Semiconductor Device Modelling and Simulation
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Lecture – 42
Drift-Diffusion Model (Continued)

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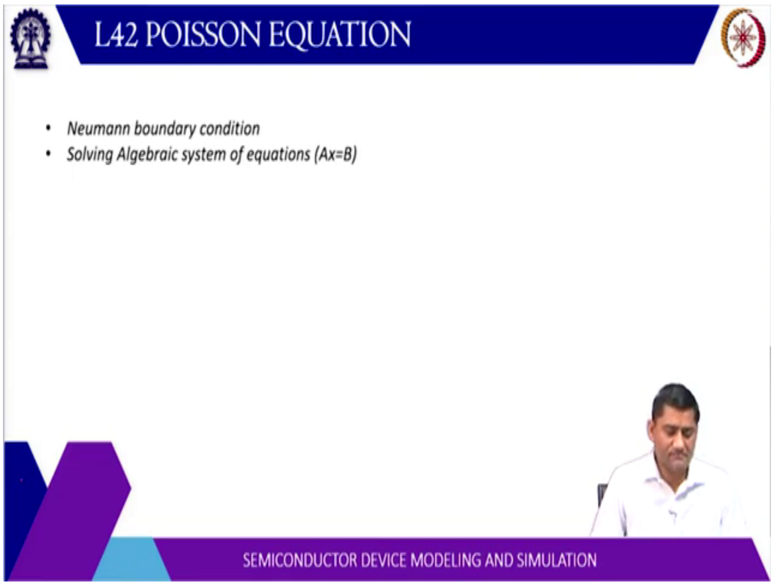

Hello, welcome to lecture number 42. So, we will continue our discussion on finite difference and we will solve the Poisson equation for using the finite difference method. We have already discussed dirichlet boundary condition. So, in this lecture we will discuss about the Neumann boundary condition and how to discretize the equation? And then of course, a brief process of solving the algebraic system of equations will be discussed.

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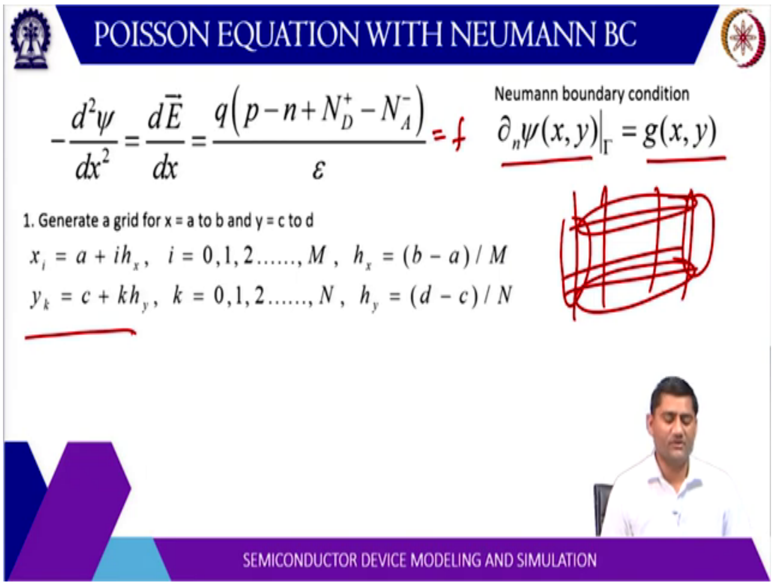

Now, this is the Poisson equation and it can written as some function f. And the Neumann boundary condition the characteristic is that the derivative of the function is defined at the boundary. So, if this is your domain, so now, instead of defining the values here, the derivative is given by this function g. So, it can be defined for all the four boundaries here for 2-D domain. And of course the first step will be we will generate a grid.

Now, this can be uniform or non uniform grid and that we have already discussed, in which case, to use the uniform grid, in which case to use the non uniform grid.

