Numerical Methods and Simulation
Techniques for Scientists And Engineers

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Lecture 17
Examples of Differential Equation Heat Condition

So, let us look at solution of these initial value problems that we have been doing lets you know generalize to more realistic situations.

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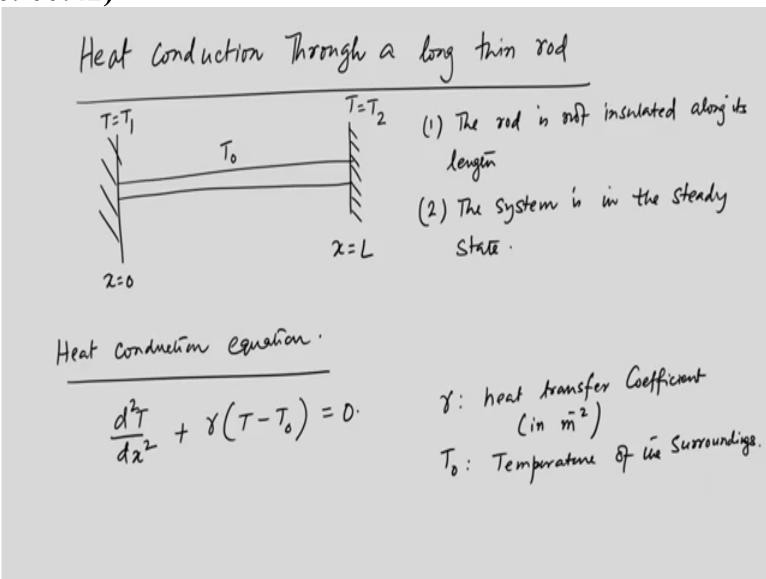

So, let us just talk about the heat conduction equation or rather the conduction of heat, heat conduction through long thin rod. So, let us specify the problem before we get with get on with the formalism. So, there are 2 rigid ends which are shown here and this is the rod so it is between 2 rigid ends. Now this rigid ends are marked as x equal to 0 and x equal to L so the rod is of length L and say the temperature outside is T0 and heat is of course so this is at a temperature T equal to T1 and this is at a temperature T equal to T2.

Suppose T1 is greater than T2 or T2 is greater than T1 the heat will flow through this long rod and we are assuming that one that the rod is not insulated along its length so there is no insulation there. So, the heat can actually the exchange of heat can take place between the rod and the surroundings. And also that we are talking about a steady state the system is in the steady state. So, the heat conduction equation will take a form it is d2T dx 2 + a gamma T - T 0 and this is equal to 0.

So, gamma is called as the heat transfer coefficient and the unit is in you know meter inverse square 1 over meter square and T 0 is as I said is the temperature of the surroundings okay. So, far we have seen a solution of these first-order differential equation and now we are seeing a second-order differential equation. And of course we know that the second-order differential equation can be converted into a first-order differential equation or rather a pair of equations which have to be solved self consistently and this is what we are going to do.

So the first method that underlines a solution of such equations are the heat conduction equations through these rod is called as a shooting method. So, let us talk about the shooting method.

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Consider $m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0$

Consider a new variable $y = \frac{dx}{dt} \Rightarrow \frac{dy}{dt} = \frac{d^2x}{dt^2}$. (A)

$m\frac{dy}{dt} + cy + kx = 0$. (B).

$\Rightarrow \frac{dy}{dt} = -\frac{cy+kx}{m}$.

Eqns. (A) and (B) are required to be solved simultaneously.

Lets write $\frac{dT}{dx} = z$. (3)

$\frac{dz}{dx} = \gamma(T - T_0)$ (4)

(3) & (4) are to be solved simultaneously.

And the shooting method is based upon converting the boundary value problem into an equivalent initial value problems. This is the main point we will and initial-value problem and let us see what it means so the boundary conditions for this particular problem are given by T at x equal to 0 we will simply write it as T at 0 this is equal to T1 and T at L equal to T2 okay and let us specialize for a given case for the sake of concreteness say L equal to say means consider L equal to 10 meters gamma equal to 0.01 per meter square and surrounding temperature is say 20 degree centigrade and the T 0 is given as 40 degree centigrade.

