Semiconductor Device Modelling and Simulation
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Lecture – 41
Drift-Diffusion Model (Continued)

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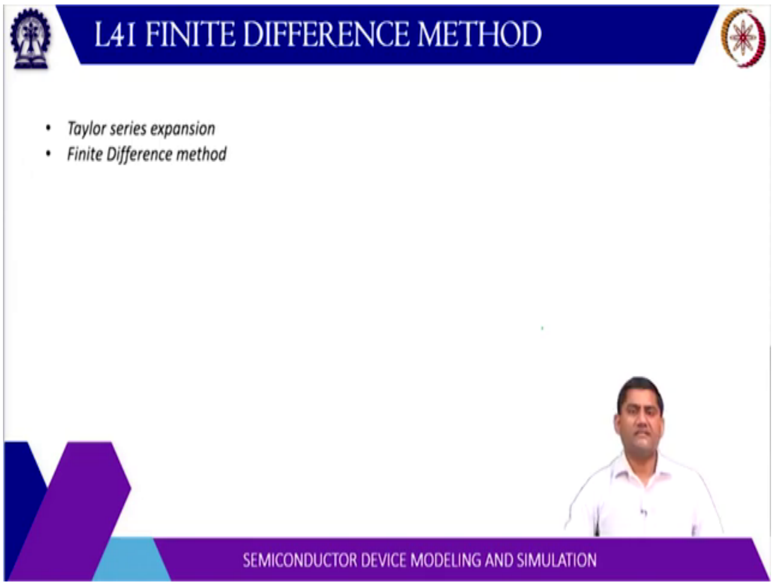

Hello, welcome to lecture number 41. So, far we have discussed the drift diffusion method and now to if to be able to solve it. We need to have some idea of the finite difference method. How do we discretize these equations? And eventually, how do we solve them? So, in today's lecture we will discuss the finite difference method, a part of it. And so, here we will learn we will recall that Taylor series expansion. And we will learn how to write the finite difference expression for different derivative terms.

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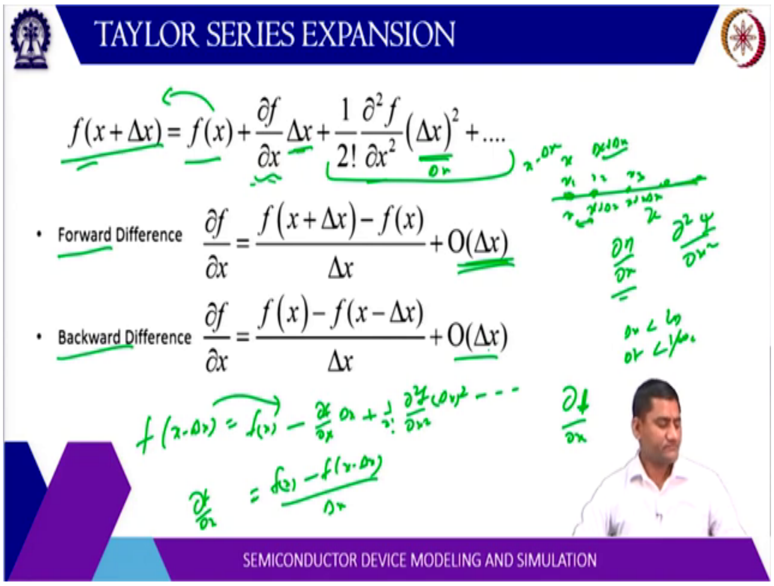

So, all of that any function f x in the vicinity of x let us say, f of x + delta x can be written as a series expansion function of multiple derivative at x. So, f x + delta x can be written as f of x + derivative times delta x plus double derivative times delta x square plus third order derivative times delta x cube and so on with some factor. So, this is a Taylor series expansion. So, we will use this to express these derivatives in terms of the values of the function.

So, what we do, basically? Let us consider a line. So, let us say this is your x axis and we want to find out. We have this del n by del x. This term appear there or d 2 psi by dx square. This term appears in Poisson equation. So, how do we write them? And so, let us say this position x this is x + delta x + 2 delta x or we can write x 1, x 2, x 3. So, when we try to solve this equation in computer, we cannot specify a place from expression that is not possible all the time.

So, what we do? We choose a domain and we discretize it. And when we discretize, we try to calculate these values of these discrete points. So now, what we are doing? We are calculating the values of unknown. Let us say x at this discrete point. So, unknown can be n or it can be a potential psi so. And this delta x has to be sufficiently small, as suggested in the previous lecture.

