Computational Physics
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Lecture – 33
Partial Differential Equations Part 01

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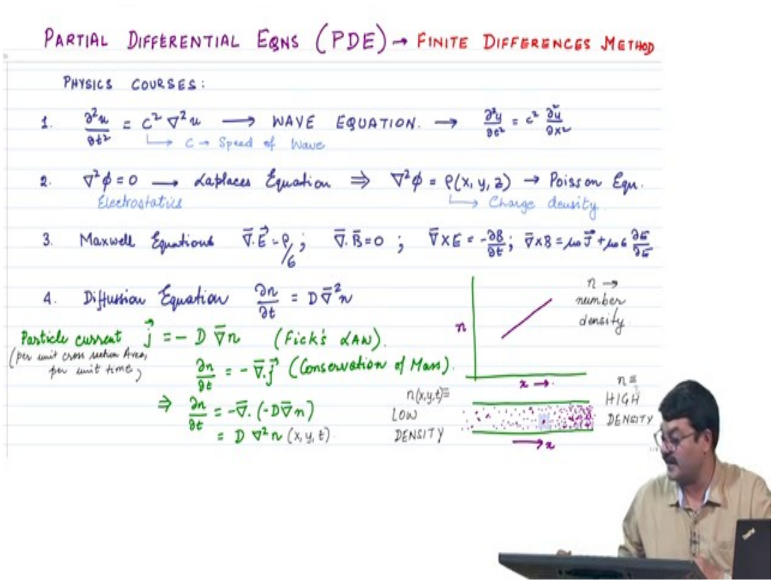

So, welcome back, in today's class we will be discussing about partial differential equations or PDEs; PDE for Partial Differential Equation and in particular we will be discussing the so, called finite difference method. In the last class you have already solved a second order differential equation, which was something like d 2 y dx 2 plus something into divide x and so on so forth.

And, there the finite difference method was already introduced where you solved y versus x. So, that was basically a differential equation and that was only a 1 variable problem. Whereas, in partial differential equation as you might know you essentially have quantity suppose temperature or displacement as a function of x and y a multivariable. Basically, it is a differential equation in multi variable in multiple variables and you have to solve those right.

Now, in your physics course you must have come across various partial differential equation the most common being the so, called wave equation, which is basically a double derivative of u in time, u might be a displacement, it might be a density location of the density peak and so on so forth. And, that is related to c square, where c is the speed of the wave into grad square u right.

Now, grad square has been written as the laplacian or like the divergence of a gradient, vector operator and in more simpler cases you might have come across the wave equation as del 2 u del y 2 equal to c square del 2 u del x 2, but this gradient this d 2 d 2 dx 2 in general in 3 dimensions can be written as grad square right.

And, other than the wave equation you must have come across the so, called Laplace's equation in electrostatics grad square phi equal to 0, where phi is the electrostatic potential and this equation is valid when there is no charge in the place where you are calculating phi in more general, in electrostatics you would have come across the so, called Poisson's equation, which is grad square phi again being the electrostatic potential equal to rho xyz the charge density as a function of xyz.

And, you can solve this equation to at the points where there is a charge density we calculate the electrostatic potential. Maxwell's equations of electromagnetic theory are written as partial differential equation divergence E equal to rho is rather rho by epsilon. And, the basically divergence B equal to 0 curl of E equal to minus del by del T and curl of B equal to mu 0 J J being the vector, the current vector plus nu 0 epsilon into del u del T.

So, these are all examples of partial differential equations moreover you might have come across in your statistical physics course about the so, called diffusion equation and that relates the single derivative with respect to time. So, suppose n is a quantity n will being could be suppose the density, number density of molecules in a certain volume. And, del n del t equal to D; D being the diffusion constant into grad square n right. So, in contrast with the wave equation you have a double derivative with respect to time here, here you have a single derivative with respect to time.

So in the next rest of the class we will be solving the diffusion equations under different conditions. So, let us discuss the diffusion equation a in a bit more detail this is of course, a partial differential equation. And, let us suppose that n right is the number density of particles over space. So, suppose this is some box or a channel and here you have higher density of molecules, which is suspended in water say.

And, here you have a lower density. Now, you might have read about Brownian motion and what you expect is that these particles from the higher density regions are going to diffuse slowly and come towards the lower density part right. So, n is the local number density of particles and if you plot n versus x x being this direction suppose right, then n is increasing as a function of x.

