Advanced Mathematical Techniques in Chemical Engineering
Prof. S. De
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Module No. # 01
Lecture No. # 32
Solution of non-homogeneous PDE

Welcome to this session of this class. In the last class we were looking into the solution of spherical polar coordinates using separation of variable and we took up two problems; in the first problem we considered a two-dimensional spherical coordinate with phi symmetry.

The solution we had constituted by the r to the power n and the governing equation we got, which is the Legendre polynomial, is basically an eigen function in the theta direction, and in the r direction we got an Euler's equation. We solved them and constituted the complete solution. In a three-dimensional problem it is no more a phi symmetry, but it will be maintaining periodic boundary conditions in the phi direction, therefore we formulate the eigenvalue problem in the phi direction, which is exactly similar to the cylindrical polar coordinate system - a three-dimensional problem corresponding to theta direction in that case.

Now, since we have formulated the eigen functions and eigenvalue problem in the phi direction, let us look at what will be the formulation for the theta direction and what is the solution of r direction; then we will be multiplying these three functions together and sum them up and we will constitute the complete solution.

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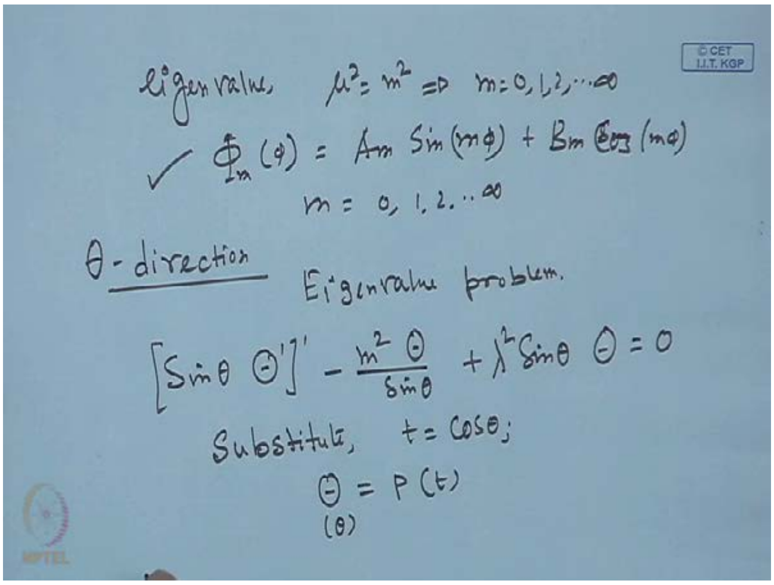

Since we have looked into the phi direction part, now let us look into the theta direction. In theta direction we need to have an eigenvalue problem, therefore we have a negative separation constant; so if you write it down this becomes sine theta theta prime prime of that minus m square theta divided by sine theta plus lambda square sine theta theta is equal to 0. So, this is the equation that we will be getting, we substitute t is equal to cosine theta, so you will be getting capital theta is equal to P of t and capital theta was a function of theta.

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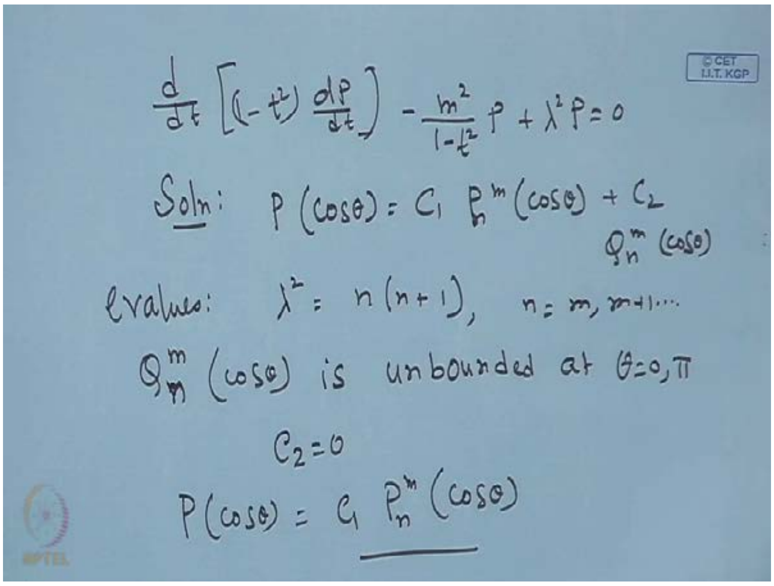

In this form, the equation will be in the form of a Legendre equation, and we have already seen that the Legendre equation becomes d dt of 1 minus t square dP dt minus m square 1 minus t square P plus lambda square P is equal to 0.

This is a Legendre equation, the solution is generated by the Legendre function and Legendre polynomial P of cos theta is equal to C 1 P n m cosine theta plus C 2 Q n m cosine theta, where the Eigenvalues are lambda square is equal to n into n plus 1, where n runs from m m plus 1 up to m plus infinity and Q n superscript m cosine theta is unbounded at theta is equal to 0 and pi - that is the property of the Legendre function.

