# Computational Science in Engineering

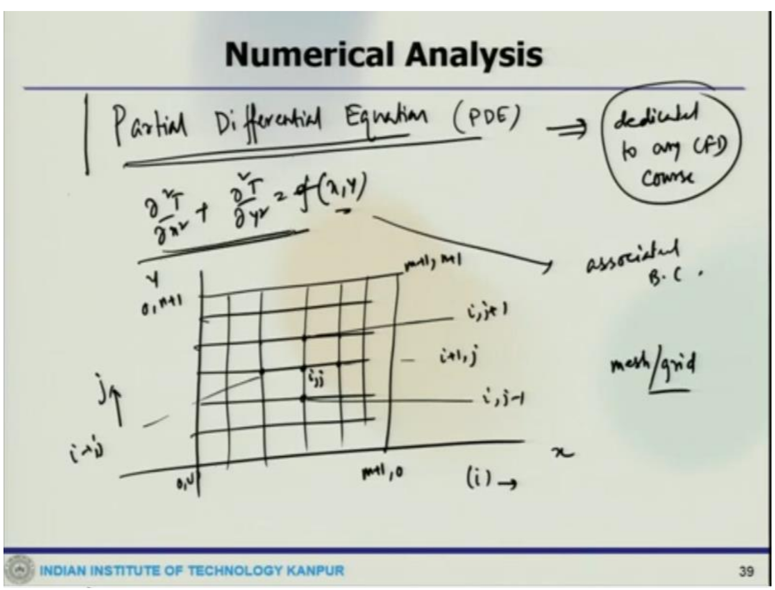
Prof. Ashoke De
Department of Aerospace Engineering
Indian Institute of Engineering – Kanpur

## Lecture – 40
## Numerical Analysis

So, we have looked at in details the solution or different ways to solve the ordinary differential equation. So, now here we are going to talk about a little bit on the partial differential equation, but we will not go in very details, because that is not the kind of lecture that can cover of the detailed discussion on numerical methods of partial differential equations. But essentially, when you look at the typical numerical methods or approach for the solving partial differential equation, that actually goes to a very dedicated lecture.

Or course on partial differential equation solution, which is like computational fluid dynamics, or any CFD course, or compressible fluid mechanics, whatever be the name in that kind of course, if you look at that pretty much talks about from the beginning, how to solve the partial differential equations. So, here we will just touch upon some of the quick ideas. Whatever we have discussed in details using that, we will just look at what kind of system it leads to, but we will not go into very much detail.

**(Refer Slide Time: 01:26)**



So, let us look at those things quickly. As I said, we will restrict the discussion to only a few some important or touching points not in very details, as any partial differential equation or the numerical approach for solving PDEs goes to so this is dedicated to any CFD course, or part of CFD course, where you can see how different ways you can solve these PDEs different methods, so that we will talk about error stability everything. Here we will just touch up on how we can solve it, because we have already seen the linear system.

So, let us look at a particular system how let us look at this Laplace equation of

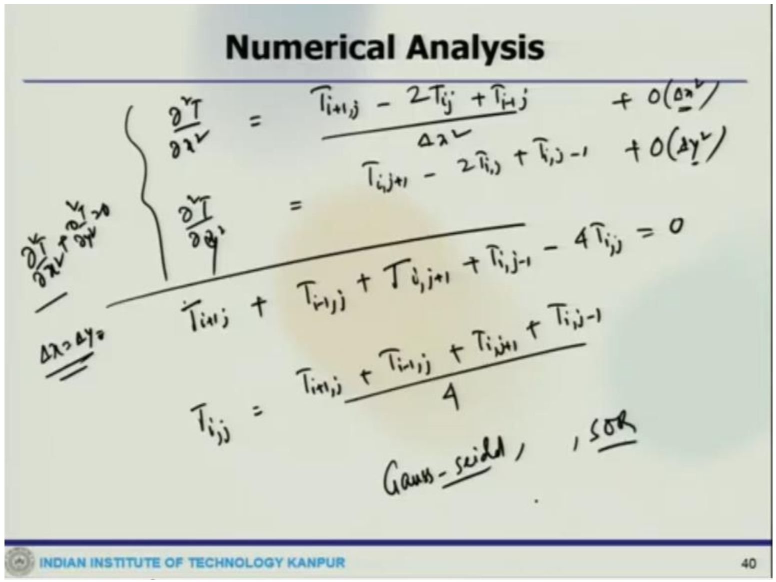
$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = f(x, y)$$

So, typically, when you solve these things, so, this goes in as you can see in a 2 dimensional system.

