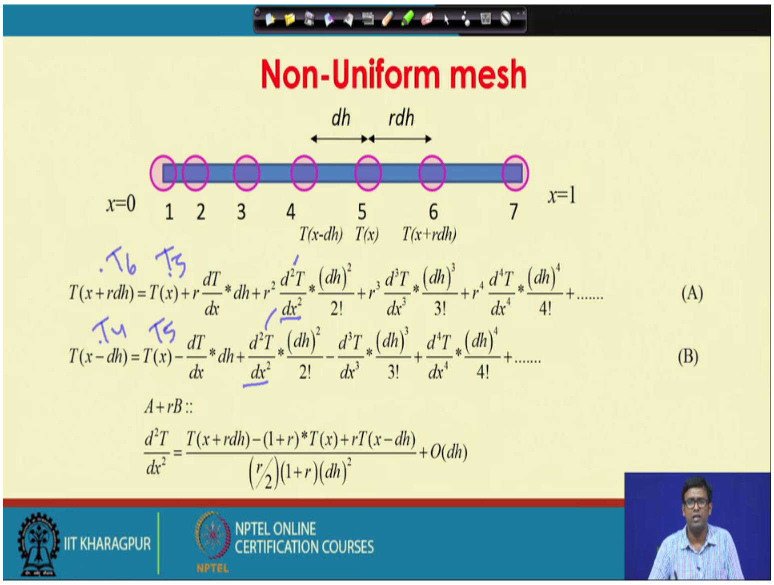

Now, one thing is that we assume that uniform mesh in a sense, all the grid points are equi spaced from each other. It is also possible that this is not an uniform mesh, rather an non-uniform mesh. And in certain cases specially in fluid flow calculation we see that lot of most of the variations are near one particular boundary, so you put more mesh points there, we and we use less mesh points away from that boundary.

Then what we use a non-uniform mesh that all grid points are not equi spaced. And here we are taking a multiplier r by which the spacing between two grid points are increased. And if we have a non-uniform mesh, we can still write Taylor series expansion for different points point 5 is T x; point 6 temperature will be T x plus rdh, which is a difference here point forced temperature will be T x minus dh.

So, Taylor series for point expansion for T x plus rdh and T x minus dh can be written. And now we have to eliminate d T d x term, because we want the expression for d 2 T;

we want the expression for d 2 T d x square in terms of T x plus rdh T x, and T x minus dh, which is T 5, T 6; this is T 5 and T 4, we want the expression for d 2 T d x square in terms of that. So, what we will do we have to eliminate d T d x, so we will add A with r times of B, so that this terms are eliminated. And A plus r B will give me d 2 T d x square is of little complicated expression.

However plus the error now is of the order of dh not of dh square. So, there is one caveat here, if we use uniform mesh, we get using 3 points, we get second order accurate error for d 2 T d x square as well as for d 2 T d x square. For non-uniform mesh using 3 points, we will only get a first order accurate error. So, the we need to have more more and more mesh points in order to have list error solution as compared to the case we have seen previous for the uniform mesh case.

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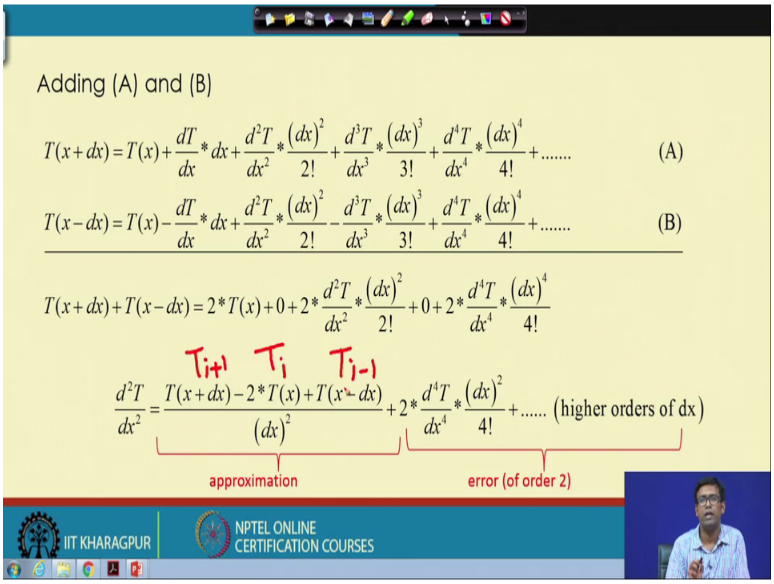