So, the associated constant must be equal to 0 to have a finite bounded solution, therefore, P of cosine theta is equal to C 1 P n superscript m cosine theta - those are the Eigen functions.

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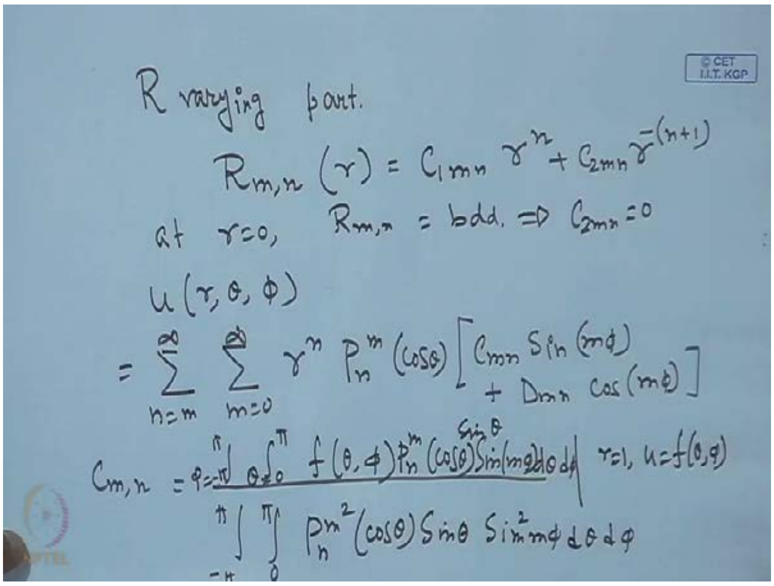

Now, if you solve the R varying part, the solution will be in the form of Euler's equation. We have already seen it earlier, so we write it as C 1 m n r to the power n plus C 2 m n r to the power minus n plus 1, therefore in order to have a bounded solution at r equal to 0, R m n is bounded, so we have the associated constant is equal to 0, so C 2 m n is equal to 0.

We will be getting the solution as u r theta phi, so the solution in the r direction will be C 1 m multiplied by r to the power n, the other constant becomes 0, so this becomes double summation n is equal to m to infinity; this will be m is equal to 0 to infinity r to the power n P n superscript n cosine theta C m n sine m phi plus d m n cosine m phi.

Using the orthogonal property of the sine functions, cosine functions and the Legendre polynomial we will be getting the constant values C m n - from phi is equal to minus pi to plus pi, from theta is equal to 0 to pi, f of theta phi, those are the initial condition; the non-homogeneous boundary condition at r is equal to 1, so using r is equal to 1 your u was some function of theta and phi; using that boundary condition we evaluate this one using orthogonal property, it will become f of theta phi P n m cosine theta sine m phi d theta d phi divided by minus pi to pi 0 to pi is the theta P n m square cos theta sine theta sine square m phi d theta d phi.

We can get the eigenvalues and we can get the integration constants. In the numerator also it will be multiplied by sine theta because the Legendre function will be orthogonal to each other with respect to weight function sine theta, so there will be a sine theta somewhere here in the numerator as well.

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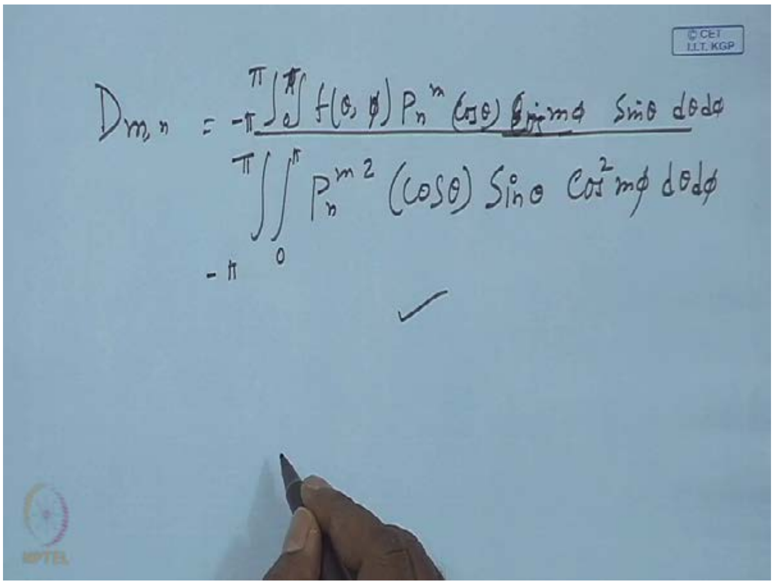

We can get the integration constant D m n as well, the same thing f of theta and phi P n m cos theta sine m phi, this becomes cosine m phi (Refer Slide Time: 08:31) sine theta d theta d phi - this is the weight function and here we will be getting P n m square cos theta sine theta cos square m phi d theta d phi, limits will be theta from 0 to pi and phi from minus pi to plus pi. So, we can evaluate the integration constant D m n and C m n, we will be able to completely solve the problem in the spherical polar coordinate; that goes the solution of partial differential equation in spherical polar coordinate using the separation of variable type of solution.