So these are all T's are in all degree centigrade and T at 10 which is L because L is 10 so this is equal to 200 degree centigrade. So, we have kept a rod fixed between 2 ends x equal to 0 and x equal to L the ends are maintained at temperatures 40 degrees and 200 degree centigrade's the outside temperature or rather the surrounding has a temperature of 20 degree centigrade the heat transfer coefficient is given as .01 meter per meter square and length of the rod is 10 meters.

And we are going to solve this problem by using what is called as a shooting method. But before we understand shooting method let us see that how a second-order differential equation can be converted to a first-order differential equation. So, consider this equation which is for a forced or rather a damped oscillator to begin with so this is a damping term which we have seen earlier and this is that the term with Hookes law and there is a damping term which is proportional to the velocity.

So, if we consider a new variable y which is equal to dx dt such that a dy dt is nothing but equal to d 2x dt 2 so we can write down this equation the original equation as m dy/dt + cy + kx equal to 0 or a dy dt it is equal to a - cy + kx over m, so let us call this as equation a equation a and this as equation b, so equations a and b are required to be solved simultaneously all right. So, this is the condition rather this is the simplification that we achieve that a second-order equation is brought down to a first-order equation.

In the same spirit let us write dt dx equal to z and that gives us dz dx is equal to - gamma T 0 or let us just write it by inverting the sign or rather absorbing the sign so this is equal to that alright. So, let me give this as equation 1 and so this is 1 and the boundary conditions are written as equation number 2 and these equations are now written as 3 and 4. So, 3 and 4 are to be solved simultaneously all right.

So, this is what the situation is as of now that we have been able to reduce a second order equation the heat conduction equation into actually a pair of first-order equations which have to be solved self consistently or rather simultaneously okay.

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A guess for z is needed.

$z(0) = 10$.

Solve Eq. (4) using a fourth order Runge Kutta method.

In the 4th order RK method, integrate from $0 \rightarrow 10m$, Step size = 2m.

$T(10) = 168.3797\,^\circ C$.

$T(10) < T(L)$ as per the boundary condition.

$z(0) = 20$

$T(10) = 285.8980\,^\circ C$

$T(10) > T(L)$.

In the shooting method a guess is needed a guess for z is needed, so let us have the gas at x equal to 0 to be equal to 10 okay. So, this is the initial condition and we have to solve this dz dx equal to gamma T - T0 and of course also dt dx equal to z simultaneously but at this moment let us only consider on equation number 4 and if we solve equation 4 equation for using a fourth order Runge-Kutta, so just to remind you of the fourth order Runge-Kutta it takes 4 points in an interval h and calculate their slopes at all these points.

And in fact a slope at a given point depends on the slope or rather the value of the function at the previous point and then different weights are taken for these slopes and we iterate the solution with you know the value at the beginning of the interval plus this slope this effective slope which comes out of these 4 slopes that we calculate and then it is multiplied by the h which is the size of the interval for this particular issue.

So in the fourth order RK method one can take I mean the integral is from or rather one has to integrate from 0 to 10 because L is 10, L equal to 0 from a equal to 0 to l equal to 10 and we can take a step size which is h this is equal to 2 meters okay. So, this is 0 to 10 meters and steps as equal to 2 meters and so on and if we do that then the T10 comes out to be equal to 168.3797 and of course T means the temperature for x equal to 10 which means the other end of the rod the far end of the rod rather the right end of the rod.

And this is actually given as 200 degree centigrade so this value is less so T 10 is less than TL as per the boundary condition so which means the shooting method which starts with a guess value for z at x equal to 0 that 10 is actually insufficient to have the boundary condition so what 1 can do is that 1 can actually take a larger value for this it is a larger value because this is an effectively a linear equation.