However, so what we end here is basically this one of the previous expression, if we see the if we see the previous expression, what we are ending here is a equation of d 2 T d x square in terms of one particular locations temperature T i temperature of the location next to it, and temperature of the location previous to it.

And these locations at the finite points what we consider to be our grid points or the mesh; we consider constitutes of all this finite points. So, now, we will get similar equation for each and every point in the mesh, so we will get an equation system essentially.

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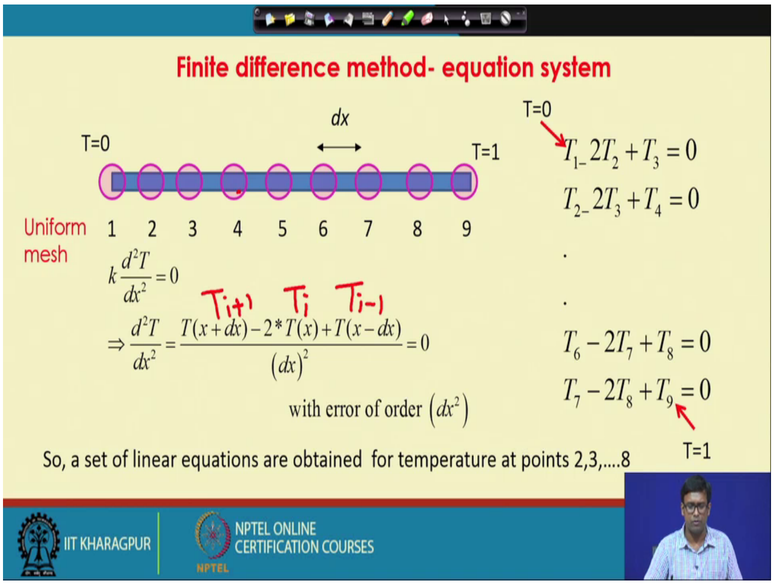

And let us see, so this is what we are getting for a uniform mesh d 2 T d x squared is equal to 0 will give me T x plus d x minus 2 T x plus T x minus d x by d x square. So, for any point any point i if this is if this is T i, this is T i minus 1, and this is T i plus 1; and these two are the boundary points. So, for except point 1 and point 9, because their temperature i already know from the boundary conditions; for point 2, 3, 4, 5, 6, 7, 8 for all this seven points, I will get seven such equations.

And this and there will be an error of course d x of the order of d x square. These equations are T 1 minus 2 T 2 plus T 3 is equal to 0. So, there are total seven equations, and all these equations look very similar only, because the weights of each the central term and the next to next and previous terms are same.

And in this equation we also have the boundary condition, which is T 1 is equal to 0, so we have to substitute this here; we have T 9 is equal to 0; we have to substitute it here. And we will set of get a set of linear equations for temperature 4.12 2 to 8 for this seven point.