So, you need points in both an x and y and the obviously, this would be associated with all boundary conditions, that means this is the domain let us say. So, this is the point which starts from so this you divide into multiple points like that. So, it goes and any intermediate points, which will say that this is i and j, so this side you go i this side you go in the indexing j and this could be any point (m + 1, 0) and this point will be (i + 1, j), this point would be (i, j + 1), this point would be (i – 1, j), this point would be (i, j – 1) like this.

So, this side would be (i – 1, j + 1), this would be (i + 1, j + 1), this is (i + 1, j – 1), (i – 1, j – 1). So, these are the indexing which is done and this could be (m + 1, n + 1) and this is (0, n + 1). So, this is how you need? So, this is called some sort of a mesh or grid, where you distribute and you try to find a solution for this particular system.

**(Refer Slide Time: 04:10)**




Now, the first term that you can write. now, so far, we have looked at different for different formula. So, this is you write like these

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + O(\Delta x^2)$$

$$\frac{\partial^2 T}{\partial y^2} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} + O(\Delta y^2)$$

So, you can see, it involves some of these tensile around that particular point. And so, both the cases this would be order of $\Delta x^2$ the truncation error, this case $\Delta y^2$ and as you refine your step size, the error truncation will be reduced.

And if these two you put it in this equation and you let us say

$$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$$

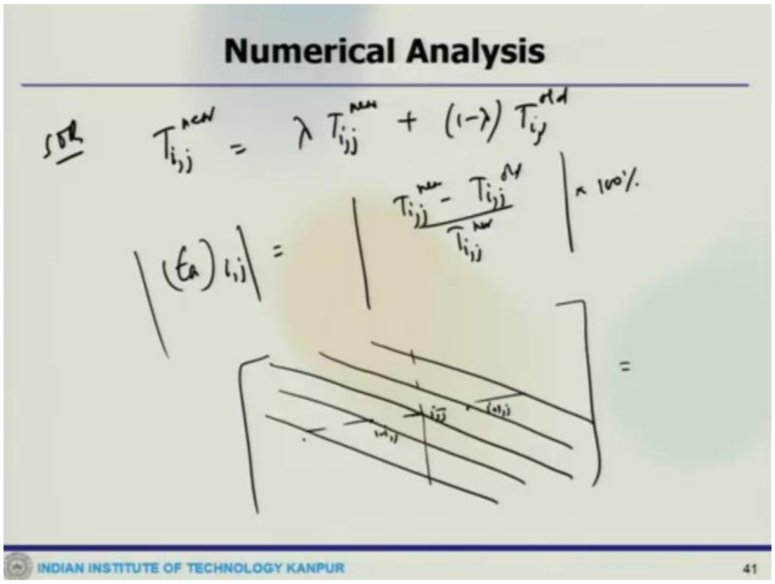
So, this is called the Laplacian difference equation that you get and you need as I said you need the boundary conditions all these different positions to solve this and you may have these boundary conditions to solve this.

And now, there are different ways one can solve it so, it will form a actually matrix and like if you write

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4}$$

So, this can be solved by loop and now, we can use the methods that we have already discussed in our linear system like kind of iterative method like Gauss Seidel or SOR kinds of things, where if you use the SOR kind of approach.

**(Refer Slide Time: 06:52)**




Then what you can find out that

$$T_{i,j}{}^{new} = \lambda T_{i,j}{}^{new} + (1-\lambda) T_{i,j}{}^{old}$$

Now, depending on the lambda it could be over relaxation system or another relaxation system or one can solve like an any obviously, direct method is not advisable there as you can see from the system. So, the methods that we have already discussed in our linear system anything you can apply like any iterative methods that you can apply to solve this problem.