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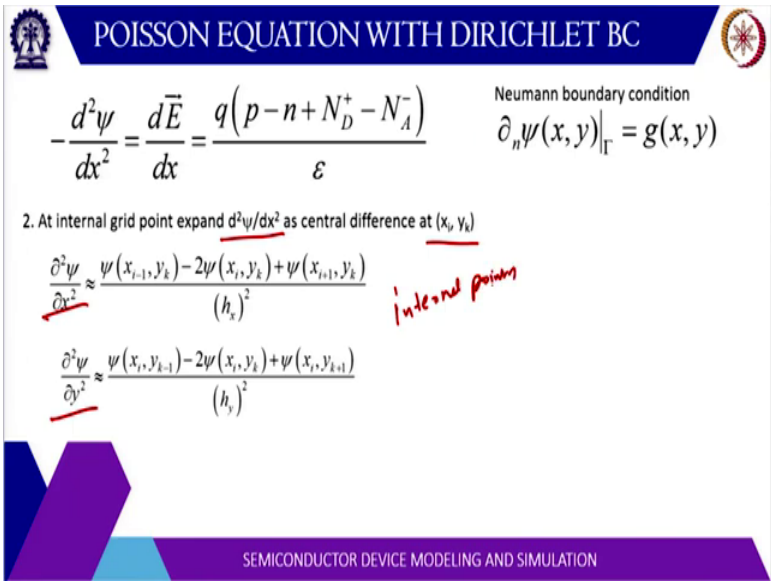

Then again we will expand d 2 psi by dx square, a central difference at all the internal points x i and y k. So, this is d 2 by d x square d 2 psi by d y square.

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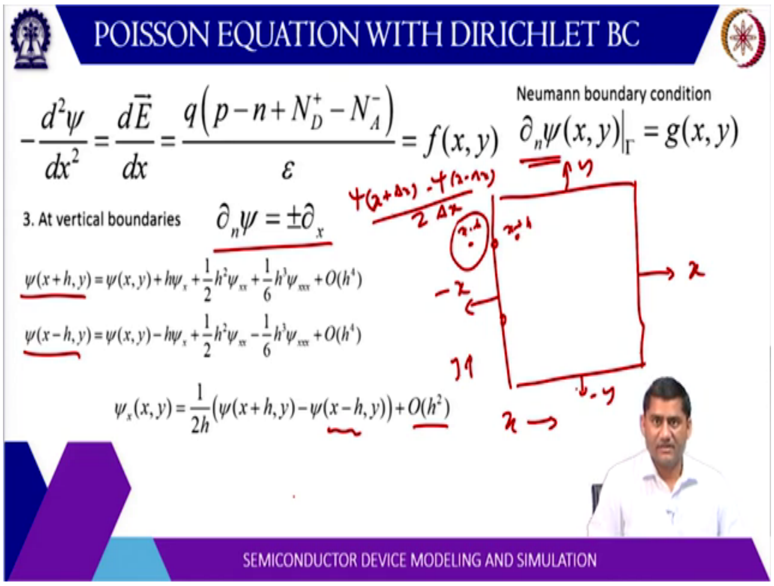

Then let us come to the boundary condition here. So, in Neumann boundary condition let us say this is vertical boundary. So, this is, let us say, x axis and this is y axis. So, there will be two vertical boundary for 2-D domain and there will be two horizontal boundaries. So, at vertical boundaries, the normal the derivative d n the normal vector this will point in minus x direction. This normal will point in x direction.

For horizontal boundary this will point in y direction and this will point in minus y direction. So, if we write the derivative then of course we are using the central difference. So, the derivative can be written as psi of x + delta x – psi of x – delta x divided by 2 times delta x. So that of course is obtained from the Taylor series expansion so, at x + h and x – h and when you subtract, you get this expression which is odd of h square accurate.

Now, if you notice here at the boundary point, the point on the right side which is x + h will be inside the domain. The point which is on the left side x – h will be outside the domain. So, outside domain we do not have any information about so, this point will be the fictitious point, so, this x – h, so, this point will be fictitious point. So, how to address this issue?