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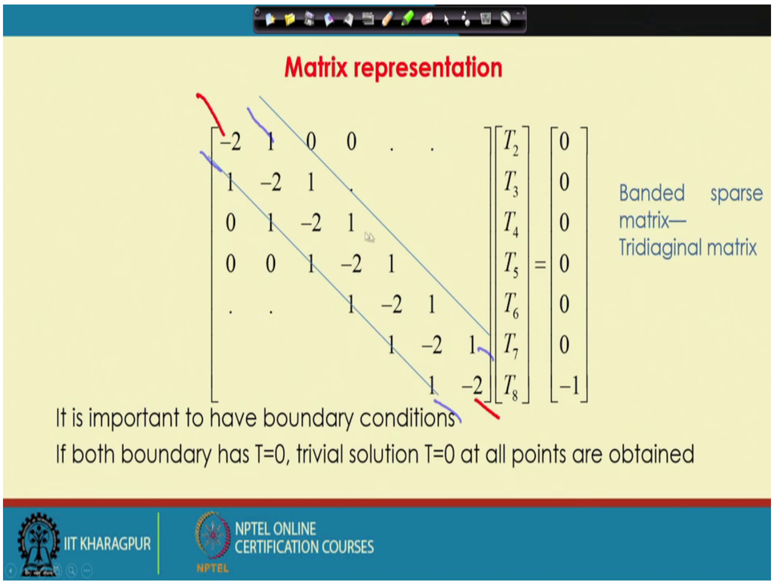

So, in order to find out what is temperature distribution here, we have to solve this set of equation. And what we get a in a matrix form, we get a particular matrix equation. And this is if we look into this matrix, there is one diagonal term there is one diagonal term, and there are two of diagonals next to it and rest all this terms are 0. So, this is a sparse matrix, where most of the terms are 0.

This is also a banded matrix if we recall the very first discussion on types of matrices, these are sparse matrix this is most of the this is the banded matrix because most of the non zero terms are clustered near the diagonal term with a bandwidth up to one term away from the diagonal one term below the diagonal. So, we can say that this is called a I am sorry this is a banded sparse matrix called a tridiagonal matrix.

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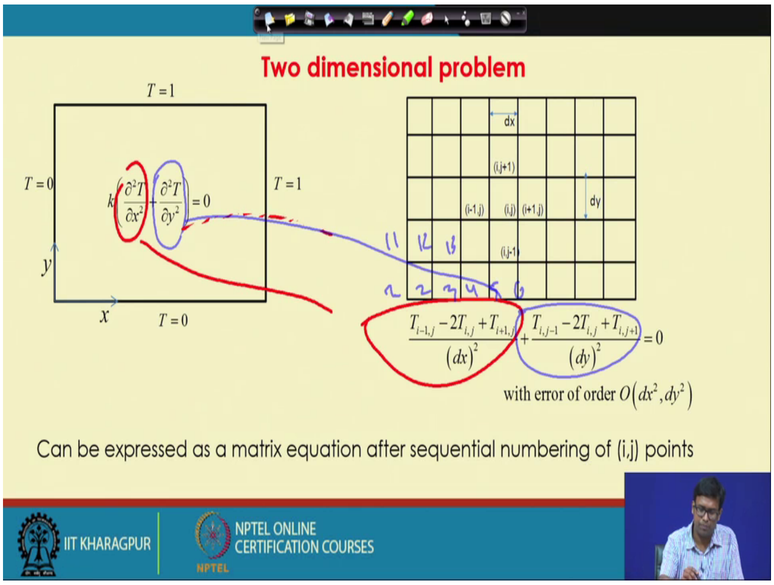

Another thing which is important here is that that this matrix if we will have a solution of this matrix only due to the fact or we will have a sorry. We will have a solution of this matrix because we have substituted the boundary condition that is why we can write it in a matrix form.

And then if the right hand side boundary T 9 is equal to 1, if that was not 1 this would have been 0 and the entire set of equations would have given me a trivial solution T is equal to 0.

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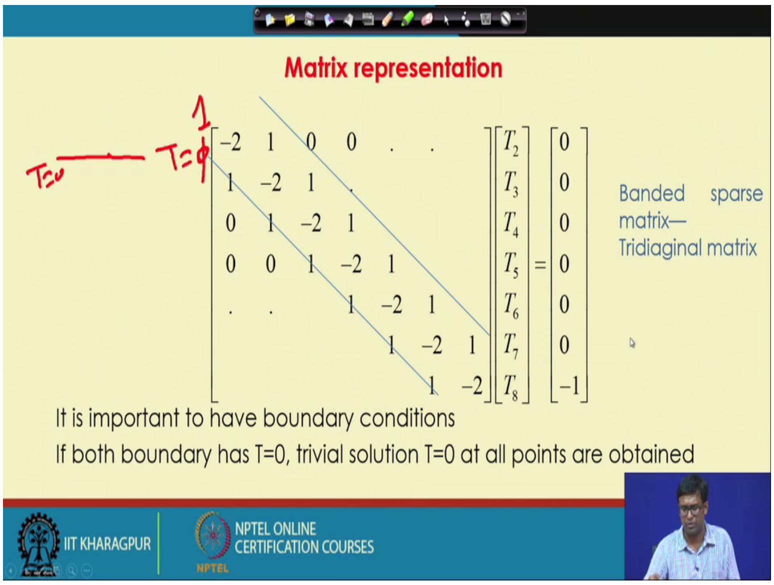