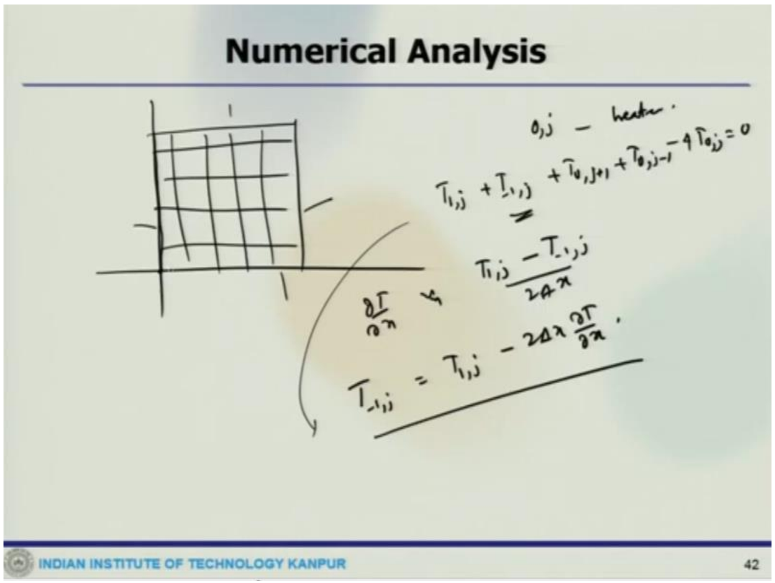
And finally, one has to look at the relative error which would be of the order like the magnitude would be

$$\left|(\epsilon_a)_{i,j}\right| = \left|\frac{T_{i,j}{}^{new} - T_{i,j}{}^{old}}{T_{i,j}{}^{new}}\right| \times 100\%$$

So, that percentage one has to see, so, that it remains within the tolerance limit. Now, typically, if you look at this particular system here, so, this gives you an essentially if you like in a matrix form, so, this actually gives you a system like an if you see this is a 5 diagonal system, so, any point of time if this is i and j.

So, you get all this (i + 1, j), so, you can see that (i + 1, j) then there will be (i – 1, j) then (i, j + 1), (i, j – 1), so, this is what you have (i, j – 1), (i, j + 1). So, this actually gives you a penta diagonal system all the time. And you can solve that penta diagonal system by different approaches that that has been given.

**(Refer Slide Time: 09:00)**




Now, the boundary conditions, obviously in this particular to solve that problem, when you have this boundary, where you are solving these, then either you could have all these boundaries could be this lead boundary or you could have the gradient of the Norman boundary conditions which are given or some sort of derivative boundary condition that could be given. So, that would lead how you can solve this.

For example, let us say node 0, j, which is the basically left side of the plate here, it is heater. So, then what I can write there at those points

$$T_{i,j} + T_{-1,j} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0$$

So, now there is an imaginary point you can see this is or lying outside of the plate is required for this equation, although this exterior point might seem to present in the problem, it actually serves as the vehicle for incorporating the derivative boundary condition into the problem.

So, this is done by representing the first derivative at that point 0, j like if we write

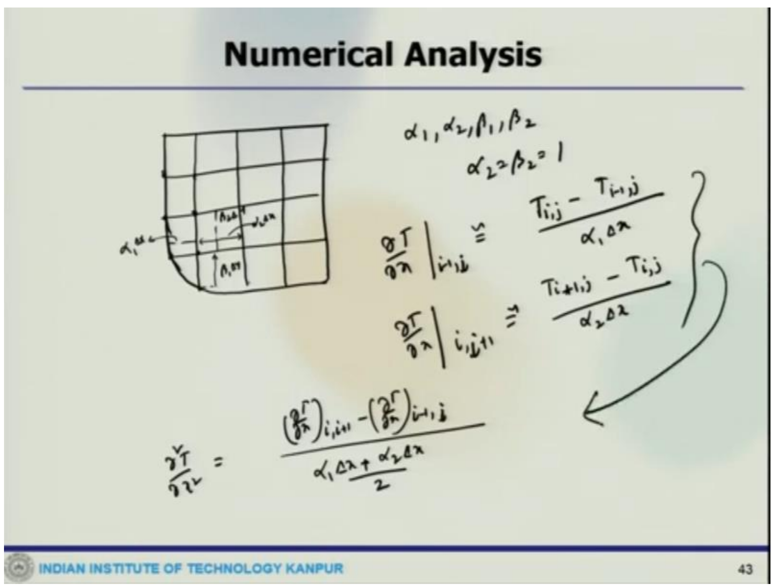
$$\frac{\partial T}{\partial x} = \frac{T_{1,j} - T_{-1,j}}{2\Delta x}$$