Because it is a linear equation you want us to actually take a larger value in order to get this. Now if you repeat the same procedure using a fourth order RK method then this T10 comes out to be 285 and 8980 and these are as you understand these are all in degree centigrade I am putting this thing later of course when you do the computation you do not need to worry about it but now you see that when we increase Z at x equal to 0 from 10 to 20 the temperature at far end of the rod comes out to be more than what the boundary condition says.

So, here T 10 or rather T 20 sorry T 10 10 is the L equal to 10 so this is equal to TL and so on so which means that we now have crossed the boundary what the boundary condition gives whereas in the earlier case we actually fell short of the value that we need to satisfy at the boundary.

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$$\left.\begin{aligned} z(0) &= 10 \Rightarrow T(10) = 168.3797 \\ z(0) &= 20 \Rightarrow T(10) = 285.8980 \end{aligned}\right\} \text{are linearly related.}$$

$$z(0) = 10 + \left(\frac{20-10}{285.8980 - 168.3797}\right)(200 - 168.3797)$$

$$= 12.6907$$

$$\frac{dT}{dx} = z(x).$$

$$y' = f(x, y).$$

Solve it using RK method.

Now you see that since the nature of the equation is linear you have a linear equation that is dt dz or dz dx is equal to a linear function which is gamma T - T0. So, what happens is that this 2 guesses that is z equal to 0 10 z at 0 10 giving us T 10 equal - 16 8.3797 this and z at 0 at this is 20 is T at 10 so this is 285.8980 they these are linearly related. Of course this linear relationship will go away if you have a nonlinear equation.

But since the equation is linear it is they are linearly related so if they are linearly related a linear superposition can be done. So, z at 0 it is equal to 10 + 20 - 10 divided by 285.8980 – 168.3797 this and then 200 – 168.3797 and this will give us a z at 0 to be 12.6907. So, in the shooting method had you started with a z of 0 equal to 12.6907 you would have landed up with the exactly correct result.

So, this value should be used to determine the correct solution okay. And because there is a function of x now z at different x's can be you know built and this will be the input to the equation dt dx equal to z of x okay and if you compare it with your familiar equation y prime equal to f xy then you have to solve it again by Euler method or some Runge-Kutte method whichever I mean that is left up to you that whatever approximation you want so solve it using maybe RK method second order fourth order and so on. And which we saw are quite accurate.

So this is about the shooting method in which we shoot a value z equal to z at x equal to 0 is taken some value and then you try to see how the boundary condition is you know closely met. If you meet the boundary conditions quite low I mean closely then z at x equal to 0 is specified by that and then once z at x equal to 0 is specified this will be the initial value for the other differential equation that you are going to have that is dt dx equal to z, z of x or so z of x is obtained that is the initial value is obtained from this the shooting method.

And then once again you iterate this and get this value for the the correct value for the T as a function of x. Because you have a d 2t dx 2 so what you are interested in is find out the temperature distribution throughout the length of the rod. So, at one can ask the question what is the temperature at x equal to say for example 7.5 meters. So, one needs to calculate what is you know T at x equal to 7.5 by solving this equation.

And one such equation we have seen earlier where we wanted to calculate the value of the function at you know at some discrete points okay. So, this is about the shooting method it is quite simple and quite useful as well let us now look at the finite difference method okay.

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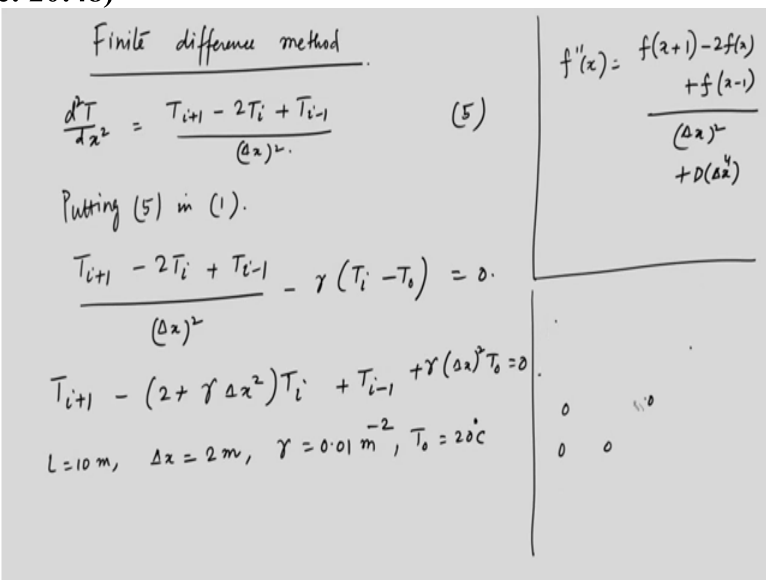

