Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 13
Numerical Solution of PDE-Method of lines

Hello every one, in this lecture, we are going to learn about the implicit and the explicit solution strategies for solving partial differential equation. Now, in the last week, we have already done at some of the exercises using the separation of variables for based on the analytical methods. In this class we are going to do the exercise for a (parabolic) similar kind of parabolic equation or a parabolic partial differential equation using the method of lines which we have so far discussed in the last two or last couple of classes on the technique of discretization and learning about the different (stability) numerical stability schemes.

Here we are going to have a solution of partial differential equation heat equation essentially using both the implicit and the explicit scheme.

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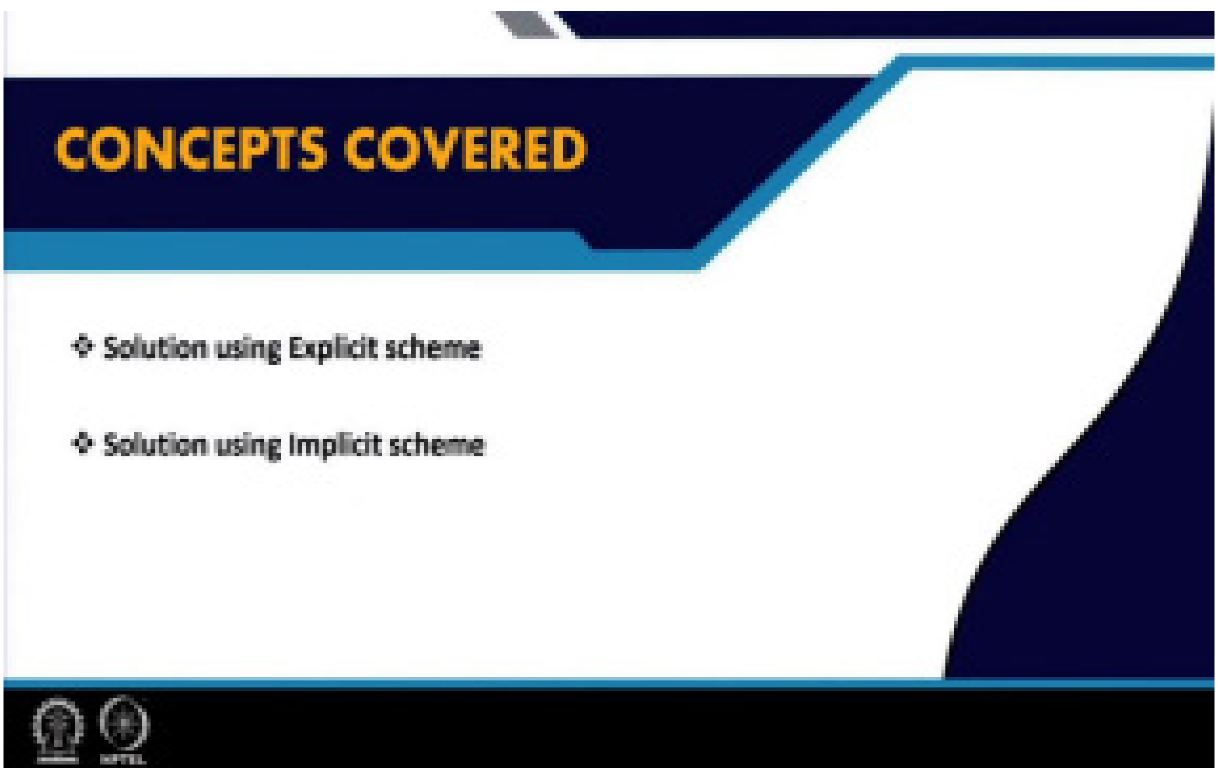