And that physically we can also see that if T is equal to 0 here and T equal to 0 here, there will be no heat transfer across the rod; so temperature everywhere will be0. So, it is important that we make T is equal to 1 here. So, that there is some temperature distribution inside it that temperature is not trivially 0 and as I said like this is a banded sparse matrix under tridiaginal matrix.

Now this is for a 1D matrix. For a 2D matrix, the equation is k del 2 d del x square plus delta 2 t del l y squared is equal to 0 temperature boundary temperatures are defined at all four boundaries, there are four boundaries now. And if I try to discretize it, it should be a 2D meshing, there will be mesh points in x direction or along i, i minus 1, i i plus 1 along i as well as there will be meshing in j and spacing in x meshes in along i is d x and along j is dy.

And we can convert this two terms del 2 T del x squared and delta 2 T del y squared similarly using Taylor series that this del 2 T del x square can give me T i plus 1 is partial derivative. So, keeping j constant it is a the same thing Taylor series will be applied in x direction keeping y constants, and also del 2 T del y squared will be given as this particular term and the order will be of d x d y square.

And now if we, so we if there are m into n points, we will get same m into n equations. And if we can re number the points like 1, 2, 3, 4, 5, 6 say here 11, 12, 13. If we can renumber the points from i, j k to i j to one particular number which will move along the mesh, we can form it as a matrix equation. And we can also write this to be a matrix equation with after sequential numbering of i j points. So, both this 1D, 2D even for 3D, we can also get similar matrix equation.

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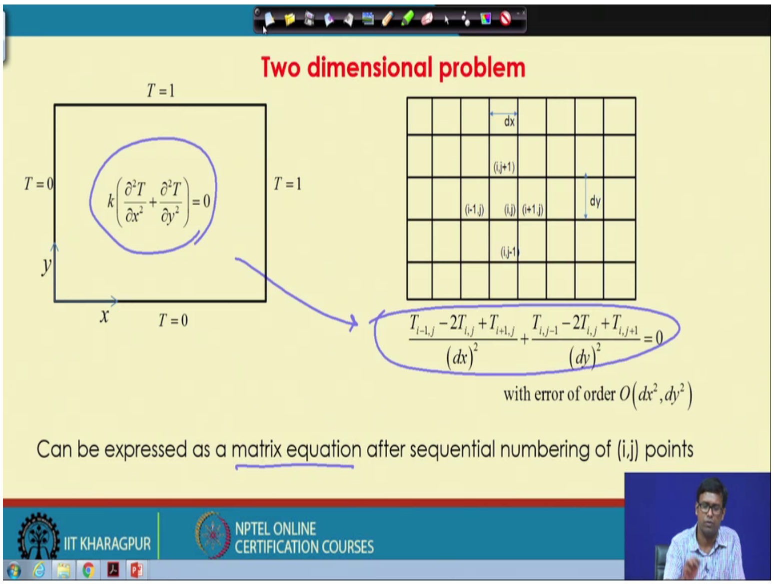

Laplace equation which we started here, Laplace equation which we started here can be converted into a difference equation and finally, we can get a matrix equation out of it. So, many physical equations can actually be converted into difference equations.