So, we can solve for

$$T_{-1,j} = T_{1,j} - 2\Delta x \frac{\partial T}{\partial x}$$

now, this is a different relationship that we obtained for that now, this you can replace back here and then you can actually get a different system to solve it. The whole idea is that when you actually discretize that kind of system, then you get this specially this different discrete equation, which we you need to solve using this kind of situation. Now, another issue which may come is like that, the boundary may not be like regular like this.

**(Refer Slide Time: 11:17)**




So, the boundary could be slightly irregular, for example, let us say we take in a situation where the boundaries going irregular and like this, and you have these points like this, so these are the points which are sitting there on the irregular boundary. and these are the different other points, so like that.

Now, so this is where you can see the boundaries irregularly shaped, now we have now here 4 parameters $\alpha_1, \alpha_2, \beta_1, \beta_2$. So, obviously, you can by looking at that you can see $\alpha_2$ and $\beta_2$ they are same, but we still retain these parameters through the following derivation so, that a generic system can be obtained and you can use that. Now, in the first derivative of the x direction which like

$$\left(\frac{\partial T}{\partial x}\right)_{i-1,j} \cong \frac{T_{i,j} - T_{i-1,j}}{\alpha_1 \Delta x}$$

and

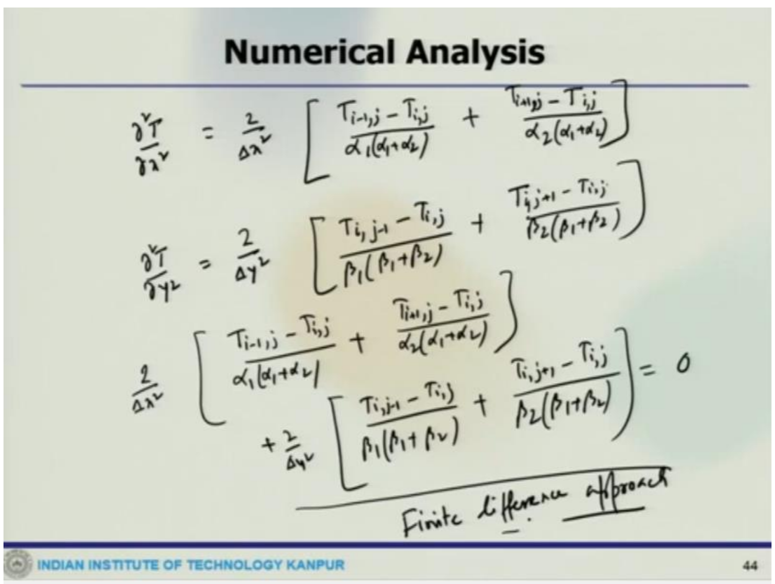
$$\left(\frac{\partial T}{\partial x}\right)_{i,j+1} \cong \frac{T_{i+1,j} - T_{i,j}}{\alpha_2 \Delta x}$$

So, that is what we get. So, what do we get now, the second derivative can be developed from this first derivatives like

$$\frac{\partial^2 T}{\partial x^2} = \frac{\left(\frac{\partial T}{\partial x}\right)_{i,j+1} - \left(\frac{\partial T}{\partial x}\right)_{i-1,j}}{\frac{\alpha_1 \Delta x + \alpha_2 \Delta x}{2}}$$

Now, if we substitute these things in this particular expression and then do the algebra.