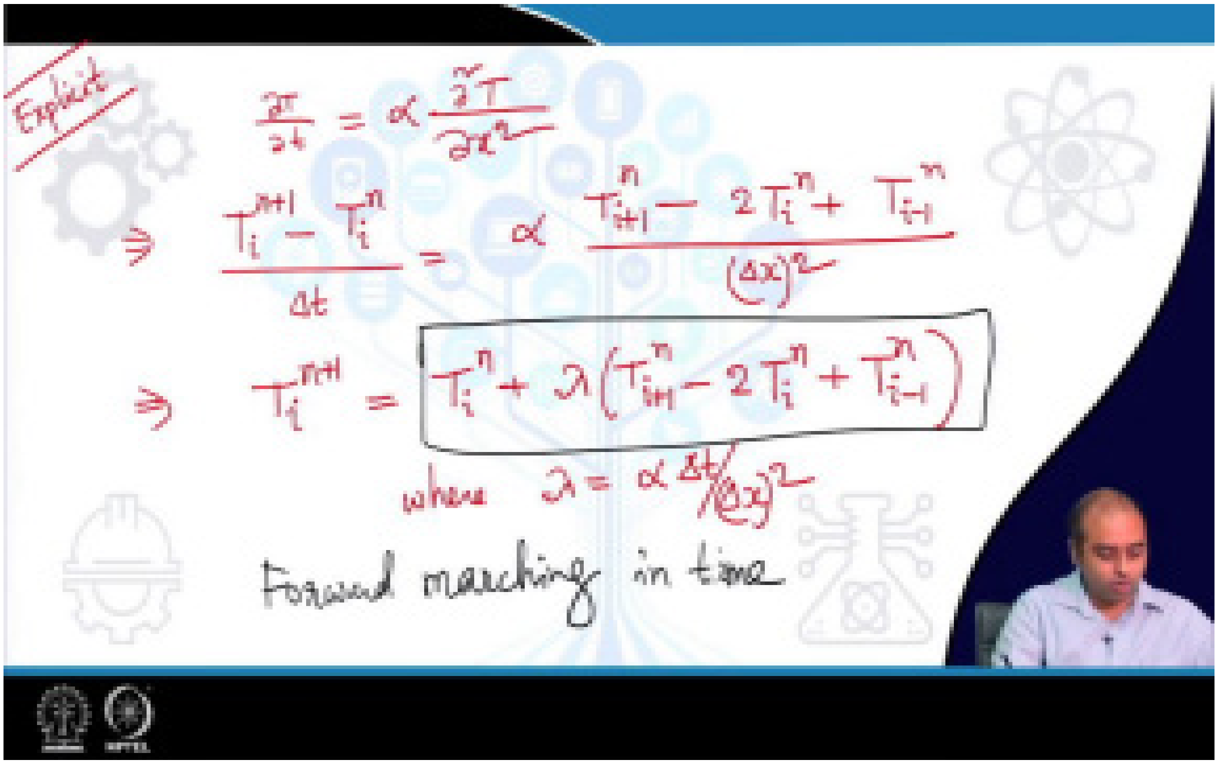

Now, let us try to look into the equation and frame the explicit formulation. So, as I have said we are going to use the heat equation in this case so, trying to write down the discretized or the difference equation. So, the subscript represent the space discretization and the superscript represent the temporal discretization. So, this is something which we have already talked about that any second order space part would be discretized using the central difference and the temporal derivatives is generally discretized based on the forward difference, so this is the explicit scheme and we can write the time update temperature equation.

So, if we know all the background information from the previous time step we can calculate from this equation, what would be the value at the future time step. So, this is the explicit formulation we have already discussed in the last class. So, we are just starting from there, so this equation is forward in time and central is space and this is the explicit scheme because the spatial derivatives is discretized at the current time, and so if you can see here in this equation on the right hand side, everything on the right hand side everything that is mentioned or calculated are going to be calculated is based on the previous time. So, that is how we do forward marching in time.

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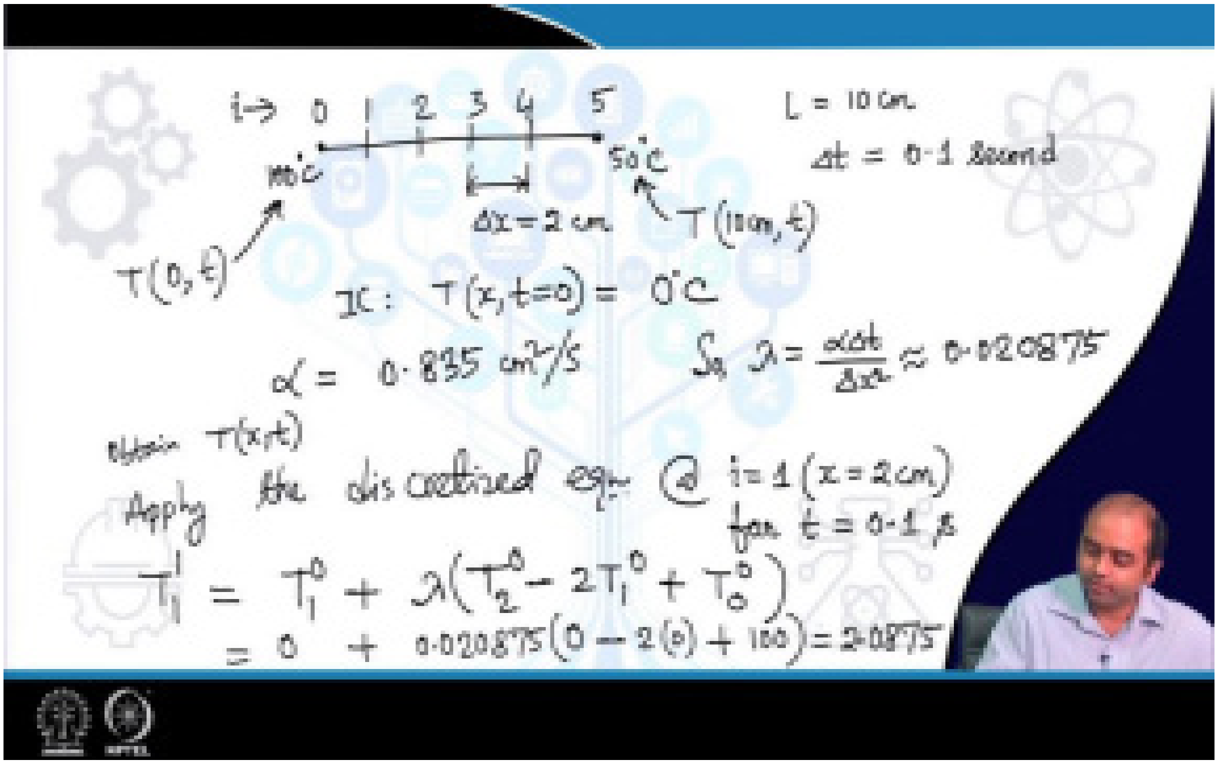