So, this is the n at high density region this is n this is a function of the number density is a function of x y and t. So, nx y t this is the low density region and to get where the diffusion equation comes from one can understand it as the so called Fick's law ok.

So, what does the Fick's law state? Fick's law states that the particle current. What is the particle current? Particle current j is the number of particles crossing per unit area per unit time right. So, the number of particles moving in this direction say per unit area per unit time that is the particle current, and that as for Fick's law can be written as minus D D being a proportionality constant grad of n n being the number density.

So, it is basically saying the current is proportional to how fast n the number density is changing as a function of x. Why is this minus sign here?. Why is this minus sign? So, the current the particle current will move in this direction right. So, it is then move the particle current will move in the negative direction, but n is increasing in the positive direction in the positive direction right.

So, hence the particle current is opposite to the direction of gradient of n and which is the Fick's law, and in addition the conservation of mass is typically written in physics as such a in such an equation del n del t and again reminding you is the number density of particles. So, in a certain volume how fast is the number density changing and that is proportional to the flow of particles the particle current, which is entering the certain volumes.

So, this is nothing, but the so, called differential form of the Gauss's law which you would have studied in your BSc right. And, this is how you write your conservation of mass and combining the Fick's law with the conservation of mass. So, basically del n del t minus divergence j instead of j you use the Fick's law you just substitute minus D grad n and what you get is D grad square n x y z t.

And, if you solve this partial differential equation for the appropriate boundary conditions, you shall know how does n change as a function of time with time and as a function of xyz. So, this is the differential equation and a partial differential equation if it is an xyz multi variables. If, basically density is changing in the x direction as well as in the y direction, there is a certain current etc if you solve it you will get the so, called solution to the diffusion equation.

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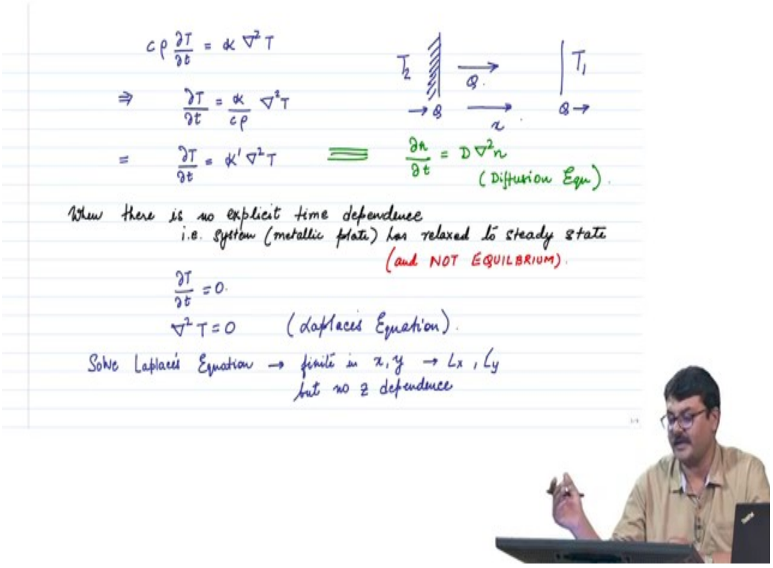

Where else have you seen the diffusion equation?

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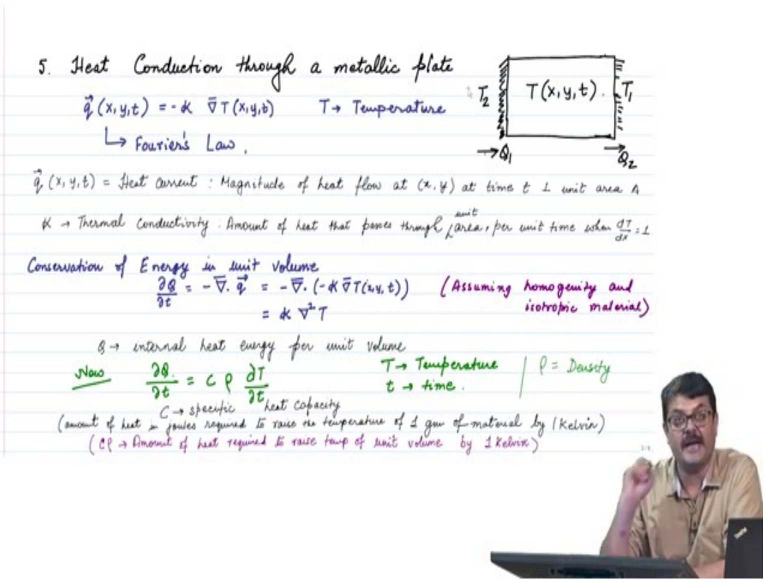