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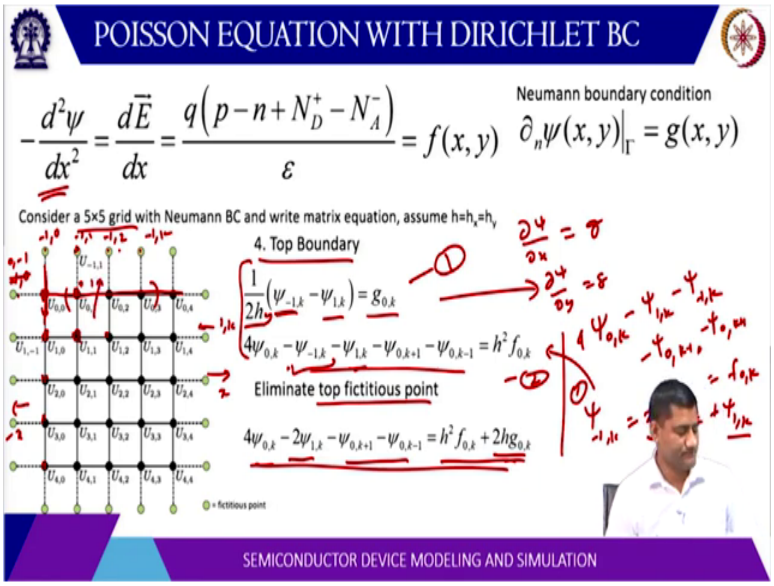

For example, we consider a 5 by 5 grid. So, this is the left, boundary, 0,0 1,0 2,0 3,0 and 4,0 and so on. So, let us consider this 1,0. So, at 1,0 we know that del psi by del x is g. Now, this is in minus x direction. So, it will have some minus sign so, this will be minus x direction. Because this side is minus x direction and this side is x direction. So, 1 over 2 h psi because this point is, let us say, 0,0. So, this will be this is psi 0,0 this will be minus 1,0.

And this will be + 1,0 that all the order is different. So, this is 0,1 and this will be 0 – 1 and this is vertical. So, this is 1,0 this will be –1,0. So, here we are writing at the top boundary. If you write at the top boundary, this will be along y direction. And if you write along the horizontal boundary, the vertical boundary, this will be in x direction. So, here you have –1 and +1 for the first column.

So, this is along the top boundary the corner point. So, here you can actually write here you can write this equation for derivative with respect to x as well as derivative with respect to y. So, this is the derivative with respect to x and this is the derivative with respect to y. So, –1,0 and 1,0. Now, this is first point 0 this will be second point. So, along the top boundary, the first value is fixed the second one the k is changing basically.

So, we can write a generalized equation for the top boundary, so that will be –1, k. This will be –1,1 this will be –1,2 and so on. So, in general we can write –1, k and this will be 1, k. So, the difference divided by 2h. This is in y direction, so, you can write y also is equal to g at these points 0, k. So, this is the boundary condition that we have written d psi by dy. Then at this point we can also write the equation for d 2 psi by dx square.

Now, d 2 psi by dx square will consist 4 points actually so, let us say if you consider this point. Then right point, left point, top point and bottom point so, 4 psi 0, k will be write here psi 0, k 4 times – psi 1, k – psi – 1, k – psi 0, k – 1 – psi 0, k + 1 will be equal to f 0, k. Now, the points which are here in the middle, so, not at the corner point. We will have this equation basically, so, all these four will be there. Now, we have to eliminate this fictitious point on the top.

So, how do we eliminate? We have two equation, equation 1 and equation 2. And here we can substitute this psi – 1, k the expression so, psi – 1, k from equation 1. So, from 1 psi – 1, k is 2 h times g 0, k+ psi 1, k and that you substitute here. So, this – 1, k will be 2h g 0, k + psi 1 k so this psi 1 k will come twice. So, your – 2psi 1 k rest are remaining same and this 2hg gets added here.