So now, let us see a simple example of a one dimensional rod, we try to explore an example problem. Let us say the two ends of the rod has a temperature of 100 degrees and at the other side it is 50 degrees and we discretize the space with equal intervals marking them as 1, 2, 3, 4 so, this is 0 and this is 5. So, these are the i values the index at different locations in (the) in this in this solution space and each grid size is of 2 centimeter.

So, this means that the rod length is 10 centimeter essentially it is a 10 centimeter and a discretized into 5 parts so, the delta x is 10 sitting there and we consider our delta T, I do not know whether it will lead to stability or it will have any issues with convergence, but for the time being let us assume that 1 second time interval is considered point 1 second of time interval without worrying too much about the stability issues.

So, define the boundary condition T at x is equal to 0 is and at all time is this and T at x is equal to 10 centimeter is this. This is the boundary conditions and the initial condition is time sorry temperature x T is equal to 0 is he is initially everywhere it is 0 degree centigrade. We define alpha to be thermal diffusivity which is nothing but thermal conductivity divided by rho Cp.

So, naturally you can find out (al) lambda is equal to alpha delta t by delta x square and if you put in the numbers this will come out 0.020875 and you can clearly understand that for based on the Von Neumann stability criteria of diffusive equation this factor lambda needs to be less than half and it is clearly it is half less than half and it is point 02.

So, of course, this will lead to no no issues on the stability of the problem. So, you can also from here you can also determine what should be the maximum delta t for which you can try to solve this problem. So, higher is the delta t the faster is the time dynamics you can solve with. So, now, it is asked that you find a solution obtain T x comma t. So, how do you work out this problem we go step by step.

So, we apply the discretized equation apply the discretized equation at i is equal to 1 which means x is equal to 2 centimeter for time t equal to point 1 second that is fast delta t. So, T11 all of you can understand what do we mean by T11 which is calculated from T01 plus lambda into T02 minus 2 T01 plus T 0 this is from the discretized equation.

So, if I put in the numbers here, so, I will get 0 because this is based on the initial condition that is why I have written down 0 next is 0.020875 that is lamda the first one is again 0 second one is 2 into 0 and the last one please note that this is the boundary condition so, boundary condition value is 100.

So, the boundary condition is valid at all times including the initial time so, do not get confused with this one. So, whenever there is a boundary coming in the vector you should take into the boundary condition irrespective of whether it is in in equivalence to the initial condition or not you should apply the boundary condition that is why this is a boundary condition and I have written. So, from here you can find out that it is 2.0875.

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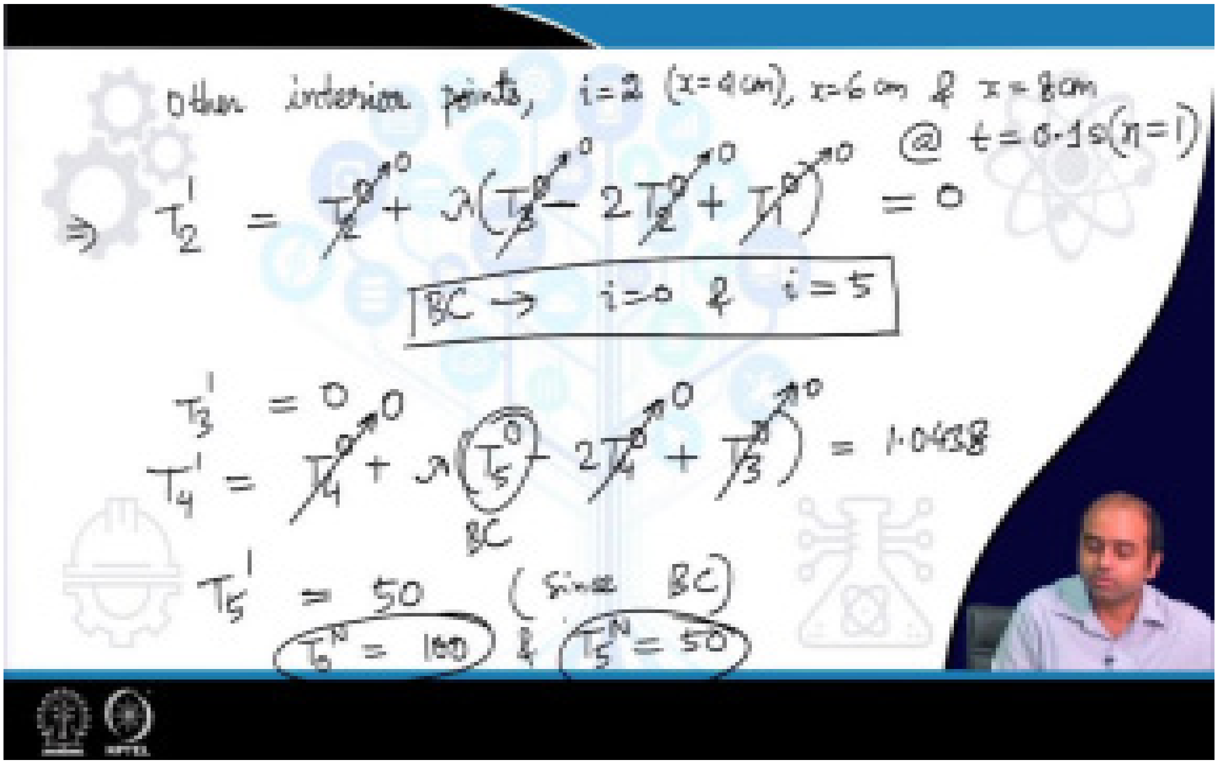