so instead of reducing it to a equivalent first-order equation one can actually directly solve it by using the second-order formula and this 3 point formula is very familiar to us we have done it while we discussed derivatives and differentiation of functions. So, we will use this second-order derivative form as d 2 t dx 2 equal to T i + 1 - 2T i + Ti - 1 and divided by Delta x square and so on. So, if we put it in equation 1 let us call this give it a number we have come all the way till 4, so we can give it a number maybe 5.

We are using going to use this second-order formula here so let us call this as equation 5 and putting 5 in 1 what we get is the following we get a Ti + 1 - 2Ti + Ti - 1 and this divided by Delta x square - a gamma Ti - T0 if you want we will write down this thing once more the formula for the second order derivative. So, a second order derivative is written as let us write it as f double prime x and this is equal to f x + 1 say for example and - 2 fx - or + f x - 1 and this divided by Delta x square where Delta x is the difference between x + 1 and x or x and x - 1 and so on.

And what one misses out is a term of the order of Delta x to the power 4, so this is what has been done here and we are we are familiar with this. So, if this is the substitution so this is equal to 0 so this is the equation that one gets. So, if you rearrange these things one gets an equation which is T i + 1 - 2 + gamma delta x Square T i and + T i - 1 and + a gamma delta x squared T 0 tha is equal to 0 ok.

So, this equation if you notice this equation can be easily written down in terms of a matrix equation and this matrix equation can be solved then by solving the determinant of the coefficient matrix and one can arrive at a solution. So, let us again go back to this same problem of this rod of length L etcetera. So, L is equal to 10 meter so let us take Delta x that is we will evaluate the value of the the temperature at you know sort of after Delta x distance and let us take this Delta x to be 2 meter gamma equal to .01 per meter square and T0 equal to 20 degree centigrade.

So, if these are the values that are given then this equation can be written as let me write it in the next page. But you it will be more you know easy for you if I write it here so let me here so this is 2.04 and - 1 it is – 12.0400 – 1 00 – 1 2.04 - 1 and 0 0 - 1 - 0 - + 2.04 okay but this is the coefficient well it is slightly difficult to write it here because we need to write down ok let me write it in the next page.

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Written in the matrix form,

$$\begin{pmatrix} 2.04 & -1 & 0 & 0 \\ -1 & 2.04 & -1 & 0 \\ 0 & -1 & 2.04 & -1 \\ 0 & 0 & -1 & 2.04 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{pmatrix} = \begin{pmatrix} 4.08 \\ 0.80 \\ 0.80 \\ 200.8 \end{pmatrix}.$$

Solving one gets a vector.

$$\{T\}^T = [65.9698 \quad 93.7785 \quad 124.5382 \quad 159.4795]^T$$

So, written in the matrix form 2.04 - 1 0 0 - 1 2.04 - 1 0 0 –1 2.04 - 1 0 0 – 1 2.04 so this is coming from as you can see it is coming from this Ti the diagonal elements are coming with 2 + gamma delta x square delta x equal to 2 meters delta x square equal to 4 4 into .01 because gamma is .01 so that is .042 + 0.04 is 2.04 and then I can multiply the whole thing by negative and then we can land up with this so we can have a negative sign here.

So we can multiply it by a negative sign and make this cents positive and the rest of the things are negative. So, we have a Ti + 1 that will come with a minus sign and a Ti - 1 which will come with a negative sign, so it will be a tri diagonal matrix as we see it here. And so this multiplied by T 1 T 2 T 3 T 4. So, this is equal to so this now it is a 4.08 0.80 .80 0.804 I mean this is what this will be like 200.8 and so on.