Now, next what I am intending to do is that we will be starting with the solution of non-homogeneous partial differential equation. Whatever we have done till now is that we have looked into the solution of the nature of the partial differential equation which is homogeneous.

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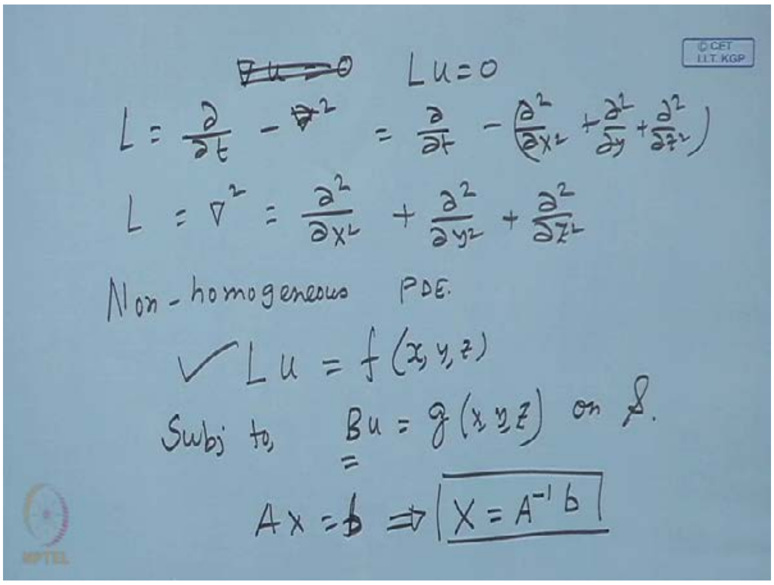

If you remember we have done a solution something like this, L u is equal to 0; we have not solved L u is equal to f, that means this L can be a Laplacian operator, it can be a parabolic operator del del t Laplacian - that means, del del t minus del square del X square del square del Y square plus del square del Z square or it can be entirely a Laplacian like del square del X square plus del square del Y square plus del square del Z square.

Now on, we will be solving the non-homogeneous partial differential equation - the compact form of non-homogeneous partial differential equation will be L u is equal to f, this f can be a function of x y and z, so subject to the boundary condition B, u is equal to in general will be a function of x y z, B is the boundary operator, this is valid on a surface s.

This non-homogeneous partial differential equation, if you bring the parallel of discrete domain, for example, in the matrices it was A X is equal to b where a is the matrix, X is the solution vector, b is the non-homogeneous vector. If you remember whatever we have done earlier, the solution vector is if you take inverse on both sides we get A inverse b.

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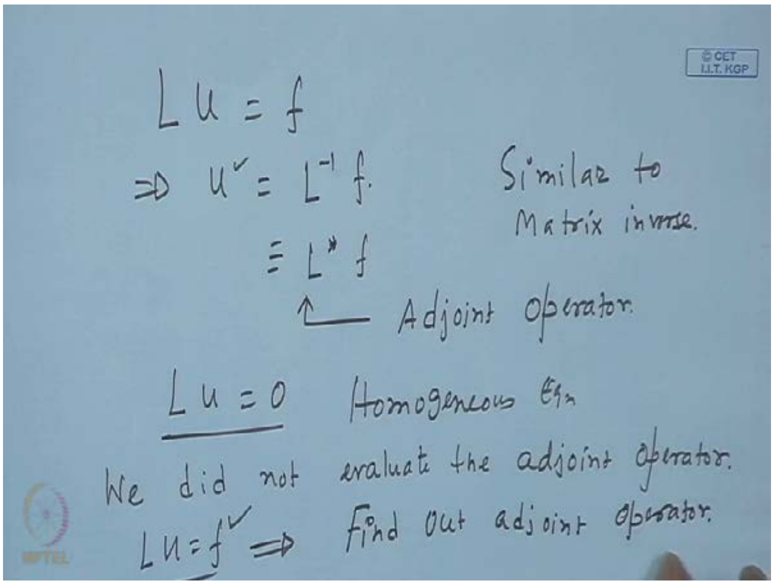

Therefore in the similar case here, the solution of L u is equal to f, you take a inverse operator the solution u becomes L inverse f, so it is similar to matrix inverse; this is equivalent to L star f. What is L star - we made L star as L inverse and this is considered as same adjoint operator.

So, in order to solve the matrix form A X is equal to b, the solution vector was X is equal to A inverse b. Similarly in this case, the solution function is u equal to a L inverse f and we call this L inverse as adjoint operator. So, it is the adjoint operator for the case of solution of non-homogeneous partial differential equation we need to find out and then connect it with the actual problem.