So, basically now if you talk about heat conduction through a metallic plate right. Now, you this is again a problem which you would have studied in class now suppose this is a metallic plate, and T 1 end you fix the temperature at T 2. At the other end you fix the temperature at T 1 at T equal to 0 at time T equal to 0. And, you want to find out what is the temperature distribution within the metallic plate, now if the plate was at a temperature different temperature T 0.

And, you put them between 2 regions and ah temperatures T 2 and T 1, then the temperature of the plate itself shall evolve in time, but after it reaches a steady state, after a considerable period of time, the temperature variation along the plate on the plate will be basically independent of time and T will be a function only of x and y . So, to study the problem what one uses is the so, called Fourier's law and this is very similar to Fick's law which is and then what you say in the Fourier's law is that the heat current.

So, in the Fick's law you had the particle current and here you have the so, called heat current which is a function of x y and t is proportional. So, this is the so, called proportionality constant, the thermal conductivity right. And, the heat current is proportional to the gradient of temperature. So, that is what is the Fourier's law is so, what you did in the Fick's law was del n del t the particle current was proportional to gradient of the number density.

Here in this in this case, the heat current is proportional to the gradient of temperature right. And, just to remind you I have written down that q x y t the so, called heat current is nothing, but the magnitude of heat flow. At point x and y at time t per unit area that is the heat current how much heat is passing through a unit area right at time t and that is function of xy and t, kappa is the thermal conductivity what is thermal conductivity it is the amount of heat.

It is the amount of heat that passes through a unit area per unit time when dT dx equal to 1. So, that is the heat current and just like the conservation of mass you can also write the conservation of energy in a unit volume right and del Q del t, Q is capital here. So, here Q is capital here right. And, Q is the internal heat energy per unit volume. So, how much heat energy per unit volume is increasing in a certain time the rate of change of heat energy per unit volume.

And, that is proportional to the gradient in the heat current sorry the divergence of the heat current right. It was very similar to this divergence of current. And, again here you have divergence of current being heat current being denoted by small q and the total amount of heat in a certain volume is a scalar quantity being represented by capital Q right. And, this small q the heat current by the Fourier's law can be written like this minus divergence of minus Kappa, Kappa being the thermal conductivity into gradient of temperature.

Temperature is a function of x y t and that in turn can be written as Kappa into grad square T right. Now, to put it in the diffusion equation form I would ask you to remind yourself that del Q del t is this quantity del Q del t the amount of heat per unit volume the amount of heat change per unit volume, the rate of change of it is because the derivative with respect to time is the specific heat capacity C into the density into d T. So, this T the T at the numerator capital T being the temperature and the small t being the time right.

So, as the temperature increases if the temperature increases fast quickly, then the energy in that volume also increases quickly and that is related to the specific heat capacity C and the rho being the density the density of the material right. So, just remind you what is C specific heat capacity C is the amount of heat in joules to raise the temperature of 1 gram of material by 1 Kelvin right. And, so, C rho is essentially the amount of heat required to raise the temperature of a unit volume right we are talking Q is per unit volume.

So, the amount of heat required to raise the temperature of unit volume of material by 1 Kelvin. And, this relationship holds if you just look up your whatever BSc physics course. And, this so, del Q del T equal to this this quantity we are going to basically substitute here right. And, that is exactly what I have done here and then you get gets C rho del T capital T by del T time equal to Kappa grad square T and this is nothing, but the diffusion equation again right. Where I am writing Kappa by C rho as Kappa dash right and this is very similar to the diffusion equation you saw just here right. So, this is absolutely similar.