So, this are coming from this Gamma Delta x square and T0 and so on okay. So, these are things that are important so if you solve this so one gets a vector for the T so this is the column vector so these are 65.9698, 93.778 5 124.5382 159.4795 so these are the values of temperature at these points which are you know these are the internal modes. And these internal modes are the values are obtained and of course this is a solution by using this finite difference method okay.

So, finite difference does not I will rather require you to you know boiled it down into or rather convert it into reduce it into a first-order equation but you can use the second-order formula in order to or you know to calculate the values of the derivatives and express it as a linear equation and then the linear equation can be solved using matrix method. So, a generalization of this last one which is called as a finite matrix method or rather finite difference method will show it for a very general case.

And the general case is and in which will actually because there is no time here will also evolve it in time that is will not talk about a steady state but will talk about time variation as well which is the actual heat conduction equation.

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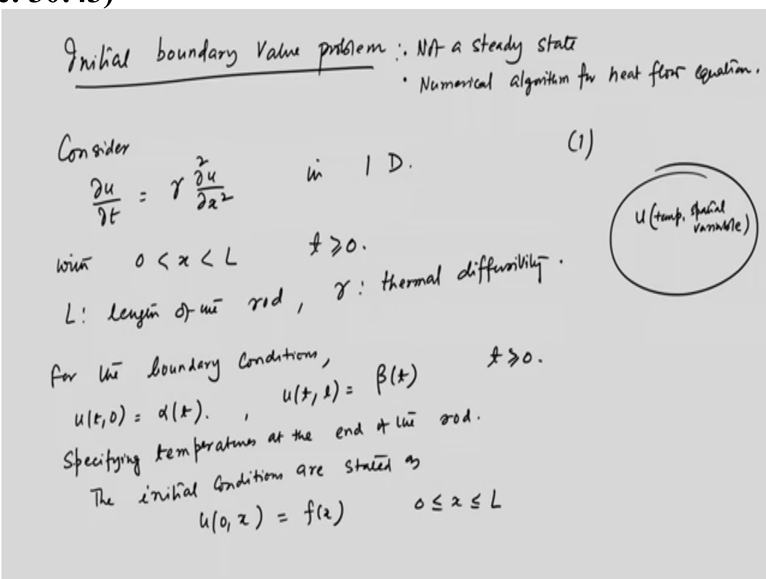

So, in the next what we do is that we do initial boundary value problem, and just to flag things that this will be an not a steady-state and not only that it is so we will learn the numerical algorithm for heat flow equation. So, we will use a slightly different notations but things remain the same so to consider one dimensional equation of this type which is del u del t equal to gamma del 2 u del x square you see that was only dealt del u T del x square which was equal to some constant or rather dependent on the time the temperature T.

But here we have a time derivative the first time derivative is actually related to the second space derivative. So, this is in a 1D and with of course 0 less than x less than L and T is greater than equal to 0 so L denotes the length of the rod the rod and gamma the coefficient of heat transfer or it is also called as the thermal diffusivity all right. So, this is called as a thermal diffusivity. Now for the boundary conditions so let us call this as equation 1, u t 0 equal to alpha t and you t l equal to beta t for t to be greater than equal to 0 okay.

So these are the n temperatures which are given as alpha t and beta t and of course they depend on time here previously we have specified these temperatures are the 2 ends. So, the also the initial conditions so these are specifying temperature at the end of the rod. So, in order to solve this problem let us also write down the initial condition. So, this is u at 0 x this is equal to f of x for 0 less than x less than L okay.

So when I write function u then the first of its argument denotes temperature and the second L denotes special variable okay. So, keep this in mind while we write down this now we no longer have a one-dimensional problem even if we are interested in the heat flow phenomenon in 1 dimension. But we still have a two-dimensional space in which the spatial variables span 1 dimension and the time variable rather the temporal variable this pan in another direction okay.