Now, let us look into the rest of the meaning of the interior points other the interior points. So, the other interior points corresponding to i is equal to 2 which is means x is equal to 4 centimeter, then we have x is equal to 6 centimeter and x is equal to 8 centimeter at t is equal to the first time step point 1 second which is n is equal to 1. So, for T21 you will be having T20 plus lambda T30 minus 2 into T20 minus sorry plus T10. So, you can clearly understand that none of the temperature conditions on the right hand side is at the boundary conditions.

So, the boundary locations so, what are the boundary locations the boundary indexes are i is called to 0 and i is equal to 5. So, in this case you can clearly realize that for T2 all there is there is since on the hand side all the terms that we are seeing on the hand side this is 0 this is 0 because these are all initial condition this is 0 and this is also 0 none of them is a boundary condition.

So, T2 is equal to T2 at the first time interval is also 0. Similarly, T31 is also 0, but for T4 if I try to write the discretized equation, you will realize that it is T40 plus lambda T4 sorry it is T5 T50 minus 2 into T40 plus T30. So, this is 0 this is 0 because these are initial conditions and interior points is 0, but this is not 0 this is a boundary condition.

So, if you put in the numbers on this case, you will get that T4 is equal to 1 point 0438 and of course, T51 is equal to 50 because that is the boundary condition value this is since it is a boundary condition. So, please note that at the boundaries. So, essentially what I mean to say that T5 T0n is equal to 100 and T5n is equal to 50 for all time points. So, this is something to be realized here that at the boundary conditions is valid for all time points.

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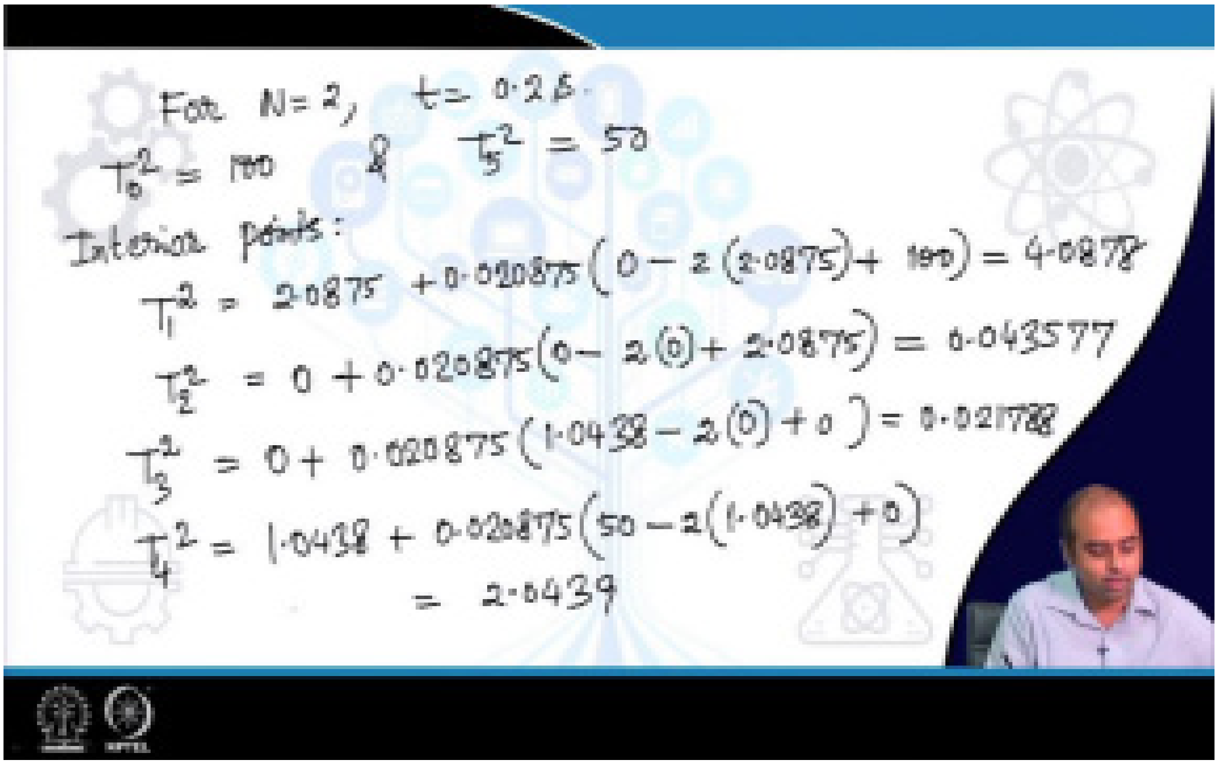