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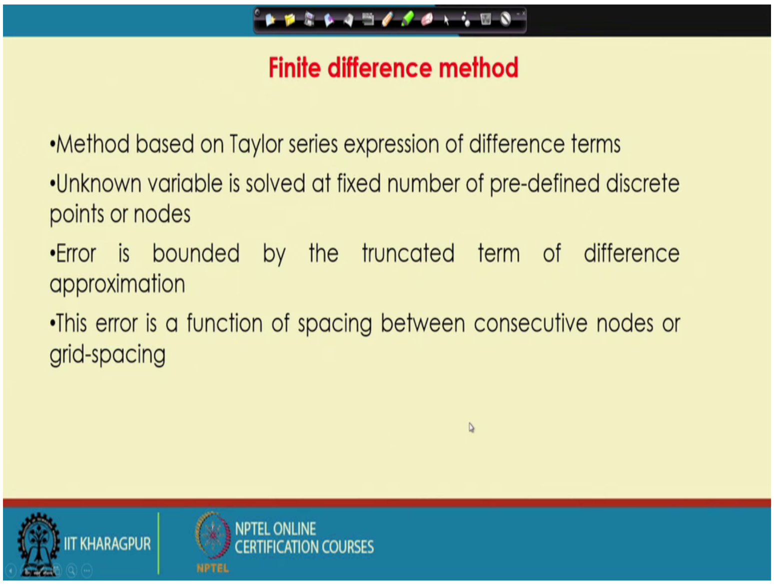

And this method is called a finite difference method this is based on Taylor series expression of different terms unknown variables are solved at fixed number of pre defined discrete points or nodes which are doing here. The error is bounded by the truncated term of the difference equation. And this error is a function of delta x or delta y or d x d y or d x which is the distance between two grid points in the space. If we increase the number of mesh points, then the distance between two mesh points reduce dx reduces and the error which is of the order of d x square or of the order of dx reduces and we get more accurate solution.

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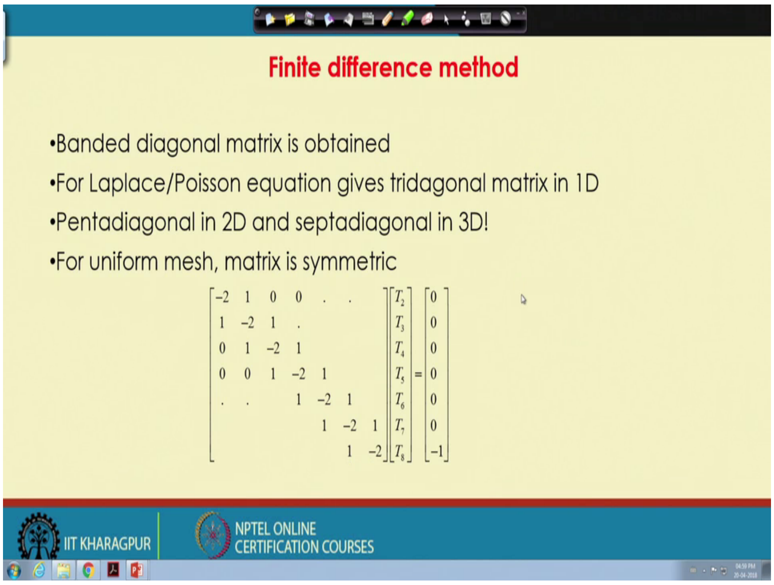

Now, finite difference method when we use we have seen we get a banded diagonal matrix. For Laplace or Poisson equation which we have shown here we get a tridiagonal matrix if you are solving one-dimensional problem. For two-dimensional problem, it is a penta diagonal matrix.

So, it is a matrix of five bands, bandwidth for tridiagonal bandwidth is 3 for penta diagonal bandwidth is little more than 5, but there are five diagonals. For say a 3D problem, it gives a spectra diagonal or there are 7 diagonal, 1 diagonal and six off diagonal bands in which all the nonzero terms are available remaining everything is 0. So, these are sparse equations sparse matrices and also banded matrices which we get.

And if we use an uniform mesh then the matrix is symmetric. If we see the matrix we obtained in the 1D case using uniform mesh, this is a symmetric matrix also. And there are certain issues with this particular tridiagonal matrix there are certain issues also its symmetric matrix which we will discuss in later classes. But today we will also looking to tri diagonal matrix or in the next class we will look into the tridiagonal matrix solution algorithm.