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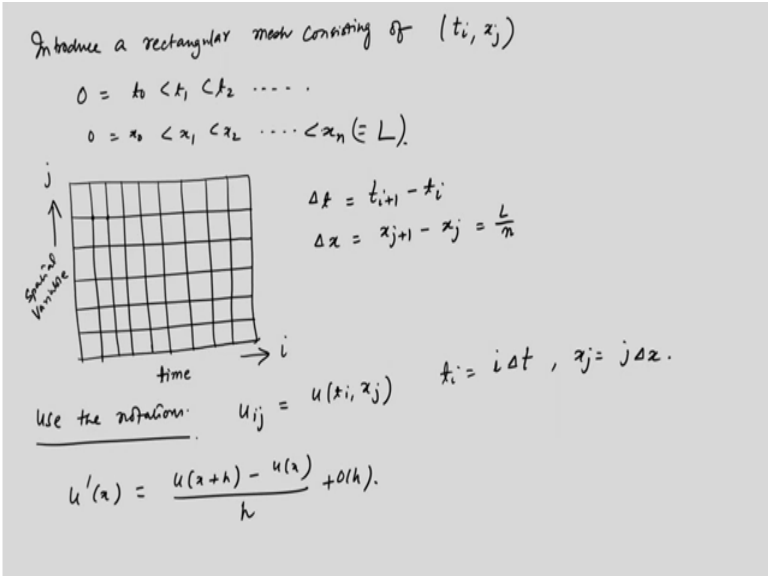

So, we have to introduce a rectangular mesh and so this rectangular mesh consisting of t i so the i index will go with time and the j index will go with space so this is 0 equal to t0 less than t 1 less than t 2 and so on and 0 equal to x 0 less than x 1 less than x 2 and less than x n equal to L this x n is equal to L. So, xn is equal to L, so we can assume a uniform so it basically you know makes our space as a mesh in which along the i direction say this is the I direction time will run.

And along this vertical direction let us call that as j direction the special variable will run. So, we have such you know grid points okay and these are our points say x i and tj or rather ti and xj, so these are these mesh points that we actually calculate the value of the temperature. So, the temperature at a given time and at a given a point can be calculated. So, you can have a sort of uniform mesh size or you can have a non-uniform mesh size in x and y direction it is not very essential to have it a uniform one.

What I am trying to say is that your delta T which is the time lag between our time gap between 2 successive times and your Delta x which is between 2 successive points they may or may not be same this is equal to L over n and so on okay. So, this is not that, they do not have to be same and in fact we consider them to be different. So, we will use the notation that you i j this is equal to u t i and x j t i equal to i delta t do not confuse that this is not the root over - 1 with this simply an index for this mesh in this the time direction.

And xj it is equal to j Delta x similarly that is the mesh in the x direction ok. So, we are quite aware of the derivative formula so we will use the for writing down these time derivative will use this forward difference formula mainly. So, this is the forward difference formula and you are also you know familiar with the center difference formula, there is a forward difference and so on okay. So, this is the one can also use the you know the center difference in which we take a ux + h + - u x - h and so on which has a better accuracy because the terms that you actually miss out is of the order of h square.

And similarly we will use the second order derivative formula which we have written down here this one we will use that for the 2 sides of this equation, equation number 1.

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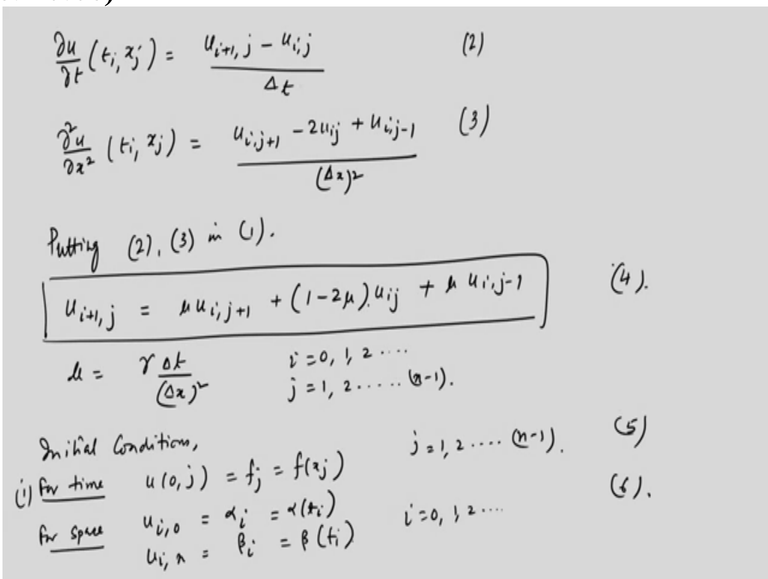