Now, as I said before now when the system reaches steady state right, steady state suppose this is the your material and you are holding one end one edge of the material at temperature T 2 the other edge is being held at temperature T 1 right, then you can solve the diffusion as then you can solve the so, called diffusion equation. And, once it reaches steady state there will be no explicit time dependence in the temperature at T will be a function of only x and y, which means that the temperature is not going to change as a function of time.

So, del T del T can be written equal to 0, which means grad square T equal to 0, which is nothing, but the Laplace's equation which you also solve for electrostatics. Just to remind you steady state is not equilibrium, because in equilibrium you would have the temperature uniform over the entire space. A steady state means that there will be a current there will be a heat current a certain amount of heat is going to enter this end and in steady state an equal amount of heat is going to leave this surface from the other end, there will be a temperature profile there will be a T as a function of x and y. But, that is not going to change.

In steady state there will be a net heat current and what would be the heat car what would be the temperature profile across in this region we can find it out by solving. So, called grad square T Laplace's equation, when appropriate boundary conditions are given right. Now, you might have handled such problems in 1 dimensions in your college and your BSc or your masters considering that y and z being infinite plates being infinite in this direction.

And, this and suppose this is the x direction and you find out how the temperature varies around along x, but suppose instead of considering a fully blown T as a function of x and y and z suppose a long z. There is no temperature difference the T does not vary along z that, but it varies along x and y only right. Suppose, T varies along x and y only and you have finite boundary. So, this is of a finite dimension and not extending along y. And, the question is to solve the temperature profile 1 has to solve the Laplace's equation and given the appropriate boundary conditions .

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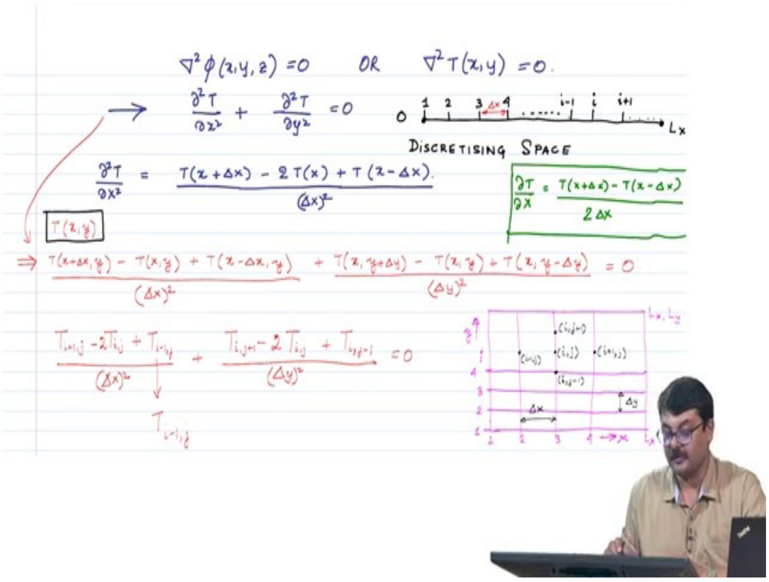

So, what is the Laplace's equation it is nothing, but grad square phi equal to 0 or in this particular case basically grad square T as a function of x y equal to 0. And, if there no explicit z dependence let us solve the Laplace's equation that is take the case, where it is a function of only x and y. Then, we can write this as del 2 T temperature del x 2 plus del 2 T del y 2 right equal to 0 and just to remind you from the last class by the finite difference formula one can write del 2 T del x 2 as T at x plus delta x plus T at x minus delta x minus 2 T calculated at x divided by delta x square.

So, what are we doing we are basically discretizing space. So, suppose your space started here at x equal to 0 and it the tip the metal plate ended at L x right. So, what we are going to do is calculate the temperature at discrete points within this range right. So, if you have continuum we have infinite points between 0 and L x, instead on the computer we are going to calculate temperature and discrete points between 0 and L x

So, suppose called the one end of the plate which is 0 basically the first point, and the neighboring point to be the second point, and then the third point, fourth point and so on the i minus 1th point ith point and i plus 1th point. And, the distance between say the third point or the fourth point is delta x right. So, you are calculating temperature at discrete points of space separated by delta x and the distance between 1 and 2 is delta x.

And, then basically this is how you can write down the second derivative right. Basically, you are calculating the temperature at suppose x plus delta x like, i plus 1.