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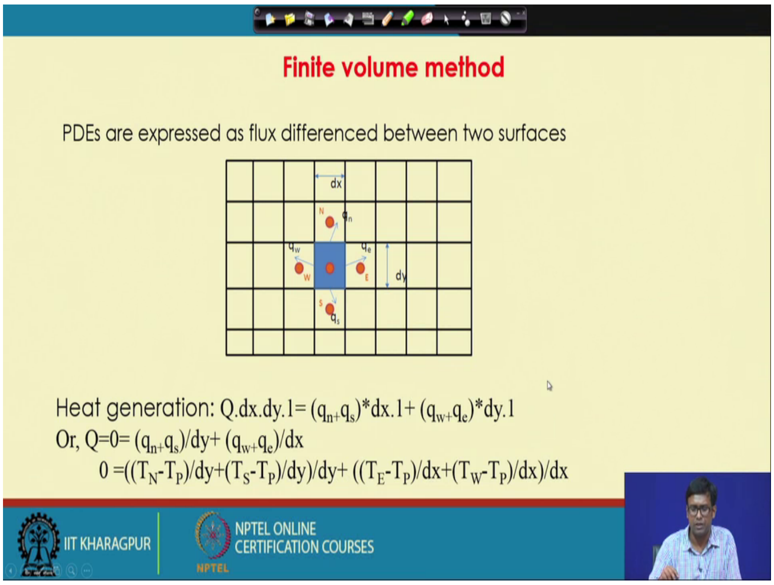

There are other methods like finite volume method. In finite volume method, instead of doing a Taylor series approximation, we do a little more physics based approximation, which is that heat conduction equation from a particular volume control volume can also be considered as the rate of conservation of heat or conservation rate of conservation of heat flux in the volume, heat generation within the volume is equal to heat loss as fluxes from the CV surface.

So, we write it that heat generation is equal to we calculate fluxes from each of the cell surfaces heat generation is equal to the net heat fluxes into the area. And if heat generation is 0 for study conduction, we get that the sum of the fluxes multiplied by area and then we divide by the volume. So, sum of the fluxes divided by d y sum of the y fluxes divided by d y and sum of x fluxes is divided by dx is equal to 0, which can be converted into an equation fluxes are difference of temperature divided by divided by the area.

So, we can which can be contributed into a temperature based equation and we can get similarly matrix equation.

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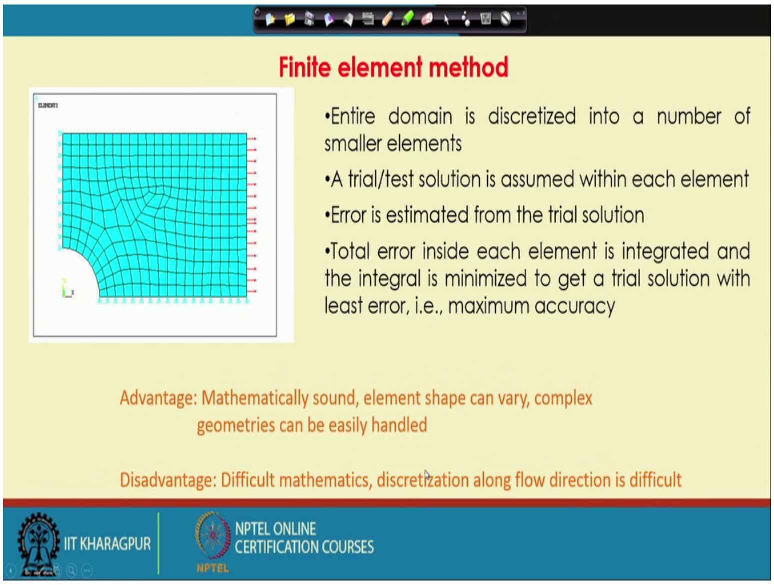

The other method is finite element method which is a very rigorous method specially applicable for irregular geometries find a difference we have developed it for a regular Cartesian geometry. Finite element can be applicable for complex geometries. Here the entire domain is discretized into a number of smaller elements the trial or test solution assumed within each element.