Because this delta x should be less than this d by length and delta c should be less than this 1 over omega c the plasma of frequency. Now, if there are derivative and other terms are coming into the picture, how do we take care of this? So, let us say there are different ways to write the derivative. So, let us consider df by dx this is a derivative and we want to calculate the derivative at position x. So, what we can do?

We can write the Fourier series, expansion, Taylor series, expansion at x and we can write at x + delta x. So, if you see this, we know the f x and let us write the Taylor series expansion at x+ delta x. So, from this you can find out del f by del x del f by del x will be you take to the left, so, f of x + delta x – f x divided by delta x. And then these are the error terms basically. So, this is order of delta x because we are dividing by delta x.

So, this will also get divided by delta x so, the order becomes delta x. And this we are calling forward difference. Why forward difference? Because we are taking a point which is ahead of it, so, this is x here, so, we are taking a point at x + delta x. And then we are defining the derivative instead of x + delta x let us say, take x – delta x. So, the Taylor series expansion of x – delta x will be f of x – del f by del x times delta x + 1 over 2 factorial del 2 f by del x square times del x square and so on.

So, if you see here then del f by del actually f x you take this side – f of x – delta x = del f by del x times del x and del x you divide this thing. So, you have f x – f of x – delta x divided by delta x. So that is called backward difference because you are considering a point which is x – delta x and the accuracy is order of delta x.

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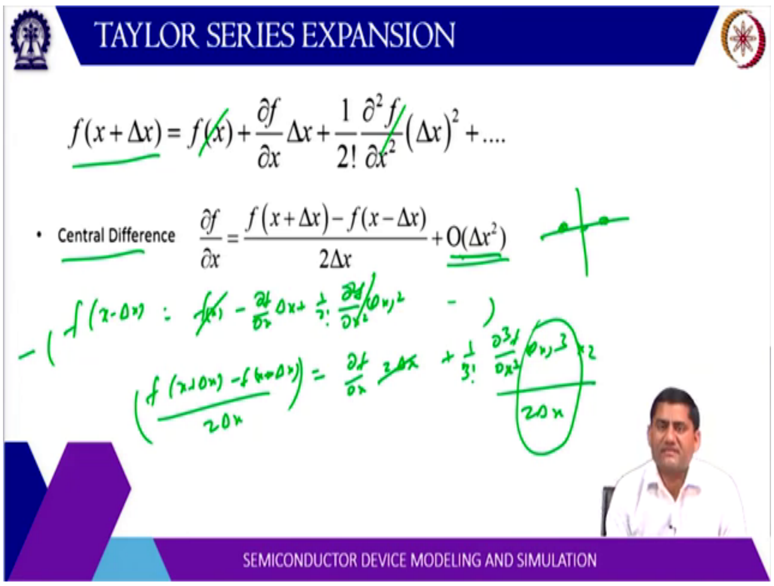

Similarly, for double derivative also, we can write so, double derivative so, let us try the central difference first. Now, central difference the advantage of central difference is that it is accuracy is higher. Now, how do we get it? So, let us we evaluate on the Taylor series expansion for f of x + delta x let us write f of x – delta x which will be f of x – del f by del x times delta x + 1 over 2 factorial del 2 f by del x square times delta x square and so, on.

Now, you take the difference of these two, subtract second equation. So, what you have of x + delta x – f of x – delta x is equal to this f x, this f x will cancel. So, you will have del f by del x times 2 delta x then this will also cancel out. And then third term will be there which is 1 over 3 factorial del 3 f by del x cube times delta x cube. And this will become two times f. Now, you divide by 2 delta x so, divided by 2 delta x divided by 2 delta x divided by 2 delta x.

So, del by del x is this thing f of x + delta x – f of x – delta x divided by 2 delta x. And the accuracy is delta x cube by delta x so that is order delta x square. So, the central difference is it is called central difference because we are considering the points on both side. So, when we are calculating, we are derivative at x position x. We are considering the value at x + delta x and we are considering value at x – delta x.

And it is higher accuracy with of course, requirement that now you have to consider three point instead of two points. So, for f x you have to use the value at x + delta x and x – delta x.