So, if you take to right hand side the sign changes basically from minus it becomes plus and this adds up. So, we have eliminated the top fictitious point. So, at the boundary we use these two equations to write a equation which has all the points within the boundary. So, for internal points step one is ok so, this is for internal points and this is for boundary points. Same thing we can do for left boundary right boundary and the bottom boundary.

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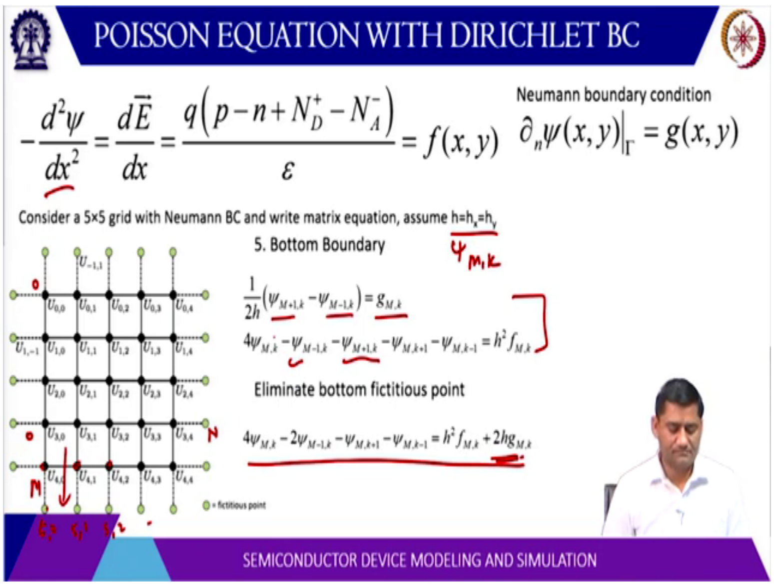

Then for the bottom boundary this is the bottom boundary, so, this all will be let us say this is changing from 0 to M and the horizontal chain is 0 to let us say n. So, bottom boundary will have M 0, 1, 2, 3, 4 and so on so, M, k and so, it is psi of M, k. And then if you take the derivative here, so, psi M + 1 – M – 1. You notice that **(())(09:02)** M + 1 – M – 1. So, this direction is basically pointing away, so, the normal derivative is always pointing away.

In previous if you saw it was – 1. So, it was point it was also pointing away from the surface. So, psi M + 1, k – psi M – 1, k divided by 2h is g at M k. Then from expansion of d 2 psi by dx square you can use these two equations and substitute a value of M + 1 k. Because M + 1 k is outside, so, this will be 5,0 5,1 5,2 and so on. So and then you will get the similar expression as we got for the top boundary.

So, here all the points are the internal points. The only function that is appearing here is 2gh on the right side. Now, of course, here it is assumed that h x = h y. Otherwise, we have to include separately. And the equation you can still do it but it will be little involved encoding you can do but as far as explanation is concerned, it is easier to consider both h x and h y = h.

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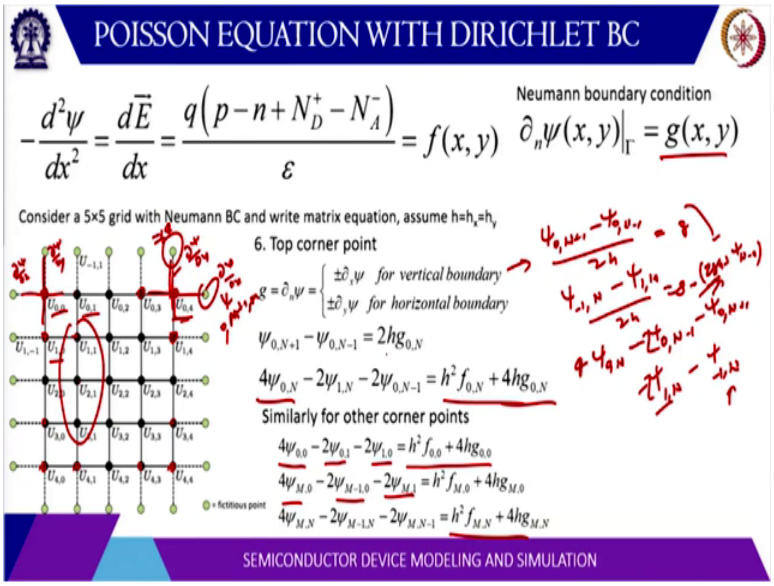