Similarly, now, for the next interval for n is equal to 2 which means T is equal to point 2 second we can calculate the interior values. So, the (bounds) so, T02 is of course equal to 100 and T52 is equal to 50. But what about the interior points so, the interior points T12 will be equal to 2.0875 which is the previous time instant value at the same location plus the value of lambda this is 0 which is the value at T2 and the previous time instant minus 2 this is the value at the same space location but in the previous time instant and this is the boundary value. So, this will give you a value 4.0878.

Similarly, you can also calculate T22 and you will find out that at previous one it was 0 previous time instant. So, the (int) all the interior points in the previous time instant was 0. So, it was the third location the next one, the current one is also 0, but the previous one was the first interval and that was non 0 and this values.

So, slowly you can realize that as time progresses, the interior points picks up the temperature initially it was all 0 and at the ends were heating, but with time you can see that slowly in the beginning only the heat was diffused to the first interior point, but at the second time instant, you realize that the heat is slowly diffusing into the remaining interior points and their temperature is also rising slowly and which it of the temperature intervals this is the point the I mean this this is what you can realize from these calculations .

So, now, you see in this case, in the second time instant and at point 2 or the second time interval or second time step, you can see that none of the interior points are 0 in fact, all have some or something or the other non 0 values. Of course, the values are more as we approach towards the ends because of the boundary effect and they are small at the center of the or the interior values are smaller and slowly it picks up the these interior point values also has a rise in the temperature with time points.

So, similarly, you can also construct what would happen to n is equal to 3 then n is equal to 4, 5 until it reaches a steady state or a steady state or with time you do not see a temperature change.

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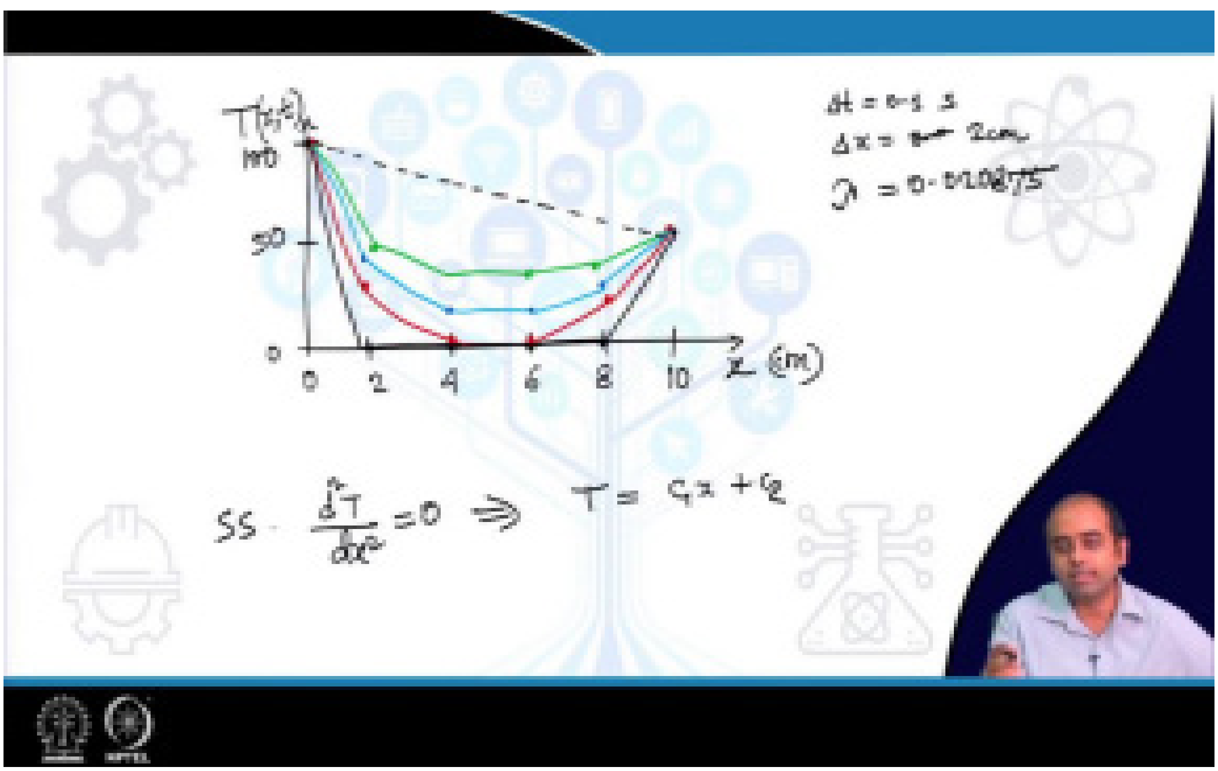