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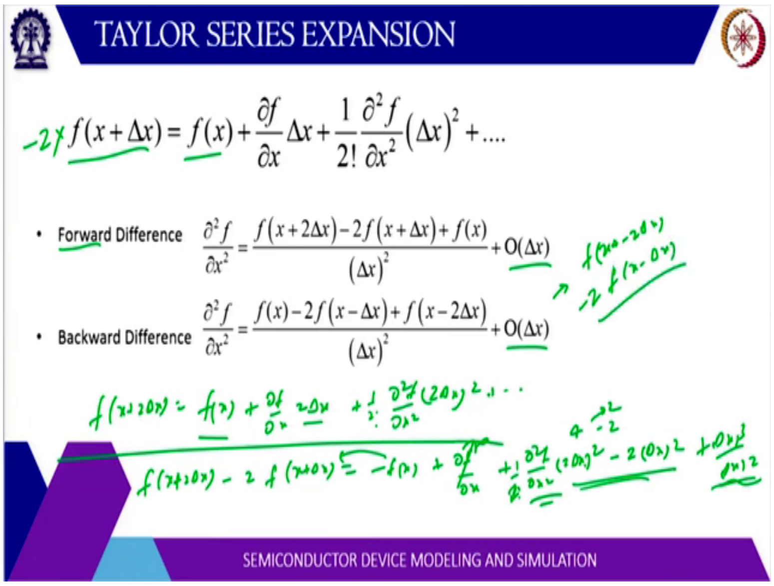

Similarly, for the second derivative you can write the forward difference. So, in forward difference we consider only the points which are more than x. So, it is f of x + delta x we can write f of x + 2 delta x that will be f of x + del f by del x times 2 delta x + 1 over 2 factorial del 2 f by del x square times 2 delta x square and so on. Now, what we do here? From this expression we substitute subtract two times of this.

So, what you will get? f of x + 2 delta x – 2 times f of x + delta x = f x – f x will be – 2 f x will be – f x f x – 2 f x will be – f x + del f by del x this is 2 – 2. This will cancel out. Then you will have + del 2 f by del x square 1 by 2 factorial this is 2 delta x square – 2 times delta x square. So, if you take this f x to other side, if you come +f x. So, this is f x + 2 delta x – 2 f x + delta x + f x divided by this is delta x square.

So, because 2 is here 2 here, so, this is 4 – 2 is 2 so, 2 divided by 2 is 1 so, delta x square if you divide you get del 2 f by del x square. But here you will have term delta x cube divided by delta x square so, the accuracy will be delta x only. So that means the terms that are neglected they are delta x accurate only. So, it has a low accuracy, so only for backward difference instead of x + delta x we take x – delta x here.

So, this is trivial you can again write it. So, here you will take the expansion of x – 2 delta x then subtract – 2 times f of x – delta x. Then you will get it.

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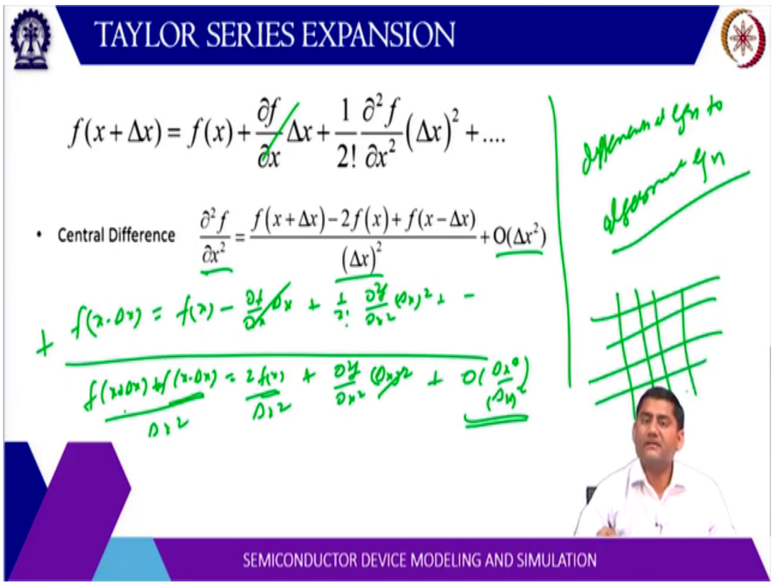

Similarly, for central difference f of x + delta x here we consider both side x + delta and x – delta x. So, let us write f of x 1 as delta x because f of x + delta x is already written. So, this will be f x – del f by del x times delta x + 1 over 2 factorial del 2 f by del x square times del x square and so on. Then if you add these two so, you have x + delta x + f of x – delta x = 2 times f x. Then this will cancel out.