This is would be the temperature at T minus delta x and this is the temperature at x right. And, just to remind you that the first derivative del T del x can be written as T temperature at x plus delta x minus temperature at x minus delta x by 2 delta x.

And, how these formulas come you can look up the book and there are Taylor series expansions and then there are first order expressions and second order expressions those are important ah, but not possible to cover in this short class. So, if you are interested and you should be please look it up. So, this was the expression when you had delta T del x 2, now when we are writing a partial differential equation right, then this expression will become this is this expression and correspondingly you will have del 2 T del y 2 and that is basically this expression right.

So, it is a very similar except now the derivative the y plus delta y is taken x is remaining constant this x y remains again x is unchanged and here again you are taking y minus delta y. Instead of x minus delta x y minus delta y, x plus delta x x remains the same y plus delta y, because now you are taking the derivative in the y direction right previously you are taking derivative and the x direction. Now, you are taking derivative along the y direction say right. Now, if that entire space so, from here this was in 1 dimension.

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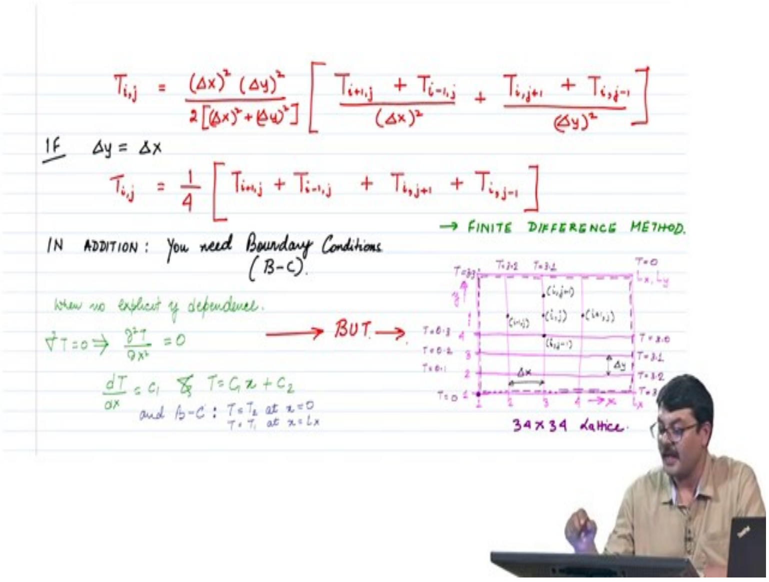

If, you think about 2 dimensions what you have is basically you have discretize space in the x direction separated by delta x, and in the y direction you have again separated you have discrete points in the y direction separated by delta y right. And, now you can calculate basically these quantities x plus delta x y and x minus delta x y, you can write them in terms of i and j where i and j are discrete they have numbers like 1, 2, 3, 4 so and on so forth.

And, each of these point suppose this is i on j the point x minus delta x would be this point right separated by minus delta x. Similarly, y plus delta y will be basically this point right, this discrete points i and j plus 1 then a neighbor in the y direction separated by delta y. So, this term can be written like this where x plus delta x has been written as i plus 1, y remains fix for j remains fix and here again xy corresponds to i j x minus delta x there is an error here.

So, this is T i minus 1 j right and the similarly this should be j minus 1. So, corresponding to minus delta x. So, you have i minus 1 and here where you have y plus delta y and y minus delta y you have basically j plus 1 and j minus 1 right. So, basically when you discretize space this minus delta x you are writing in terms of lattice points. So, basically this is your expression of the Laplacian, when you have discretized it and use the finite difference expressions for it and your aim is basically if you know all these different terms you have to find out T i j.

So, T i j the temperature at a certain point i and j can be written as i have just basically played around algebraically with this with this equation. And, this can be written as T i j can be written as delta x whole square into delta y whole square upon 2 delta x whole square plus delta y whole square please work it out, you will see that it will come. And, what remains within the brackets is T i plus 1 j T i minus 1 j delta x whole square, then T i j plus 1 plus T i j minus 1 and in the denominator you have delta y whole square.

Now, if delta y is chosen to be delta x. So, that you essentially have a square lattice right, then this expression becomes even simpler basically all these terms cancel out just put delta x equal to delta y and the expression becomes so simple right. The 1 within the bracket remains the same ah, but this becomes just one-fourth.