So, if I am trying to draw the temperature profile now, let us say this is my x sorry time which changes as a function of space and time and this is my x let us say my x in centimeter and I mark

5 points here. So, this is 2, 4, 6, 8, 10 and this is my 100 and let us say this is my 50. So, initially at a time t is equal to 0, we had the value of the boundary conditions were only satisfied.

So, it was only these two points, which has non 0 value and remaining everywhere it was 0, that was the that was the criteria we have seen. So, let me just mark it in a different way. So, let me say this is 50 so, this is we will come to something like here. So, these are the boundary points like so, initially, only these two points has known, I mean 0 so, these two points (as) the boundary conditions had the temperatures and rest the remaining points were 0. So, these are the values at the at the n is equal to 0 at the first time instant.

Now, with slowly with advancement in time, we found that, of course, the boundary condition is always true, but slowly, we found that these values also starts to rise. So, something like this next time instant, was something like this, then again, it moved to, I am only trying to write (the) just a visual description of this.

So, if I am trying to draw the values or trying to draw the card at different time in just to get an idea about the how the temperature profile is evolving, it would look something like this and then slowly we will have more time intervals updates in time like this, it would evolve slowly with time and finally, we will reach a condition where this will be almost close to a linear profile, because the steady state configuration or steady state temperature profile is linear in this time in this space domain for a purely conductive heat transfer.

So, here we had delta t is equal to point 1 second and delta x it was point sorry, 2 centimeter and a lambda was 0.020875. So, a take home exercise would be to try to obtain the solutions for longer time or larger T, what happens you try to continue to do the illustration till a steady state is attained. So, you can find out that typically, what is the timescale that you have for this problem to achieve 99 percent of the steady state value. So, you can theoretically calculate out what is the steady state profile.

So, if you do so, at steady state you will be having d2 T dx squared is equal to 0 and so, from here you can have the temperature profile at steady state to be T is equal to c1 x plus c2. So, this is the steady state temperature profile and from the boundary conditions you can work out what is c1 and c2.

So, you will know what is the steady state profile. So, what is the dynamical timescale of the problem or what is the time required in this problem to reach the steady state is something that you can investigate out from this analysis.

Secondly, important thing that you can also work out from this problem is that if you change this lambda, so, lambda is one of the stability parameter here. So, if you change this lambda beyond the one dimensioned stability criteria like you choose a identity value such that lambda is no longer satisfying 0.5, it is more than 0.5 then what happens? How does the solution change? Or how does it deviates? Or how does it diverge with forward marching in time?

So, these are some of the things that I want you to try yourself as a part of the homework exercise, so that you get a more in depth idea and insight to the problem what happens if you further decrease your delta x now, now, we have 2 centimeters, what happens if you further reduce it does it allow you to increase the this delta t, because if you increase the delta t essentially, you will be solving the problem faster, because it will require less number of solution steps to attain up to the steady state scenario, is not it? So, this is what I expect and I encourage you to try yourself.