And then the error is estimated from the trial solution, we get a trail solution which is not the actual solution put it back to the original equation and see what is the error. And then we minimize the error total area inside each note is integrated and the integration is integral is minimized to get a trial solution which will have listed at or maximum accuracy.

This is mathematically sound with different element shapes complex geometries can be handled. The issue is that it has a difficult mathematics and discretization in certain cases can be very difficult.

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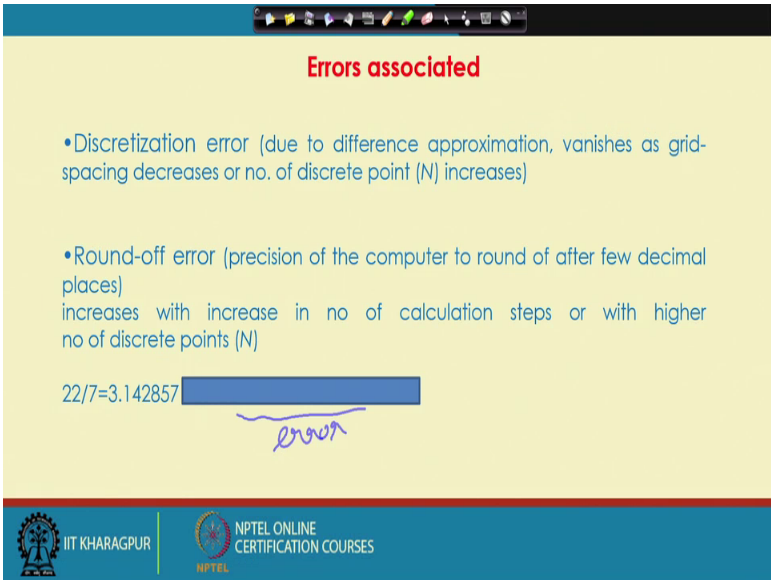

However, the errors associated is important to look into it we have discretized about discussed about discretization error which is due to converting the differential equation into difference equation this approximation. And this error is a function grids spacing as the grid spacing reduces the shaded reduces or as the number of points increases this error reduces.

There is another error called round off error or error which depends on the precision of the computer. And for example, if I am calculating 22 by 7 which is a good approximation for the pi which is a number goes which goes on and on and if we use a computer it cannot calculate pi up to the infinite decimal precision place, it will cut the value somewhere else. So, the remaining part becomes an error here which is called a round off error.

Now, as the number of points increases in each point I am doing some round off it or in any calculation in any division multiplication I am bound to do some round off error. So, whenever I have large number of points each I am doing a round off error total round off error increases. So, if we see discretization error reduces with increased increase in number of points, round off error increases with increase in number of points.

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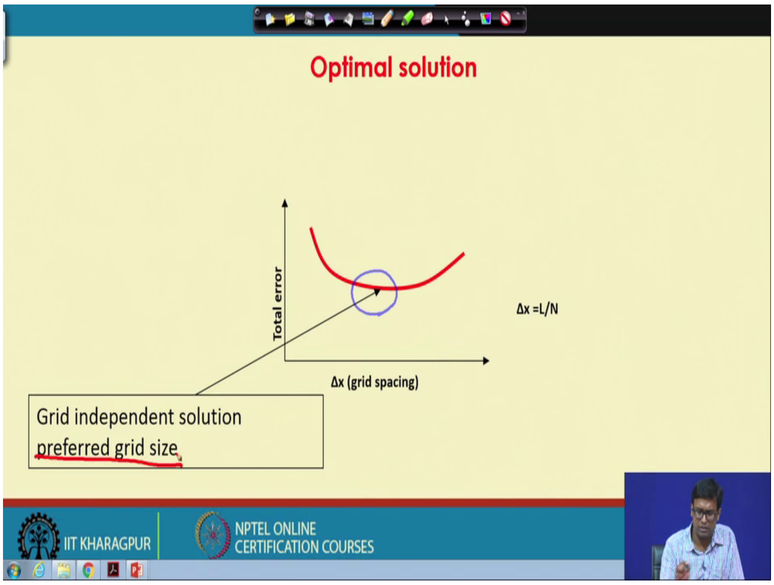

So, we go to an interesting situation that is totally if I write total error in as a function grid spacing or total error as a function of number of grid points as grid points will increase grid spacing will reduce and vice versa. As grid spacing as delta x grid spacing increases, the discretization error should also increase; however, the round off error reduces.