But, they solve this partial differential equation you need also the boundary conditions right. And, basically in the boundary conditions now when you used to solve this in suppose 1 d right you would have solve this. So, then just to remind you and I will remind you that and then you do not tell you that when you are solving this problem in 2 dimensions when you have del T del 2 T del x 2 plus del 2 T del y 2, how the boundary conditions are going to change. Just to remind you when you were doing it in 1 dimension grad square T equal to 0 would be nothing, but del 2 x del 2 T del x 2 equal to 0 all right.

There was no y dependence and then you can solve this del T del x equal to C 1 and T equal to C 1 x plus C 2. And, the boundary conditions would be that the temperature is T 2 at x equal to 0 and temperature is T 1 at x equal to lx and then you just substitute and you would get a straight line straight line variation of the temperature from T 2 to T 1 along x, but that can be done identically.

But, now if you have more complicated temperature variations right. Now, suppose this is your box and this is your metal plate, you are specifying the temperature on this on the boundaries, which is basically along this, and along this, and along this, and along this these are the boundaries right. So, you have to specify the temperature. And to take a slightly non trivial problem, suppose the temperature was not fixed T 2 on at x equal to 0 which is on this plate.

But, the temperature was 0 at this point the origin basically the 1 1 point, but temperature was gradually increasing from 0.1 and 0.2 and 0.3 as you move. Suppose j equal from 1 2 3 4 up till the end. Now, suppose you are taking a 34 cross 34 lattice right. So, the temperature would increase from 00.1 so on so forth to 3.3. And, suppose along the x direction here the temperature from here which was 3.3 would decrease 3.2 3.1 and so on so forth up till temperature is 0, at L x and L y at this edge right.

And, similarly and this edge along x here again temperature gradually increase from 0.1 0.2, 0.3 so on so forth to suppose 3.3 and along this temperature is decreasing from 3.3 from 3.3, 3.2, 3.1 and so on so forth to 0. So, we have complicated this situation right. So, now, suppose the boundary conditions are such you are the temperature are such that temperature is again increasing along x in this direction.

But, temperature is decreasing here at x equal to L x along y. So, that this point is again 0 same as here and again along this temperature is decreasing. So, these are the boundary conditions that temperatures along the boundaries are fixed, you cannot change them their conditions externally given boundary conditions and what you have to do by solving the Laplacian is find out the temperatures at these middle. I mean at these points within the metal plate as a function of x and y or i n g as you would like all right.

The boundary conditions are given you have this expression T i j, if you know the temperature of the neighbors, then you can find out the you can find out the temperature at any point. And, at iteration number note I am not using the word time, iteration number 0, we can set the temperature the unknown temperature here inside to be say 1 or 0 it does not really matter, but because you do not know you have to iteratively find out the right temperature, you have to find out the temperature distribution as a function of x and y. And all that you know is the temperature at the boundaries of the box.

And, if you know the temperature of the boundaries of the box, then you can find out the temperature iteratively here, here the temperature might be 0 in the first iteration, here you have a finite value of the temperature, there by you find out what the temperature here is and if you know the temperature here, then this is again 0 and you can find out in the next iteration what is the temperature here. So, in each iteration you try to find out the temperature of all the points leaving out the boundaries, because the boundary temperatures are fixed all that is evolving.

Because of the boundary conditions or the temperature within this square a plate the points within this plate not at the boundaries and you find out the temperatures with each iteration at each of these points. And, just like in the previous class when you see that from one iteration to other iteration the temperature at any point within the square boundaries does not change less or changes less than a certain tolerance level that you fix it might be 10 to the minus 4 see right.

Then, you say this is my final temperature distribution this is how my temperature is going to be distributed in x and y right. So, what we are going to do today is very similar to what we did in the previous class where we had only a differential equation. Now, we are just solving it in 2 dimensions right. Using this formula moreover there the boundary conditions was only at x equal to 0 and x equal to 1, here we are specifying the boundary conditions not at 2 points.

But, along 4 lines these are the 4 boundaries and we are specifying the boundaries what the temperature is at each of these points along the boundaries right. With that let us move to the computer the basic principle is the same we are going to have an endless do loop and only when the temperature variation from one iteration to the other at each of the points does not change or changes by amount lower than the tolerance we say we have iteratively reached our temperature profile. So, now, let us move to the computer and see how the thing works.