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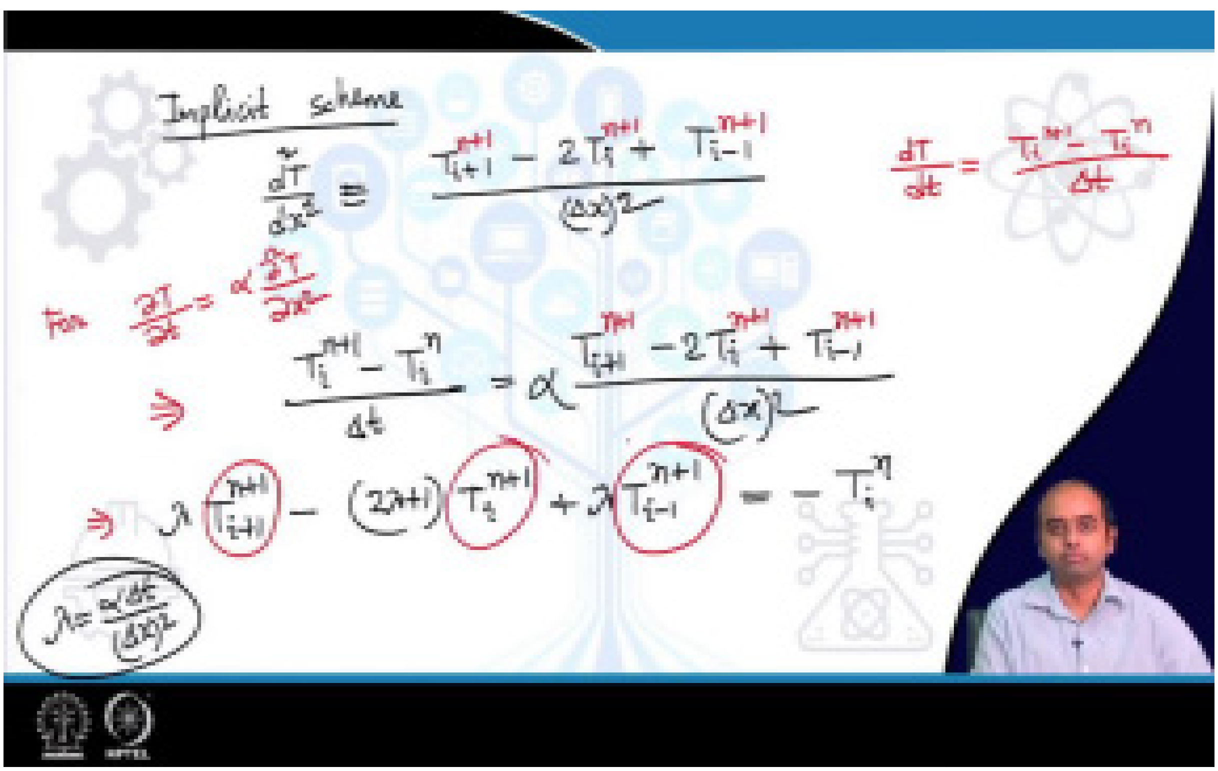

Now next, we move to the implicit scheme. So, first of all how do we frame the difference equation from the for the implicit scheme everything is same, except the fact that all the derivative time steps like dt dx or dt this double derivatives or single derivatives sorry it is d2 T dx square, these derivative term is represented in the current timescale, instead of the previous timescale, it is not timescale time instant.

So, what I mean to say that all of these are evaluated not at n time interval, but n plus 1 time interval. So, which is the current time interval n was the previous one. So, when we try to do dt the temporal derivative when we write it as T i sorry this n plus 1 this forward difference for a temporal derivative the question comes that, when we try to estimate the spatial derivatives at (what) which time interval do we consider we in the explicit scheme we considered when to be the previous time instant because that was known.

So, the problem becomes fully explicit formulations that everything on the hand side was known, and we can calculate the future timescale or the n plus 1 time instant, but now, in the implicit scheme, you can easily realize that based on this idea for the same problem that we have sorry for the same problem that we have delta t delta t is equal to alpha delta.

So, for the same problem, if I try to write the difference equation, I will be writing something like this, the temporal part stays the same. Write part on the spatial terms or the space derivative terms are evaluated at n plus 1 and not at n.

So, what is the natural consequence that you get finally, is that you do not get an explicit I cannot write something as Ti n plus 1 is equal to some known quantity that sort of description is not possible. So, here what I will get is this the equation or the discretized equation now takes this form of course, lambda here means the (delta) alpha delta t so, let me write so, this was the lambda.

So, now in this equation as you can see all the n plus everything on the left hand side is an n plus 1 terms because these are unknown and only Tn i is a known quantity. But here since all the current step all the current and the the spatial the temperature profile at the current steps are unknown for example, t n plus 1 at any i values is unknown, because that is why we are trying to calculate it here like all the solutions at different space locations or different space point in the current time is something unknown to us.

So, that means, this quantity is unknown these quantity is unknown as well as these quantities is unknown. So, all of these quantities are unknown to us. So, in the same equation if you have three unknowns of course, you cannot solve it explicitly.

So, what happens here is that if you try to frame the equations, we will we will talk about them (()) (25:57) now only or possibly in the next class, that if you try to frame the equations in a single equation, you will find three unknowns then how to solve them now, it is not possible to have explicit solution, where you try to equate something with every known quantity on the right hand side, you have to frame a system of equations now, if you frame a system of equations, you will see that for each space location, you will be landing up with one equations, is not it? With each space locations, you will be landing up with one equation, and every equation we will have three unknowns, but some of these unknowns, some of these unknowns will be same, isn't it because it is i plus 1 i and i minus 1.

So, if I try to write (the) this equation for let us say i is equal to 2 then in that case, the unknowns are T3, T2 and T1 is not it? Now, again when I (write) try to write the equation for i is equal to 3, then I will be having the unknown is equal to T3, T2 and T4. So, you will see that there are some unknowns which are common, I mean essentially at the end of the day, the unknowns are only the temperature values or the interior points, is not it? Of course, in each equations, you are having three unknowns, and we will be framing the system of equations based on each space point, is not it?