Then you will have del 2 f by del x square times delta x square 1 by 2 + 1 by 2 1 and some term again 3 will cancel out. So, you will have 4 only delta x 4 here then you divide by delta x square. So, this will be accurate to the order of delta x square and the expression for del 2 f by del x square will be f of x + delta x – 2 f x + f of x – delta x divided by delta x whole square. You can also notice one more thing here this is symmetric.

So, the f x + the single derivative and double derivative both were kind of symmetric, f of x + delta x – f of x – delta x and here f of x + delta x + f of x – delta x – 2 f x by delta x square. So, this is a central difference expansion. So, this is basically a way to convert a differential equation to algebraic equation. So, given a differential equation over a mess, we can convert it into algebraic equation.

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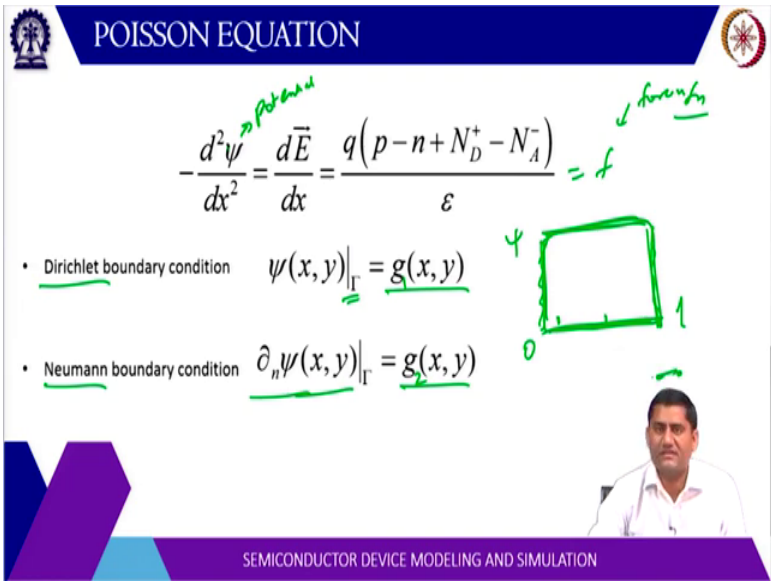

Now, let us consider the Poisson equation d 2 psi by dx square is rho by epsilon – rho by epsilon, so, minus is taken here and let us call it some function f. Generally, this is called forcing function because this one is actually forcing the condition on this variable psi is a potential. Now, when we solve for a difference equation, we generally encounter two types of boundary condition.

One is the Dirichlet boundary condition which simply means if you have this some reason here. So, the value of psi is known. So, this region, value of psi is known, here value psi is known, here value psi is known, here value psi is known that is Dirichlet boundary. That means this is fixed, let us say 0 volt this is fixed at 1 volt. And here it may be it may not be Dirichlet boundary.

So, when we fix the potential here or fix the variable at certain end, we call it Dirichlet boundary condition so, this refer to the boundary here. So, if you see a rectangular region, there are two boundaries here two vertical boundaries and two horizontal boundaries. So, Dirichlet boundary condition, especially the value and this value can be specified through certain function or simply the values.

Then another bound is a Neumann boundary condition. Here we do not specify the values but the derivative. So, derivative is expressed in terms of some function g so, let us say this is g 1 this is g 2. So, this may be a function of y. So, you can say that derivative is 0. So that means it has to be flat here. The derivative is 0 or it has certain derivative. So, when the derivative is specified at certain boundary, we call it Neumann boundary condition.

And when the values are specified we call it Dirichlet boundary condition. So, Dirichlet is some kind of hinge that it is fixed at this value. And Neumann is basically. if you tell the derivative, it has no foundation on the value because value can be anything but the derivative if it is certain less, if derivative is 0 then value will not change at least for two grid points. The value has to be same so that the derivative is 0.