If you remember that whenever we have solved till now L u is equal to 0, a homogeneous equation, we did not evaluate the adjoint operator; what we did, we just worked with the operator and got the solution, but in the case of L u is equal to f when there is a source of non-homogeneity governing equation, you need to find out the adjoint operator.

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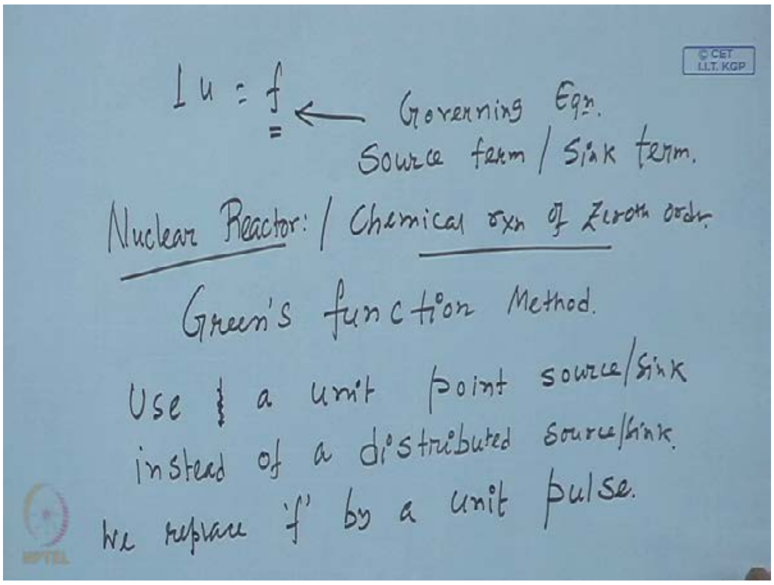

Now, there are certain steps to go through it; if you remember we are solving this problem L u is equal to f. If you want to see what this value of f is, the physical interpretation of f is - this f can be a volumetric source or volumetric sink term. Why it is volumetric - because this non-homogeneity is appearing in the governing equation and as I have mentioned earlier, governing equation is valid throughout the whole control volume. Therefore, this non-homogeneous term must be appearing throughout the whole control volume.

So, it will be either a source term or a sink term. What are the chemical engineering applications of this source and sink term? Consider a nuclear reactor, what happens in a nuclear reactor is that we pack the elements like radioactive element in a cylindrical casing and then we call that as a cladding material; typically the cladding material is stainless steel which will be having a very high melting point that will be in the order of 1450 degree centigrade, just around that.

The radioactive material is packed in a cladding in a tube which is known as a cladding tube and then there is something called positioning rod which using the neutrons, they bombard the radioactive material. The fission reaction starts and it initiates the fission reaction which propagates automatically throughout the whole control volume of the reactor.

That means, there is a source term, heat is generated by this source term and it will be conducted towards outside of the cladding material, then it will be conducted to the outside where there is a cooling fluid that will be circulated in the nuclear reactor. Typically this cooling fluid is liquid metals, for example, liquid lithium or something like that and then the whole energy will be transmitted by the convection and it will be given over to the secondary cycle, this is a part of the primary cycle and it will be given over to the secondary cycle where the turbine will run and the power will be generated; so that is typically the nuclear reactor operation, how nuclear power plant operates.

Therefore, it is extremely important to find out the temperature profile within the nuclear reactor so that under any uncontrollable situations the temperature should not go beyond a particular value, one such criterion may be the melting point of the cladding material that is the stainless steel. If it melts then whole thing comes outside and there will be a possibility of an accident, in order to avoid that we have to monitor the temperature of the wall or the cladding material as a function of time in real time domain and check if there is some problem. If the temperature increases, the appropriate control action should be taken, may be, the circulation of the cooling material should be increased, the flow rate may be increased so that more energy or heat will be dissipated from the reactor and the operation can be again under control.

Therefore, in that particular case there is a volumetric source term that will be appearing in a governing equation and therefore, you will be landing up with a non-homogeneous partial differential equation to solve.

Similarly, if we have reaction engineering's problem where there is a reaction going on in a flowing stream, if you do a mass balance of the reactant and if you have a zeroeth order reaction going on throughout the whole bulk, it is a bulk phenomenon - reaction is occurring throughout at every point in the control volume, therefore it is a bulk phenomenon; there will be a non-homogeneous term that will be appearing in a governing equation. If we are writing its mass balance equation in terms of reactant then this non-homogeneous term that will be appearing in the governing equation will be a sink term. In the earlier example where I was talking about an exothermic fission reaction where energy is evolving throughout the whole control volume of the system, it was a source term because it will be evolving out.