Then let us consider this top corner point. Now, the top corner point appears with both the boundaries, the top boundary, as well as the left boundary. So, for vertical boundary we can write d psi by d x so, for this will be d by dx this will be d by dy. So, d psi by dx you can write now this top corner point. In this example, top corner point is this one so, you can take here also because it is 0, N.

So, if you write the derivative here for x so, it will be psi of 0, N + 1 – psi of 0, N – 1 divided by 2h that will be g. And then if you take the vertical derivative then it will be psi of – 1 N – psi of 1, M divided by 2h will be g. And of course, we are assuming that for both the vertical and horizontal boundaries, the function is g only it could be a different function. So then of course, we have to write it separately.

Then from this two equations so, from the d psi by dy, we will substitute expression for this point which is – 1,4 or – 1,M and from d psi by dx. We will substitute for this point, which will be a fictitious point outside along the x boundary. So, we will basically substituting this two points here for two points really substituting here. Now, so, what will happen? We have to substitute for psi N – 1 psi N + 1.

It will appear as psi N – 1 and this is psi of – 1, M so, 0,N + 1. So, if you substitute here, 4 psi of 0,N then – psi of 0,N – 1 – psi of 0,N + 1 – psi of 1,M – psi of – 1,N so, from here psi of N + 1 here you will get as 2gh + psi of N – 1. So, this will have negative sign. So, it will be 2 psi N – 1 and – 2gh. And similarly for this one it will come 2 psi N h and 2gh become 4gh and it goes to other side it removes 4gh at 0,N.

So, for the corner points we can simulate that for other corner points also. So, this is the corner point psi 0 command 4 times – 2 times bottom point 2 times left point is equal to h square f + 4gh. Similarly, for the left boundary at 0,0 point 4 psi 0,0 – psi 0,1 – psi 1,0 2 times is equal to h square f + 4gh. Similarly, for bottom point M,0 4 psi M 0 – 2 psi M – 1,0 – 2 psi M,1 M – 1,0 this is M,1.

Then for the bottom point psi 4 psi M N – 2 psi M – 1,N – 2psi M,N – 1 = x square f + 4gh. So, what we have done basically? We have written the equation for all the points now. So, we have converted the differential equation into a algebraic equation for all the grid points. And there is no grid points which is outside the domain.

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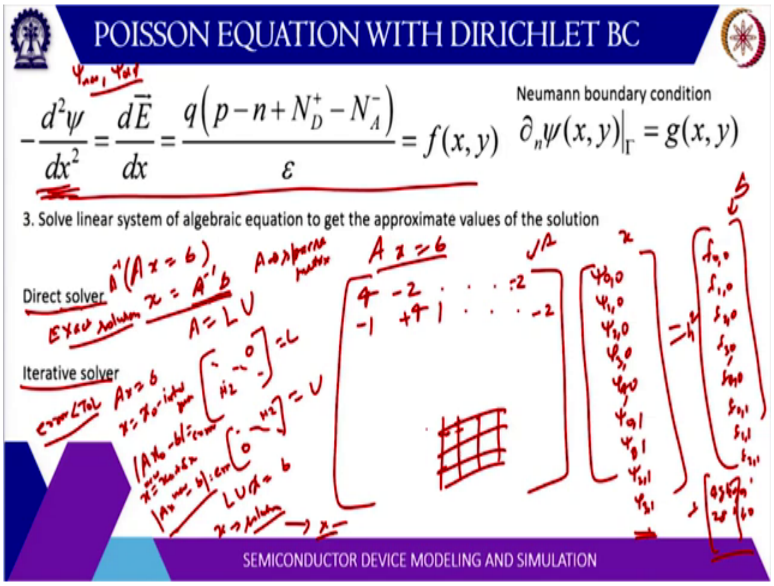