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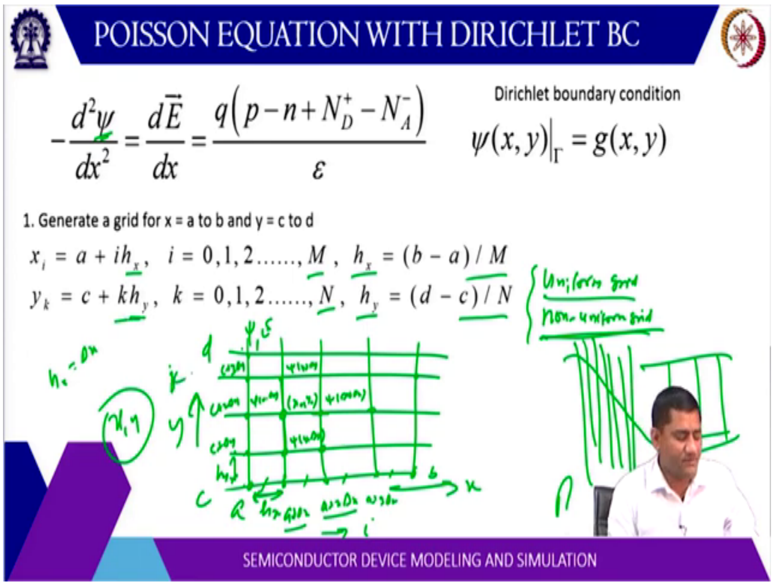

Now, how to solve the Poisson equation with Dirichlet boundary condition. So, the first step is basically is to create a grid. So, let us say this is your reason here. So, this is your x axis, this is your y axis and let us say this axis is going from a to b. And y axis is going from, let us say, c to d so, this is your region. Now, in this region we can have n number of slices. Let us say this difference is, let us say hx, let us say this difference is hy.

When the difference is across these grid points, they are equal, this is equal to this. Then we call it uniform grid when these differences are not equal when we call it non uniform grid. Now, this grid actually depends on what are the values you are trying to? what is the variation of the function that you are evaluating? So, if function is sharply varying especially if you look at the depletion region, the potential varies very sharply.

So, here we have to use some kind of fine grid. So that is able to resolve the variation but then again for a p n junction if you go to a quasi neutral region, where the change is not so, abrupt. There, you can have a coarse grid also. So, that is why this non uniform grids are useful in scenarios where you have a big structure and there are regions where you need to use fine grid then you can go ahead with the non uniform grid.

And for simple problems of course, you can always go ahead with a uniform grid. And the problem with uniform grid is that if let us say there is a small region where you need to resolve it with a small hx then number of grid points will actually increase. So, if number of grid points is more than solving the numerical problem becomes more demanding in terms of the memory and time.

So, people generally go for uniform on non uniform, depending on the requirement from the problem. So now, this is a let us say this is hx the delta x is hx so, hx is simply the delta x. So, this point will be a + delta x, this point will be a + 2 delta x a + 3 delta x and so on. This will be c, c + delta y it will be c + 2 delta y, it will be c + 3 delta y and so on. So, these are grid point. So, if I choose any grid point it can tell me what is the value of x and y?

So, this will be a + delta x and c + delta y if this grid point will be a + 2 delta x and y value is c + delta y. So, once I know the grid point, I can tell what is the value of x and y? So, this grid basically maps x and y and on top of this we have to evaluate the values of the psi or electric field. So, you can calculate psi here. You can calculate the electric field here on these grid points. So, the first step in solving is generate a grid.

So, in Matlab you can easily generate a grid and how to write hx and hy? Let us say you want to have n number of grid points. So, you divide this gap b – a divided by M or d – c divided by N. So that you will get the grid spacing.

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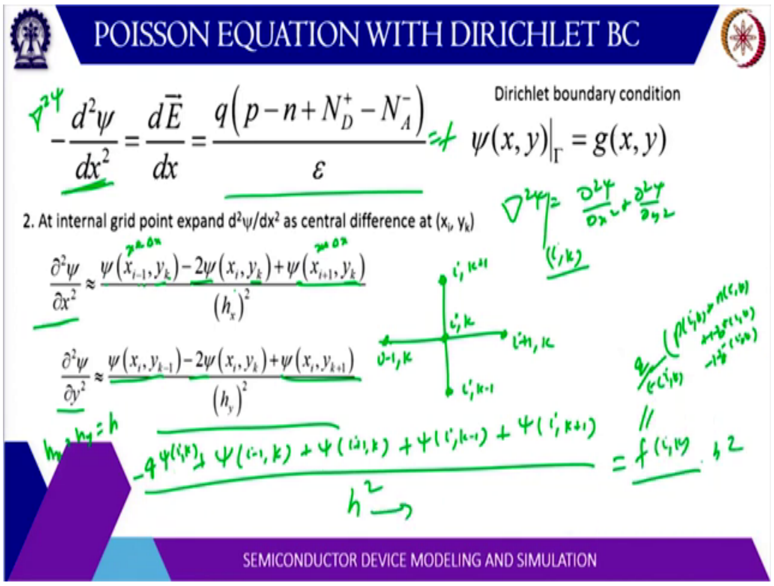

Now, here we only have the double derivative d 2 psi by dx a square. And on right side there is no derivative, so, what we will do? We will write this we will expand this differential equation at certain point x and y. So, let us say we choose this point so, here we can expand it. So, let us say this is some x naught y naught. So, we know nearby these grid points, so, this will be psi x, this will be psi x + delta x.