Therefore, we will see and as grids up to a certain point out the with grid spacing error is reducing and then it is increasing or the vice versa. If we come from this side as we are reducing grid spacing, the error is reducing up to certain point. And then as the number of points have increased grid spacing is very low, but finally, the error is increasing because one error is reduced discretization error is reduced, but round off error has been increased.

So, there is an optimal regime in which these errors kind of cancel each other and we will see a flatness in the curve there is a minima of error. We call this is a grid independent solution, because if we change the grid size slightly, there will be no change in error at this part. And this is the optimum grid spacing in which the solver should work to get the most accurate solution and this is what we called as the preferred grid size.

So, any solver any numerical method we are using to solve a physical problem like a Laplace equation coming from heat conduction equation or a Poisson equation coming from mass conservation and pressure balance equation in fluid flow, any of these equations or a stress strain relationship in a solid mechanics problem is a differential equation which is converted to a difference equation.

And when we are and then we were using a matrix method to solve this equation, but when we are doing this conversion from difference to difference equation differential to difference equations and using the matrix method we are obviously making some error that is evident that there is some error. This error has to be list or we have to in the p in the preferred gird size for the for right solution.

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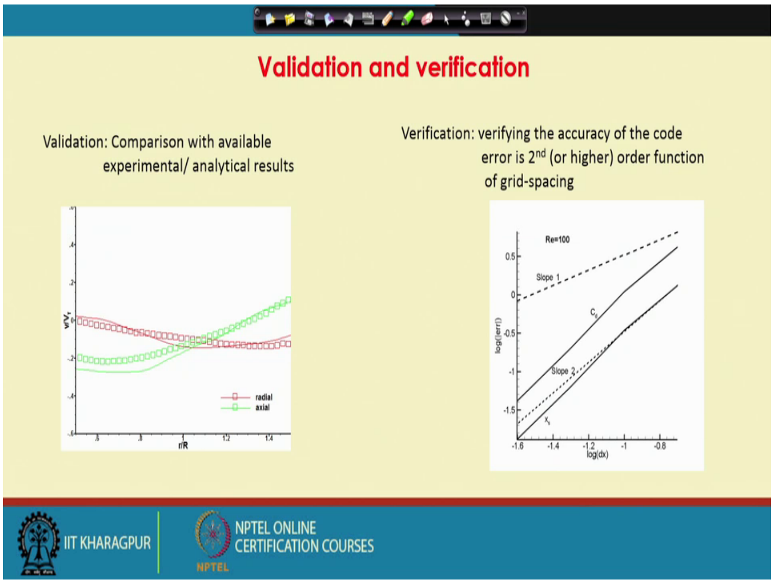

And that is why it is very important to have a validation and verification; Validation is comparing your numerical result with available experimental or analytical result and see that these differences are nominal. And verification is that actually looking into the accuracy of the code reduce the grid points see what is the difference from the analytical or experimental solution.

And now increase the number of grid points, calculate the error. And see whether the error reduces following a second order or first order whatever is the accuracy preferred slope following that particular nature. So, these two are very important things when doing a numerical solution of a physical problem. Without this we cannot have confidence over the solution method because we always know when we are converting the differential equations to the difference equation or to the matrix equation and solving it, we are making some error. This error has to be within a confidence level, so that the final solution is acceptable ok.

Next class, we will see how this matrix equation which is coming from a physical problem like a Poisson equation or Laplace equations transform difference equation can be efficiently solved.

Thanks.