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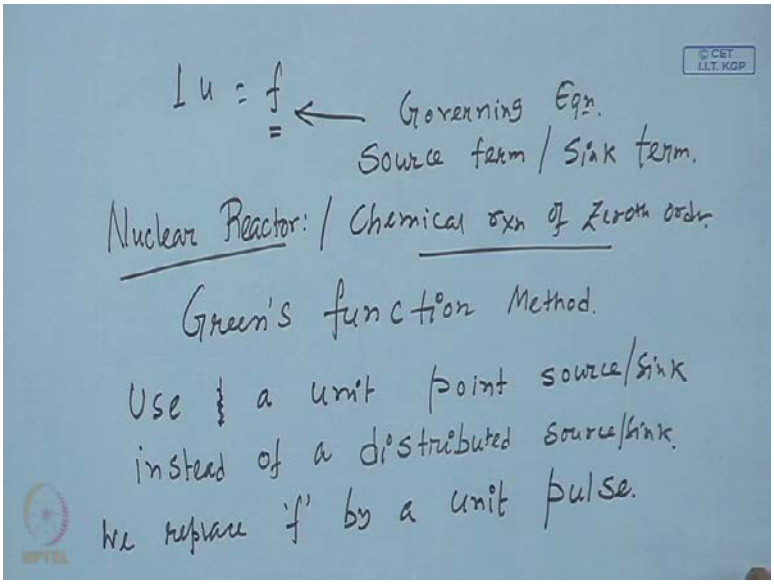

In source term the non-homogeneous term is positive, in case of sink term the non-homogeneous term is negative. So, in those particular cases one can have chemical reaction of zeroeth order kinetics, one can have a sink term here, one can have a source term here. There are many other applications also where you will be having a non-homogeneous governing equation.

So, let us see how we proceed further for the solution of this, the method that is used is called Green's function method. It is difficult to solve this problem keeping this non-homogeneity at a time, so we do some kind of unit source or we use a unit point source, instead of a distributed source or sink throughout the whole volume. In order to simplify the problem, if you remember the f is basically a bulk phenomena - it is occurring throughout the whole bulk of the system, we do not do that - we use a unit point source and try to see how this unit point source influences your solution, for example, this has a corollary of the RTD experiments, Residence Time Distribution experiments in a chemical reactor. If you remember those concepts that we put a die inside a reactor and try to trace out the path of the die, how the die moved and by that we came to a conclusion that how the reactions will be occurring and what are the dead zones in the reactor.

So, we get an interpretation from the tracer experiment by putting a unit pulse there. Similarly in this case, instead of considering the fully distributed sink or source term in your governing equation, we replace the source or sink term by a unit pulse. So what we are doing, we replace f by a unit pulse, so the corresponding solution u is called the Green's function.

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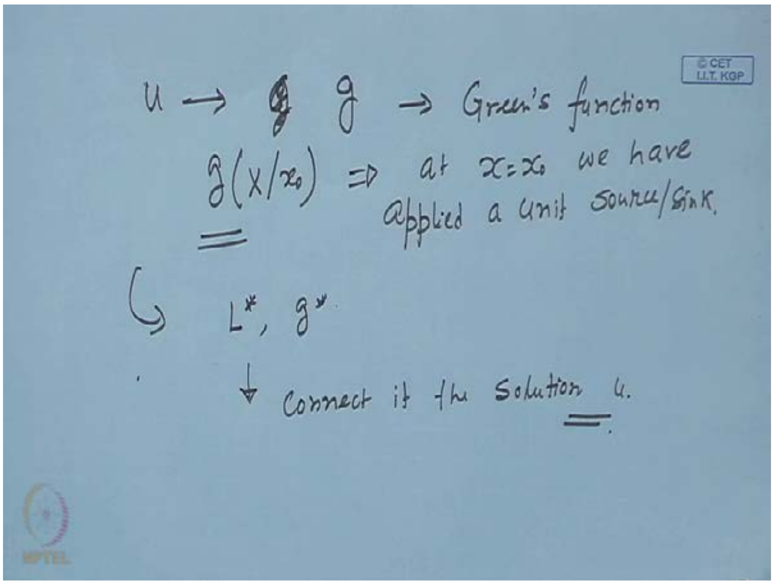

When we replace f by a unit pulse, the u is replaced by Green's function g and we write down g as a function of x slash x naught, that means, at location x equal to x naught we have applied a unit source or sink. Therefore, we define the Green's function g where the distributed non-homogeneous term is replaced by the unit source or unit sink term. Once we get that g we find the adjoint operator and adjoint Green's function, so we evaluate adjoint operator, adjoint Green's function and then we connect it to the solution u. Therefore, let us look into the steps of solution of non-homogeneous partial differential equation.