Now, what we have to do? We have to basically solve for this equation. So, similar to the previous case, where we are the Dirichlet boundary condition we can write this Ax = b. So, if you write it here, so, your x is again the vector this column here. Now, in this case, only the internal points are not the unknown. Rather, these boundary points are also unknown. So, you can write the whole vector here psi 0,1 to psi 0,0 to psi 4,0.

So, what you can write? Here, psi 0,0 then psi 1,0 psi 2,0 psi 3,0 psi 4,0. So, this is one then psi 0,1 psi 1,1 psi 2,1 psi 3,1 and so on. So, this whole thing will appear. Now, here if you see for the left boundaries 0,0 to 4,0 will be equal to f will appear in all the cases here. So, f 0,0 f 1,0 f 2,0 f 3,0 f 4,0 f 0,1 f 1,1 f 2,1 and so on now, for the corner point 0,0 see what is the equation for 0,0 it is 4 times. So, this will be 4 here.

The coefficient will be 4. Then 0,1 0,0 0,1 1,2 and 1,0 also 2. So, the coefficient is –2 here. So, 0,1 1,0 is here so, it is coefficient is –2 and 0,1 is appearing here so, 1, 2, 3, 4, 5, 6 point so, 1, 2, 3, 4, 5, 6, point 6 point will also be –2 so that is 0,1. Then is equal to h square f so, this f will be multiplied by h square. So, you can write this thing and then + 4gh. So, this will be added with 4gh.

So, this will be you can write another matrix here. This will be 4gh 0,0. Then second one is basically psi 1,0 so, psi 1,0 is here and for psi 1,0 it is a left boundary. So, this will 1,1 will have coefficient 2 and 1,0 will have coefficient 4. You can see here. This is the 4 and rest only 1 will have 2 rest will be –1. So, for psi 1,0 1,1 will have coefficient 2 and 1,0 will have

–4. So, this is –4 and 0,0 will have –1 and 2,0 will have also have –1. So, 0,0 will be –1 this is 4 then –1 and for 1,0 4.

The neighbours of 1,0 are 0,0 and 2,0 so, 2,0 will also be 1. So, 0,0 and 2,0 are 1 then 1,1 will have 2. So, if you see here this is 1,1, so, this is 7th point so, this will be – 2. So and of course, on right side, you will have h square f 1,0 then + 2gh it will be left side is 2gh instead of 4gh the because it is a corner point, it will have 2gh. So, you can write 2gh of 1,0. So now, this is your that way, you can form the matrix basically.

And another thing you can notice here the diagonal elements are usually quite large here. And these are positive values +4 +4 like this appears here and that is coming from the expansion of this equation. Because when you take the double derivative, it has 2 times psi from the x side and 2 times psi from the y side appears 4 and rest are –1. And if they have happens to get a boundary then instead of 1 they become 2 that is it.

Now, there are two ways to solve this equation Ax = b one is called direct solver. Now, direct solver usually takes lot of memory because what you have to do? This is Ax = b. So, what you do multiply? You to multiply with A inverse, so, A inverse into Ax will be x = A inverse times b. So, you have to take the inverse of this matrix A to get and multiply with b. So, b is this side and this is x and this matrix is A.

So, taking the inverse of A matrix is computationally demanding. So, it takes lot of memory one thing that you can do use this A as a save this as a sparse matrix because if you notice many of the elements of this matrix are actually 0. So, many of the elements of this matrix are 0. So, every sparse matrix that is how it is saved in the system so that it takes less memory. And there are internal codes which can make the process of taking hours faster.