So this will be psi x – delta x, this will be psi y + delta y, this will be psi y – delta y. So, we can expand d 2 psi by dx square. Now, in 2-dimension it is basically – del square by psi and del square psi is d 2 psi by dx square + d 2 psi by dy square. So, d 2 psi by now, we are expanding it at x, y. So, in terms of the grid we will have the coordinate. Let us say for x coordinate, we are using i for y coordinate we are using j.

So, ith point and kth we call it and kth point. So, for point i, k we can expand it as derivative of x square derivative with respect to y square, this is x – delta x, this is x + delta x and in all these cases, y is same. So, we are only taking the variation with respect to x. So, d 2 psi by dx square psi of x + delta x + psi of x – delta x – 2 psi at x divided by delta x square, so, a delta x is hx and that is what we get here.

So, we have written in terms of i. So, if you consider point here, let us say this is i, k. So, this is i + 1, k this is i – 1, k this will be i, k + 1 usually i, k – 1. So, derivative with respect to x using this 3 point i – 1 i and i derivative with respect by k + 1 k and k – 1 so that is what we done here. Then we add that to is equal to some forcing function. Let us call it f. So now, if you write it here, what you will have we can use i and k instead of writing x and y.

So, d 2 psi by dx square is psi i – 1, k then this term + psi i + 1, k. Then let us say this term + psi i, k – 1 + psi i, k + 1 so, these four neighbouring points. Then 2 psi 2 psi so, minus, minus 4 psi i k and divide by if we assume that hx = hy = h so, you can divide by h square. This is the left hand side is equal to f at i, k. So, what is f of i, k? Which is q by epsilon, so, epsilon, is if it is a function of position then you can also evaluate epsilon at i, k.

And if it is constant then you can just leave it as it is then p at i, k – n at i, k then + n d + at i, k – n a – at i, k so, this will be right side. So, you see here there are terms depending on position. So, all the terms here depending on i, k and near around that. So, the derivative terms include points from nearby area and this forcing function. They simply depends on the position i, k itself. Now, it is possible if you know the electron hole distribution function.

You can easily calculate this potential psi as a function of position. Now, in some cases we do not really know what will be the distribution for p and n? So then what we have to do? We have to basically follow some iterations, so, with each iteration we will update. So that we will discussed in coming lectures.

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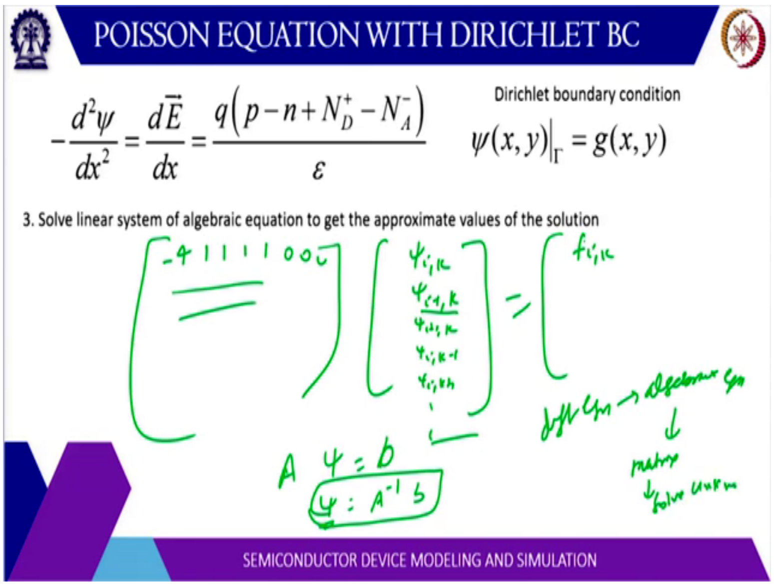

So now, what we do? We have this algebraic equation. Now, this algebraic equation can be written as in terms of matrix. So, these coefficients so, this coefficients can so, for example, psi i, k. What is the coefficient is 4 – 4 and then h square can be taken to other side, so, it becomes h square times f. So, what will happen here? If you write in terms of let us say psi of i, k psi of i – 1, k. So, psi i, k the coefficient is – 4 here i – 1, k. The coefficient is 1 here.