**(Refer Slide Time: 14:43)**




So, all these expressions if we put it back here and what we can write is that

$$\frac{\partial^2 T}{\partial x^2} = \frac{2}{\Delta x^2}\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)}\right]$$

So, similarly, one can obtain for

$$\frac{\partial^2 T}{\partial y^2} = \frac{2}{\Delta y^2}\left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)}\right]$$

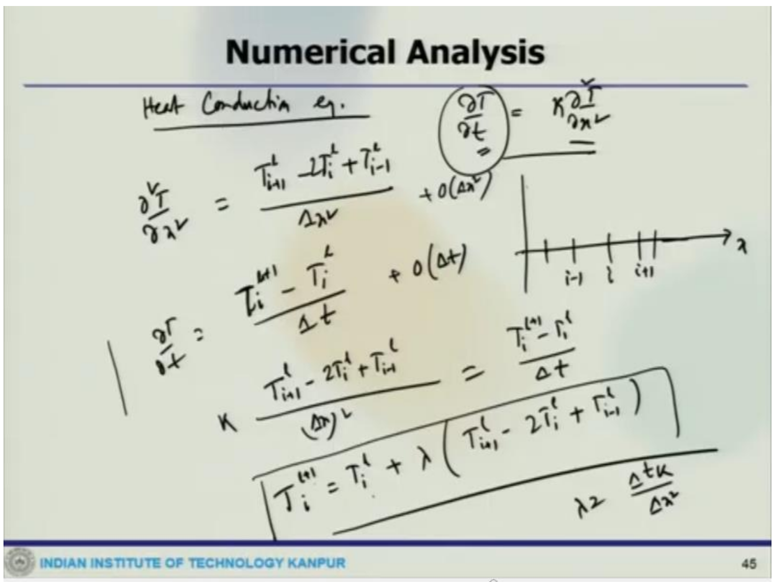
So, once we put it back in the original equation, so, what we get

$$\frac{2}{\Delta x^2}\left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)}\right] + \frac{2}{\Delta y^2}\left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)}\right] = 0$$

So, now, you can do that and kind of take it out. So, the kind of approach that we are taking here like what are we defining at the different node and we are trying to find out the solutions at different nodes.

So, this is called a finite difference approach which will allow you to get solution in different among all these different nodes i, j such that nodes. So, any finite difference approach corresponding to this kind of PDEs will lead to the nodal solution. So, finite difference approach actually provides you the nodal solution obviously, any PDEs which you define, then this is domain leads important that already we talked about and the boundary conditions are important.

**(Refer Slide Time: 17:49)**




Now another equation which we can look at the heat conduction equation, which involves the temporal derivative

$$\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2}$$

this is one equation. So, this is a parabolic equation previous one what we have looked at is the elliptical system here obviously. so, this would be straightforward, because this goes in one direction.

So, this is in the x direction, so, we have different node like i, (i + 1), (i – 1) but here the important thing is that, we have a temporal derivative sitting there. So, we have to write like what is the time level. So, that is important. So, $\frac{\partial T}{\partial t}$ can be discretized. So, this has an error of order of $\Delta t$ and this guy has an order of $\Delta x^2$. Now, once we put this back, so what we get?

So, essentially this can be written as

$$T_i{}^{l+1} = T_i{}^l + \lambda\left(T_{i+1}{}^l - 2T_i{}^l + T_{i-1}{}^l\right)$$

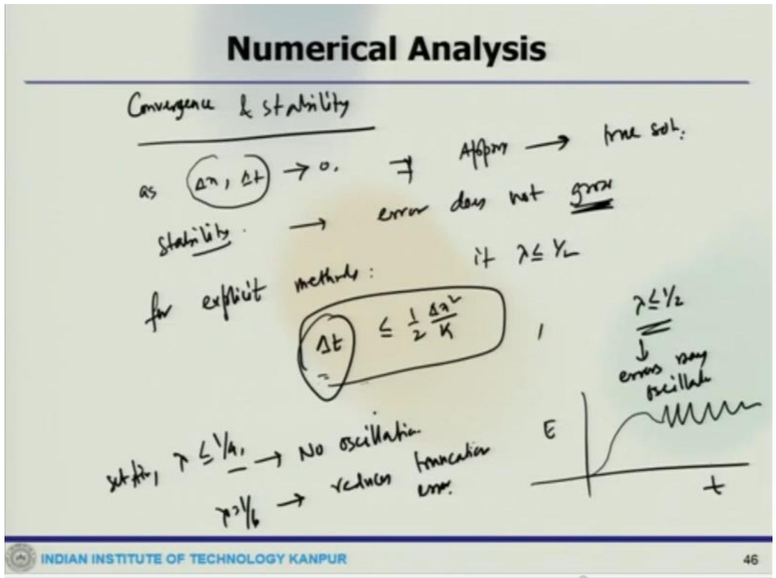
So, where

$$\lambda = \frac{\Delta t K}{\Delta x^2}$$

So, this equation is valid in the any interior nodes not at the boundary nodes and then provide explicit mean. Now, if you look at this equation, this is when we can solve like an explicit method or implicit method, because this is integration over time, and we have already discussed and this is in 1 dimension.