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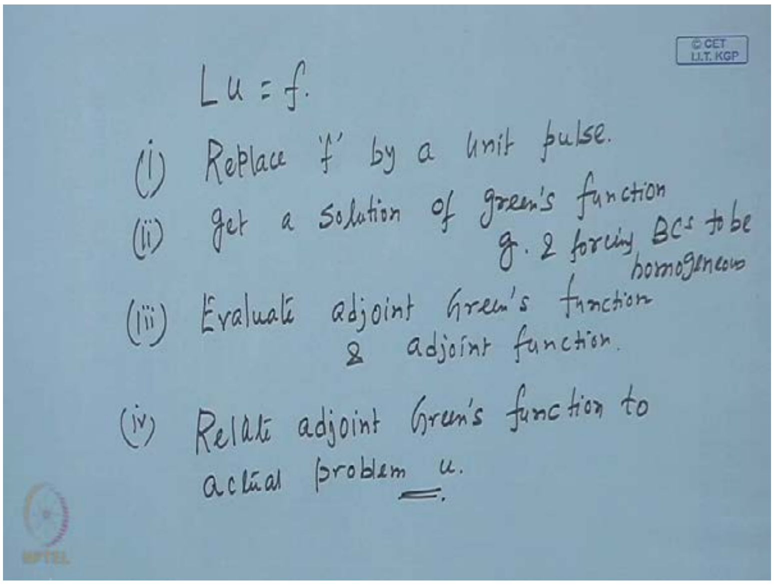

If you remember our aim is to evaluate L u is equal to f, so step 1 is to replace f by a unit pulse - get a solution whenever you are replacing f by unit pulse, u will be replaced by g, that is, the Green's function; so get a solution of Green's function g. Then evaluate adjoint Green's function and adjoint operator. Actually if we remember we found out the adjoint operator and adjoint function, both of these will be coming out automatically.

Now, remember one more thing, whenever you are formulating a Green's function by doing these steps, the non-homogeneous term is replaced by the unit pulse, but at the same time you are forcing the boundary conditions to be homogeneous, that means, suppose the boundary conditions of the original problem are non-homogeneous we force them to be homogeneous and we are dealing with these things by keeping only one non-homogeneity at the governing equation.

So, we do not want to get any interference from the non-homogeneous terms appearing in the boundary conditions, we are dealing with only one non-homogeneity and that non-homogeneity is occurring in the governing equation when it is replaced by a unit step function.

Therefore, we are keeping a unit step function in the governing equation in place of non-homogeneous term f and then we are formulating the Green's function by replacing u by g, but at the same time we are forcing the non-homogeneous boundary conditions to vanish because we would like to trace what is the effect of unit step function in the governing equation, how it will translate its variation over the actual solution; we do not want any interference from other non-homogeneities appearing in other boundary conditions.

So, we get a solution of Green's function g by replacing f by a unit pulse and forcing boundary conditions to be homogeneous. We evaluate the adjoint Green's function and adjoint function and then we connect or relate adjoint Green's function to actual problem u. So, these are the steps we are going to follow in order to solve the non-homogeneous partial differential equation.

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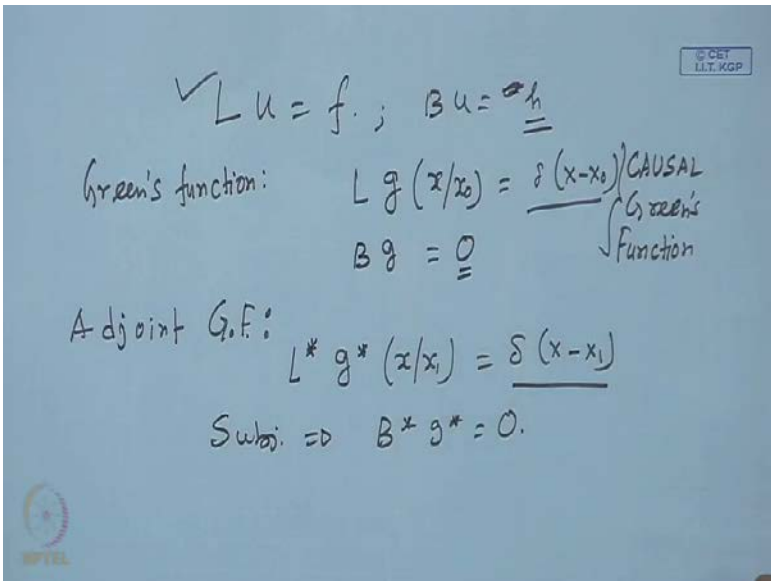

Let us look into the problem and see the formulation of adjoint Green's function. If L u is equal to f is the problem we are looking for the solution, then the Green's function formulation will be L of g x slash x naught is equal to delta x minus x naught.

So, what have we done? We have replaced the non-homogeneous term in the governing equation by a unit source term delta. It is given by a Dirac delta function and the unit step function or the source term is placed at x is equal to x naught, so it is a Dirac delta function and we replace u by g. The boundary operator was B u is equal to some h which will be a general function of x y z - it is non-homogeneous, but in this case when we are formulating the Green's function, the boundary conditions on g is equal to 0.

We force the non-homogeneities in the boundary condition to formulate the governing equation of g, then we formulate the adjoint Green's function, this will be nothing but L star g star x slash x 1 delta x minus x 1.