And psi i + 1, k coefficient is 1 here psi i, k – 1 i, k + 1 coefficient is 1 here and for others coefficient is 0 here and that is equal to f i, k and so on. So, this is for i, k then we can write for i – 1, k and so on. So, get a matrix like this, where a psi is equal to. Let us call it b. So, psi will be A inverse b. So, simply by writing a matrix and then making algebraic solution we can estimate the value of psi from this discretized equations.

So, what we have done basically? In finite difference, what we do? We convert differential equations to algebraic equation. And then from the algebraic equations we write the matrix and then problematics we solve for unknowns.

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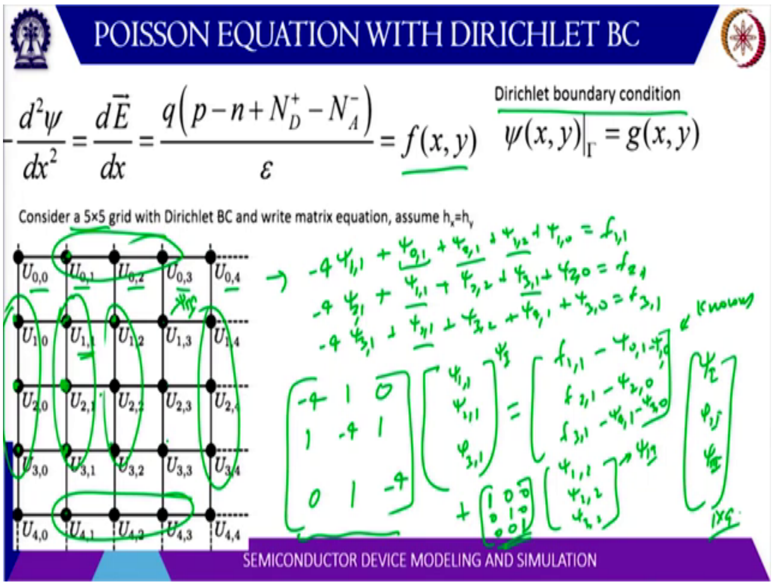

So, here you can see one example, where we have considered 5 by 5 grid point. So, 00, 01, 02, 03, 04 these are grid points. And the boundary condition is a Dirichlet boundary condition. So that means we know the value at these points we know the value at this point, we know the value at this point and we know the value at this point. So, what we have to do? We have to basically write the equations at this central points basically.

So, let us consider one by one so, let us say for 1,1 point, so, the coefficient will be –4 times psi 1,1 then 4 neighbours of 1,1 are 1,2 0,1 1,0 and 2,1. So, this will be + psi 0,1 + psi 2,1 + psi 1,2 + psi 1,0 = f 1,1 so, this is f. Similarly, for 2,1 so, – 4 times psi 2,1 + 4 neighbours are psi 1,1 + psi 2,2 + psi 3,1 + psi 2,0 = f 2,1. So, only for 3,1 – 4 psi 3,1 + psi 2,1 + psi 3,2 3,1 3,2 4,1 + psi 4,1 + psi 3,0 = f 3,1. So, if you write in terms of matrix psi 1,1 psi 2,1 psi 3,1.

So, for first equation, psi 1 coefficient is – 4, psi 2,1 coefficient is 1, psi 3,1 coefficient is 0 for second equation psi 2,1 coefficient is – 4 and psi 1,1 coefficient is 1 psi 3,1 coefficient is 1 for psi 3,1 coefficient is – 4 then psi 2,1 coefficient is 1 psi 1,1 coefficient is 0. This is equal to because we at these boundaries we already know the value. So, they can be shifted to the right side. So, this is basically your f 1,1 then psi 0,1 we already know.

So, – psi 0,1 psi 1,2 psi 1,2 is not boundary point. So, what we can write here? When you write another matrix here for second column. So that is psi 1,2 psi 2,2 psi 3,2. So, psi 1,2 has coefficient 1 so, this is 1 and 2,2 3,2 at 0 and then – psi 1,0 – psi 0,1 so, – psi 1,0. For second 1 psi 2,1 is there psi 1,1 is there psi 3,1 is there then psi 2,2, so, psi 2,2 is here, so, this is 1, this is 0, this is 0.