Now, the another way that this inverse is taken. What is done? This matrix is divided into two parts, one is the lower triangular matrix other is the upper triangular matrix. So, lower triangular matrix is a matrix whose elements below this line are non-zero. And above this all are 0. So, this is lower triangle matrix. So, this is called LU decomposition upper triangular matrix is above this line. These elements are non-zero and here all the elements are 0.

So, diagonal and up will be non-zero. Diagonal and down will be non-zero for L. So, you can do the LU decomposition then what is done here? So, A is written as L times U times x = b so then take the inverse of L then take the inverse of U which is easier? Because this is only one side of the diagonal is non-zero. So, in this case it is easier to take the inverse. So, these are basically direct solvers.

In iterative solver what we do? Let us say, your Ax = b. So, what we do? We estimate that x is some x naught some initial gas. Now, in direct solver the solutions we get are exact solution. These are exact solutions so, there is no error. In iterative solver, we start with the initial gas, so, let us say x = x naught. Then we calculate the error. And error will be A times x naught – b. So, this will be your error.

Then based on error, we update that x = x naught + delta x then this called x nu. So, we again use Ax nu and again calculate the error. So now, it will be Ax n – b there will be a new error and again update x. So that way we keep on updating the x till this error is below certain limit and that we call tolerance. So, when the error is less than the tolerance value, we stop our procedure and the last available x is designated as the solution of this matrix.

So, for last problems iterative solvers are used. They are not exact but they are accurate enough because there is some error is there. So, error margin can be kept pretty low 10 is to power –5, 10 is to power 6 and the error that is calculated is usually it is not just the Ax – b modulus. Because individual modules k N f plus and minus. So, there are different ways of measuring the error. One is called RMS error.

So that means individual error is squared and taken square root and averaged out. So that is called RMS error. So, generally we reduce the RMS error and if you consider equation, there are two types of error that can be considered. One is the difference between the psi new and psi old. So that will error with respect to this variable psi or the there are in the potential. Then error related to this equation, so, d 2 psi y square – f.

So that error can also be reduced. So, there is a some criteria for all these errors. When these errors are reduced then we call it that the solution h converts and then we have this values of x and there again. Because the values you get for the x they are in vector form and they have to be mapped to the grid to plot the values of potential. And once you know the values of potential, you can calculate the electric field and so on.

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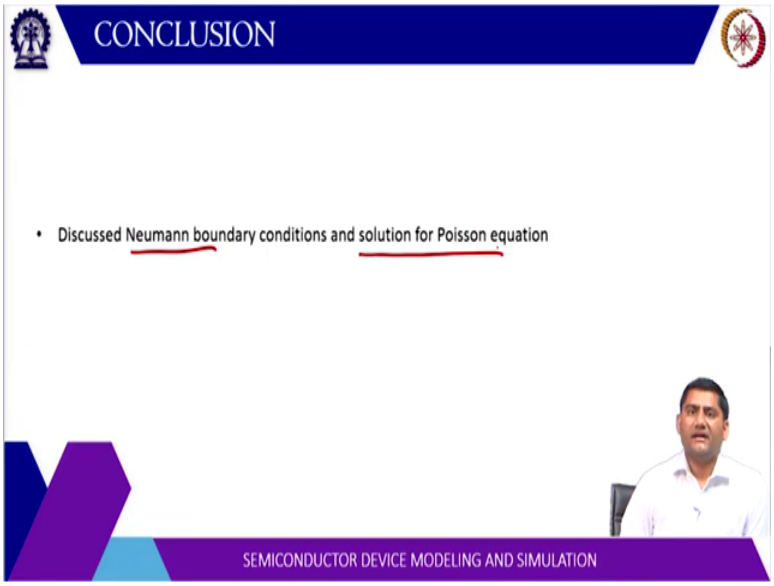

So, in this lecture, we have discussed the Neumann boundary condition and a brief procedure for solving the Poisson equation. Thank you very much.