So, in this case we find out the adjoint operator, we find out the adjoint Green's function where delta x minus x 1, x 1 is the location where we are putting the unit source in case of adjoint Green's function and of course, we put the boundary condition of g star - also homogeneous. We connect the adjoint Green's function with the actual problem and see the solution; actual problem is L u is equal to f.

Now this Green's function, the first Green's function is known as the Causal Green's function; this is adjoint Green's function (Refer Slide Time: 30:01). Now, let us look into some of the important property of the unit step function or Dirac delta function.

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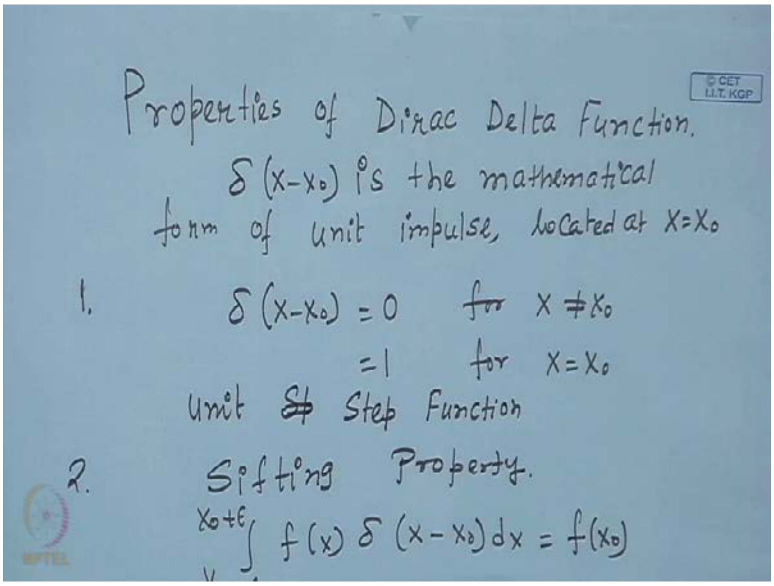

The properties of Dirac Delta Function is delta x minus x naught, it is the mathematical form of unit impulse and that is located at x equal to x naught. The first property should have that delta x minus x naught must be equal to 0 for x not equal to x naught and it is 1 for x equal to x naught. Therefore, at the location x is equal to x naught this value is 1 so it is called unit step function, for the other values of x naught it is 0.

The second one is important; this is known as Sifting Property, this is f of x delta x minus x naught dx over the domain x naught minus epsilon to x naught plus epsilon, this will be simply f of x naught. If we integrate some function multiplied with the Dirac delta function, since the Dirac delta function is equal to 0 apart from x naught, so x naught minus epsilon and x naught plus epsilon where epsilon is extremely small number; the value will be returning the value f of x naught since it will be having a value 1.

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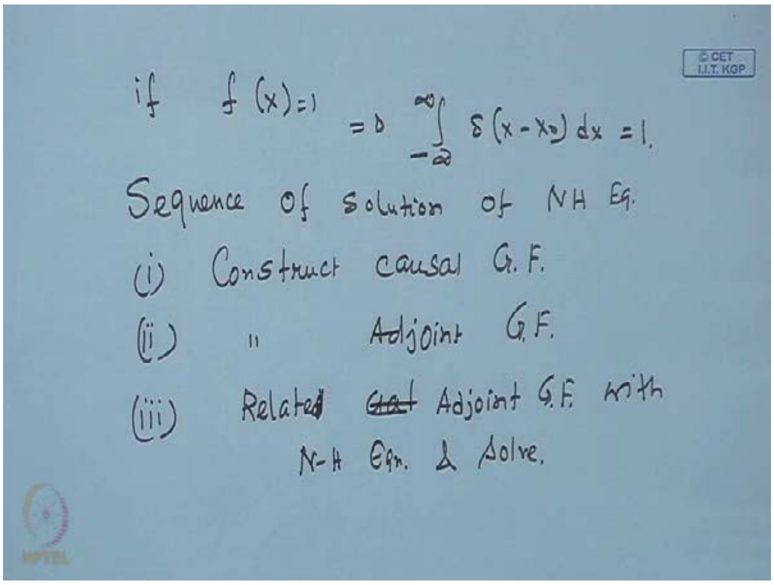

If f of x is equal to 1, then minus infinity to plus infinity delta x minus x naught dx should be is equal to 1. Next, we move forward to the sequence of the solution that we have already seen.

Let us write it down more explicitly, of non-homogeneous equation first one is construct Causal Green’s function, second step is construct adjoint Green’s function, third step is relate adjoint Green’s function with the non-homogeneous equation and solve; these are the different steps that we are going to follow.