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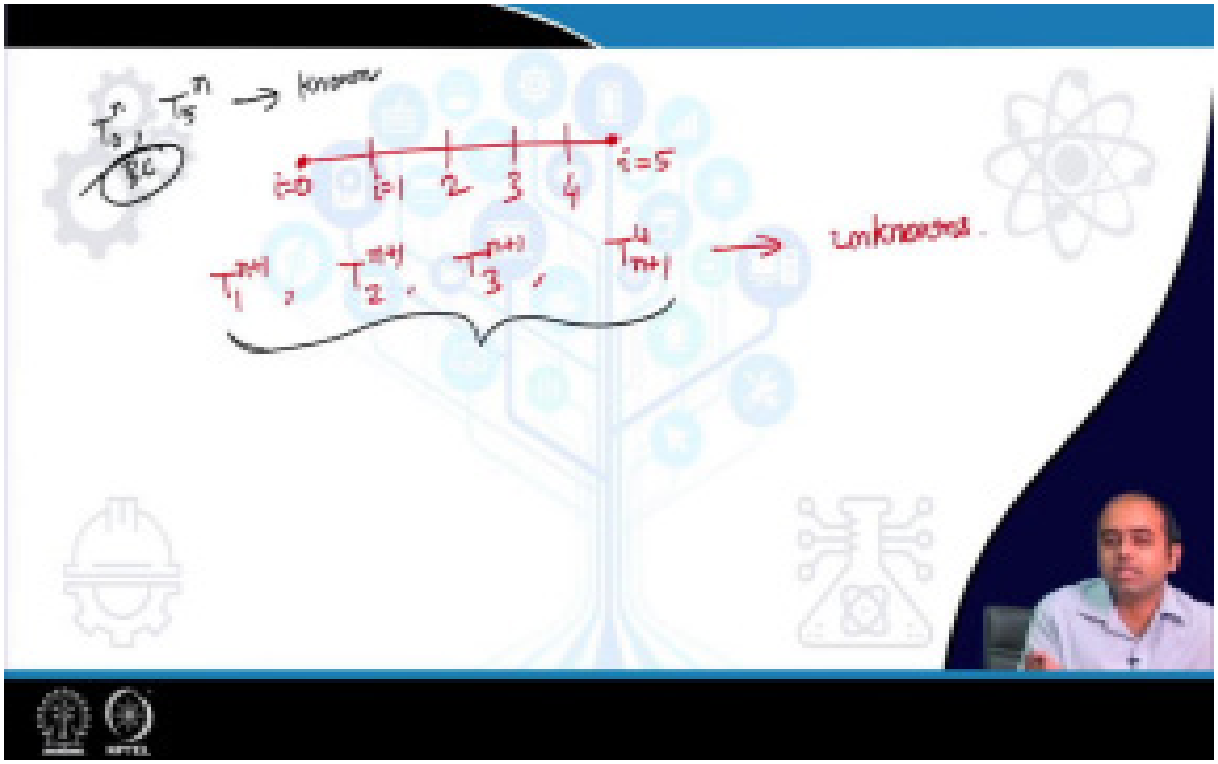

Now, just to give you an idea that here, when we talked about the same problem so, this is i is equal to 0 which is known everything is known this i is equal to 5 we are talking about is equal to 1, 2, 3 and 4. So, T n plus 1 of sorry 1 T2 n plus 1, T3 n plus 1 and T4 n plus 1, these are the unknowns is not it and of course, T5 and T0 for any n value is always known, because these are the boundary condition these are the boundary condition.

So, now, for each space point for each i is equal to 1, 2, 3, 4, you will be framing something like four different equations. So, here we will be framing four different equations. And of course, each equation will have three unknowns but ultimately we will be having four equations and total four unknowns, and out of these four unknowns, three unknowns will be appearing in each equations.

But ultimately it is four i equations and four unknowns, which (you are) you need to solve them together, because each equation do not have an explicit formulation and rather, each equation contains more than one unknown, but ultimately, it is the system of equation when the total number of unknowns and the total number of equations are same. It is just like, if you when you try to solve in your high school the simultaneous equations you write some equation as a function of x and two equations, having both x and y together, each one of them cannot be solved explicitly the same way here also, you have four algebraic linear equations and ultimately four unknowns, but since it is a system of equations, you need to have the matrix formulation, you need to have the matrix formulation and then try to solve it from there.

So in the next class, we will talk about how are dedicated algorithm is device to solve these sorts of problems where we have only three unknowns actually, these week present tri-diagonal matrix system, which we will look into possibly in the next class and try to see that how it can be used to solve these sorts of implicit formulation problems.

Of course, the implicit formulation is more energy intensive, (because) sorry, computationally intensive, because you need to calculate not single equation each time you need to calculate this multiple equations in the form of matrix and matrix inversion and these are very costly, computationally costly operations. One more thing I would like to emphasize here is that the implicit scheme is inherently stable. There are no stability issues in this implicit formulation scheme and that is why we do not study any sort of stability criteria for implicit scheme.

So, any implicit method for solving PDEs is inherently stable and this is perhaps one of the advantage or preference do you have at the cost of the increased computational load. I hope all of you have got a fair idea about the explicit formulation and understood about the background of the implicit formulation. In the next class we are going to see the same example problem and try to work out the tri-diagonal matrix algorithm. Thank you. Hope you liked this lecture.