So, we have discussed so, many different approaches, which involves in solving the ordinary differential equation. So, now, if you look at this particular expression, this is I mean at the next time level you are using the previous time level and getting the solution at the interior node. So, this is actually a manifestation of the sort of Euler's method for solving the ODEs that what we are talking here. So, that is if we know that temperature distribution as a function of position as an initial value. So, here important thing is that this particular since it involves temperature, you required the initial value, and so, it eventually leads to an initial value kind of problem.

**(Refer Slide Time: 21:16)**




So, now, what we can do that we can solve, there is one issue which will come this kind of temporal system is that convergence and stability. So, now, convergence means that as $\Delta x, \Delta t$ approaches to 0, so these results of this finite difference approach the true solution. So, that means, when they tend to 0, the approximate solutions should be tends to true solution. So, that is what it is and when you talk about the stability.

That means, the error at any stage of the competition is not amplified, but are attenuated as the competition progresses. So, these the error does not grow. So, which is important, if it grows then the solution will basically diverge, they will not converge at all. So, it already is known that for or already we have seen it for explicit methods, but we can say that the for both conversion and stable if $\lambda \leq \frac{1}{2}$ or what we can say

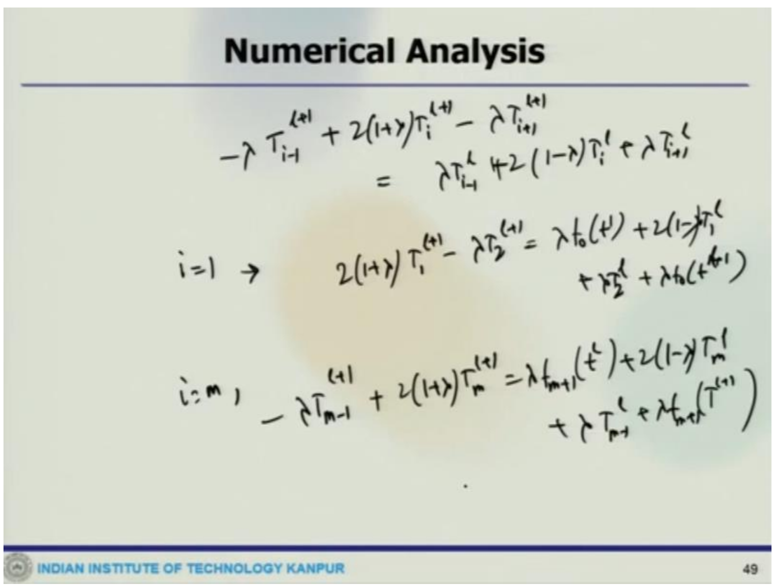
$$\Delta t \leq \frac{1}{2}\frac{\Delta x^2}{K}$$

So, if we set that $\lambda \leq \frac{1}{2}$ could result in a solution error do not grow, but oscillate. So, this is one of the stability criteria from which one can choose the step size. Addition to that, if we put lambda less than or equal to half, then it will not grow but it may for these errors may oscillate. So, like for example, with time if we plot the error, so this will grow then after that certain point it may oscillate like that.

So, this is what may happen if you setting $\lambda \leq \frac{1}{4}$. So, this will ensure that no oscillation in the solution and it is also one can say $\lambda = \frac{1}{6}$ which also reduces truncation error. So, the whole points these are some of the values which are already proposed to see what kind of stability criteria or something, but the idea is that the step size for both delta x and delta t would be such that, it should give you a numerically stable system.

And also, should give you a proper solution, I mean sometimes it may happen then the satisfaction of this particular expression will alleviate the instabilities of the sought manifested system. But it also places a strong limitation on the explicit method. Because as you can see, when you use the explicit method, then this will pose some restriction. Now, one can have higher order temporal discrimination and do that.