If you write both of them down I am skipping 1 step in which you write down both the del u del t okay let me complete it del u del t t i xj this is equal to u i+ 1 j - u ij divided by delta t and also you write the del 2 u del x square which is the double derivative with respect to space it is ti xj this is equal to u i j + 1 - 2 u i j + u i j - 1 Delta x square so allow me to be a little sloppy here sometimes I put a comma and sometimes I do not put so if I write just simply i j then I do not put a comma but if it is a i and j + 1 or i and j - 1 then I put a comma there so these 2 can be simply written down together in the put it in.

So, let us call this as you know 2, 3, so putting 2, 3 in 1 one can write down this as you i + 1 j equal to Mu u i j + 1 + 1 - 2 Mu + u i j and then you have a Mu u i j - 1 and where Mu equal to gamma delta T divided by Delta x square okay and i is from 0 1 2 etc and j is from 1 2 and all the way up to n - 1 or n small n - 1 yes I think we are writing that all right.

So, you see that this is the equation here is the heat conduction equation after we use this discretization rule and putting it into a mesh a two-dimensional mesh which we have shown in the last slide and this is the equation that we need to solve call this as equation number 4 ok. And now let us you know write down the initial conditions. So, for time the initial conditions are you 0 j equal to fj equal to f xj j from 1 to 2 n - 1 okay.

And for space u i 0 is 0 it is equal to alpha i equal to alpha t i ui n equal to beta i equal to beta t i i equal to 0 1 2 etc and so on and then let us call this as equation 5 and this is equation 6. So, these are the boundary conditions or rather the initial conditions that we have.

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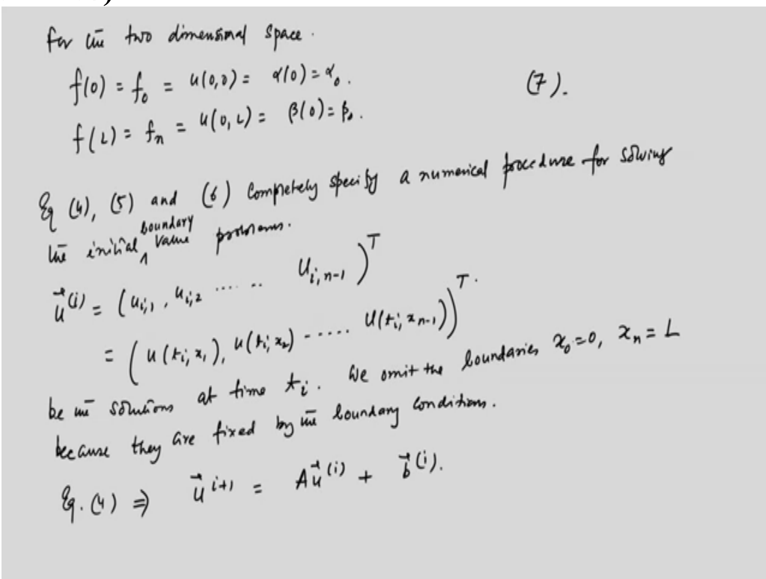

So for the two-dimensional space we need to satisfy these conditions that is f 0 equal to u 0 0 which is equal to alpha 0 equal to alpha 0 and f at L equal to f n which is equal to u 0 l equal to beta 0 equal to beta 0 so that is the those are the temperatures that are specified as the boundary values. So, these are say equation 7 now equations 4 5 and 6 so these equations I am talking about 4 and along with the initial conditions the main heat conduction equations along with these 2 we can write it down as in a matrix form.