And then psi 2,0 so, this is f 2,1 – psi 20. So, 20 is just 1. So, only for the third 1 f 3,1, so, –4 psi 3,1 + psi 2,1 then + psi 3,2. So, psi 3,2 is here. So, this is 1, this is 0. So, this is there then psi 4 is boundary point so, – psi 4,1 and 3,0 is also boundary point so, – psi 3,0. So, you here, this is the left hand side. So, this for this column where this matrix for the neighbouring column. We have this matrix and the boundary points because the values are known.

Because these are Dirichlet boundary we have shifted it to right side. These are the norms. Now, we can write the same thing for all the three columns, so, this we wrote for the first column, so, only for second column. Now, you notice one more thing here for first column, the diagonals are – 4, 4, 4. And then besides, there is a 1, 1, 1 and for the relationship with the neighbouring column is 1, 1, 1 as diagonal.

So, when we put them all three together, so, let us say we call it psi 1. Here then similarly, we can call this one as psi 2 here and we will have this will be psi 3 here we can put them all together psi 1, psi 2 and psi 3. So, it will be 3,3 and 9 elements. So, this will be 1 by 9.

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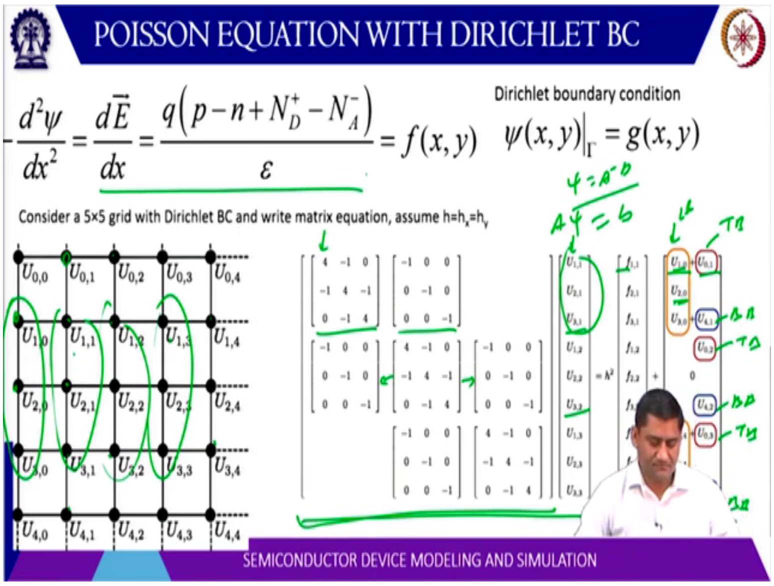

And when we write it here, so, this is basically your psi represented by U here so, psi 1,1 psi 2,1 psi 3,1. This is the vector then the next one is psi 1,2 2,2, 3,2 and this is a vector here and this is f 1,1 plus the sign should be plus here and this would be plus here. Because we are in – 4 here so, this is taken care of basically, so, this is basically inverted. So that is why this is coming here. So, this is become plus here, so, rest will become negative and this will sign will also change.

So, f 1,1 + psi 1,0 + psi 0,1 because there are two neighbours here so, psi 1,1 for psi 2,1. There is only 1 neighbour, so, psi 2,0 and this is basically left boundary. So, you notice one more thing here. For the first column, this left boundary will come here. This is the left boundary. Then for the top point there will be top boundary, so, this will from the top boundary and for the last point this will be bottom boundary.

Then for the middle points you do not have to worry about the left, right because both are covered this is left, this is right. And then the top and bottom will come here. So, this is the top boundary this is from the bottom boundary for the last column. The third column left is inner point, right is the outer boundary. So, this is right boundary and this is the bottom this is a top boundary. And then you have this expression.

This can be easily programmed into Matlab and once you have this matrix here, let us say this is unknown. So, psi can be let us say this is A psi = b so, psi is basically A inverse times b. So, you can easily solve it using direct method to get the values of the potential function.

Maybe you can write a simple Matlab code and see if you have a fixed charge distribution. you can get a potential profile from that.

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So, in this lecture we have discussed that Taylor series expansion and the finite difference method. And we have solved for the Poisson equation with a Dirichlet boundary condition. Thank you very much.