**(Refer Slide Time: 24:56)**




Now, alternatively what you can do, you can look at some implicit discretions. So, one can write that

$$-\lambda T_{i-1}^{l+1} + 2(1+\lambda)T_i^{l+1} - \lambda T_{i+1}^{l+1} = \lambda T_{i-1}^{l} + 2(1-\lambda)T_i^{l} + \lambda T_{i+1}^{l}$$

So, this is coming from previous times step and this is what you are going to solve at the current time step. So, now, this particular system, what we have written that now for this case, where the temperature levels at the end of the domain which are given and we can say that for i = 0.

So, this is where x is starting at 0 or the starting of the domain. So, and any other interior points we can have, so, this is at the boundary or the other left boundary that you have and now any other interior point where i = 1, you can have

$$2(1+\lambda)T_1^{l+1} - \lambda T_2^{l+1} = \lambda f_0(T^1) + 2(1-\lambda)T_1^l + \lambda T_2^l + \lambda f_0(T^{l+1})$$

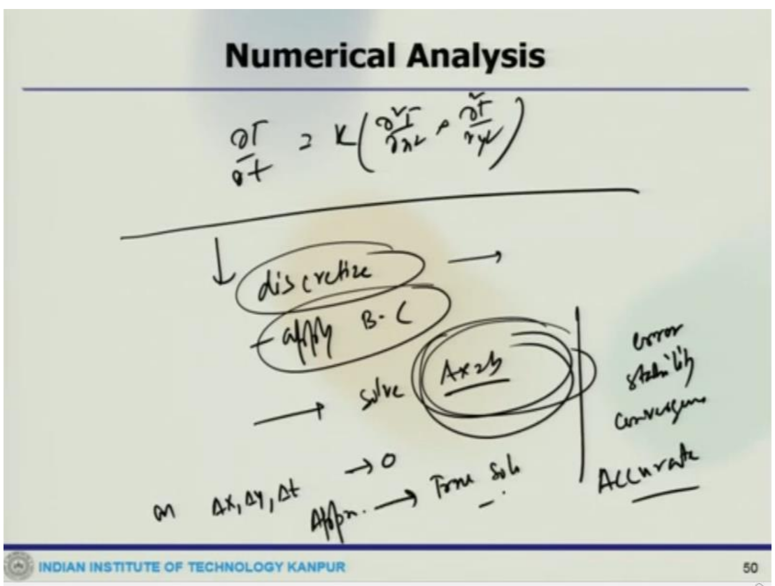
Similarly, for the last interior point which i = m that would be

$$-\lambda T_{m-1}^{l+1} + 2(1+\lambda)T_m^{l+1} = \lambda f_{m+1}(T^l) + 2(1-\lambda)T_m^l + \lambda T_{m-1}^l + \lambda f_{m+1}(T^{l+1})$$

So, these are the basically if your domain starts from i = 0, so, this is one of the boundary and this is m which is boundary. So, for i = 1 and i = 2. So, this is let us say boundary i = m + 1, this is also boundary and this is m. So, then any other interior point in between that expression that we have derived that can be written.

So, and now, we can have some like to solve this kind of method, one can use some sort of temporal discretization like Crank Nicolson is one such method which can be used Crank Nicolson method. So, you can see that what you can write like this.

**(Refer Slide Time: 31:14)**




So, similarly, one can go like no one can solve for this kind of equation

$$\frac{\partial T}{\partial t} = K\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

So, now, you see how things become a bit complicated and obviously, when you discretize the system, so first thing that you need to do you need to discretize then apply a boundary condition then you solve the Ax = b system and for that whatever we have discussed so, far that you can use different kind of method to solve it.

So, you have to discretize so, that you get the approximation then apply the boundary condition and then finally, you get this linear system. And then obviously, when you solve these, there it will include all the error, stability, convergence and finally the solution which is accurate. And for any small time or all these steps as they attempt to 0. So, the approximate solution should trend through the true solution.

Now, I mean, as I said, for any partial differential equation, there are dedicated course like CFD codes. So, this is just to give you an idea how you handle the partial differential equation. And it may also get back to yourself, essentially, when it lead to a linear system. That is where you use your concept of the solving of linear system that we have done the discussion in details. But any other details and all these things that would actually be focused of any other CFD course or something. I hope you have enjoyed the discussion. And we will stop the all theoretical discussion pretty much to conclude here. Thank you.