And basically they completely specify a numerical procedure for solving the initial value problems initial value I mean and the boundary value problems. So, it is called initial boundary value problems. So, we can write it in a matrix form with u i this is a u i1 u i2 and so on and all the way up to u i n - 1 that vector which is nothing but u ti x 1 u t i x 2 and so on this is u ti x n - 1 and that so this be the solution at time t i.

So, we omit the boundaries as we have seen in the last problem boundaries x 0 equal to 0 and x n equal to L because they are fixed by the boundary conditions. So, a compact way of writing this is that so this equation 4 which is the main equation you see so this equation for that is the main equation that can be written as, one can write this as u i + 1 equal to au i + b i and so on okay.

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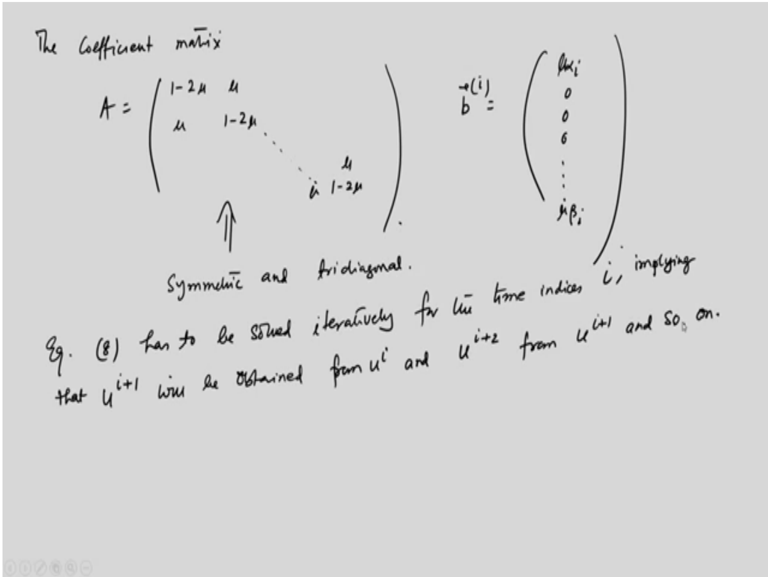

So, this is the solution and what one can write so for the for the matrix A the coefficient matrices A is written as 1 - 2 mu mu mu 1 - 2 mu and so on and so forth 1 - 2 mu mu mu and so on and this b is the vector which is mu alpha i 0 0 and so on and then mu beta I ok now this is the general you know solution of this problem. So, we will have to enough for our n dimensional matrix we will have to solve all the eigenvalues of the matrix.

So, if you see this matrix is symmetric and tri diagonal and this matrix equation which equation number that would be if we have 7 and let us draw all that as 8 so this is like this equation 8 has to be solved iteratively for the time indices i okay. So, implying that u i + 1 will be obtained from u i and u i + 2 ui + 2 from u i + 1 and so on. So, much for the heat conduction equation similar things can be talked about for the wave equation as well in which a similar formalism can be developed.

And as you saw that at least we you saw 2 methods of solving equilibrium heat conduction equation 1 is a shooting method and the other is this finite difference method which is using the formula for the double derivative that appears in the equation heat conduction equation. In this last exercise we have relaxed the constraint of having equilibrium situations so we are talking about a time variable still the flow of heat occurs in 1 dimension.

But there is a time because of the involvement of time here we have a 2 dimensional space and this 2 dimensional space can be discretized and at any discrete point that is at the corner of this mesh that we have drawn here 1 can calculate so we can calculate it here or we can calculate the value here and so on. And this will give you a feeling that this is at a time instant say T star and at a space x star if we want the value of the temperature we can calculate it from there from this formalism.

It again reduces to a equation which is a matrix equation and this matrix equation can be solved by a variety of techniques okay. so we will stop these study of the differential equations we have done a large number of methods and a large you know sort of techniques to solve these things and we will move on to simulations from the next discussion onwards.