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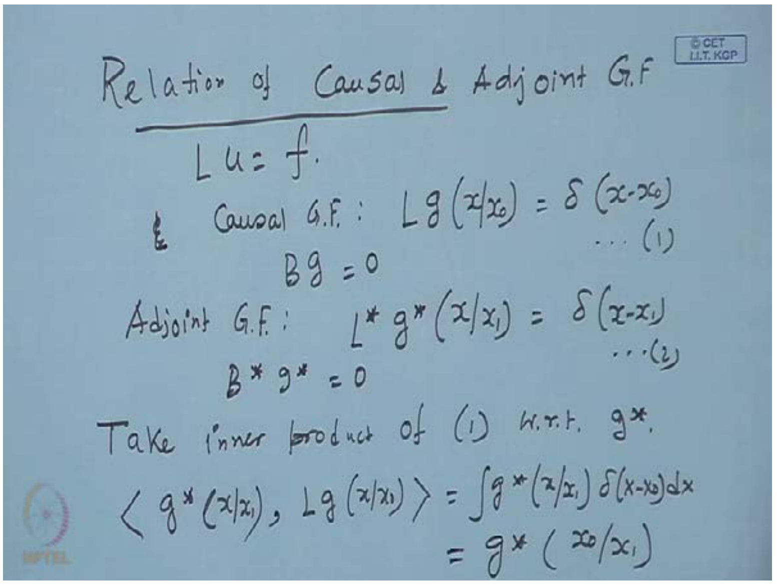

Now, let us do one small exercise to find out the relationship of adjoint Green's function and Causal Green's function. Let us do a small exercise, then the relationship between the Casual and adjoint Green's function becomes very clear.

We are going to solve a non-homogeneous equation - L u is equal to f. The first step is we construct the Causal Green's function, so Causal Green's function will be L of g x slash x naught is equal to delta x minus x naught, that is 1 subject to boundary condition B of g should be is equal to 0. Then adjoint Green's function will be L star g star x slash x 1 is equal to delta x minus x 1, is equation number 2 with B star g star is equal to 0.

We force the boundary conditions on the Green's function and the adjoint Green's function to be homogenous. In case of Causal Green's function we apply the unit pulse at the location x equal to x naught and in case of adjoint Green's function we put the unit impulse at the location x is equal to x 1; then we take the inner product of 1 with respect to g star and see what we get.

So, inner product of g star x comma x 1 comma L g x slash x naught is equal to, in case of continuous function inner product becomes an integral, we have already done earlier, so this becomes integral g star x slash x 1 delta x minus x naught dx. Now, we are having just one-dimensional problem, so g star, if you use the sifting property the integral of f of x delta x minus x naught d x will be f of x naught; so, this will be g star x naught slash x 1.

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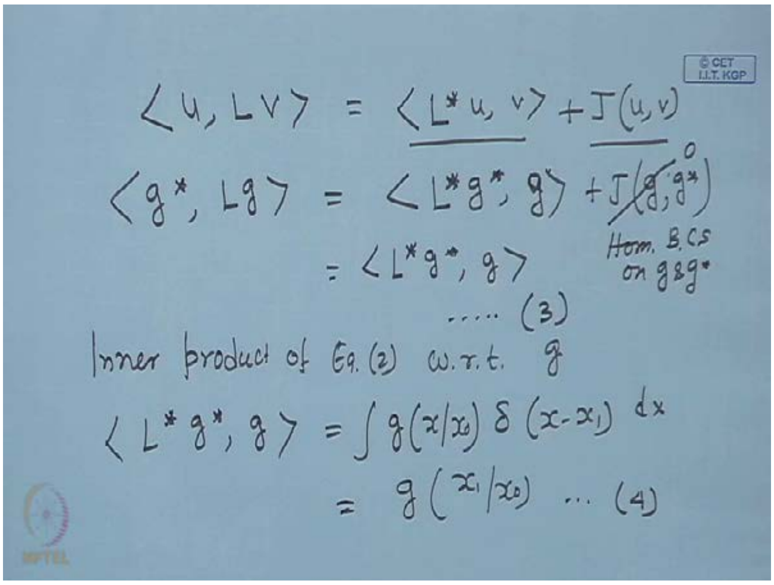

If you remember when we are looking into the adjoint operator, inner product of u and L v is nothing but L star u comma v plus J u v, so this is how we get the adjoint operator and this is the bilinear concomitant.

So, inner product of g star and L g will be L star g star comma g, so that will be the inner product of these two, plus bilinear concomitant between g and g star and bilinear concomitant of g and g star will be equal to 0 simply because we have homogenous boundary conditions on g and g star.

We have already seen that this will be nothing but inner product of L star g star comma g; that is the form when you take the inner product of equation 1 with respect to g star, this is equation number 3.

Then we take inner product of equation 2 with respect to g, if you do that we get, L star g star comma g is equal to integral g x slash x naught delta x minus x 1 dx, so using the sifting property of the Dirac delta function this becomes g x 1 slash x naught. This is equation number 4, and the equation we have obtained earlier - this is equation number 2 a; now subtract equation number 4 from equation number 2 a, if we do that then let us see what we get.

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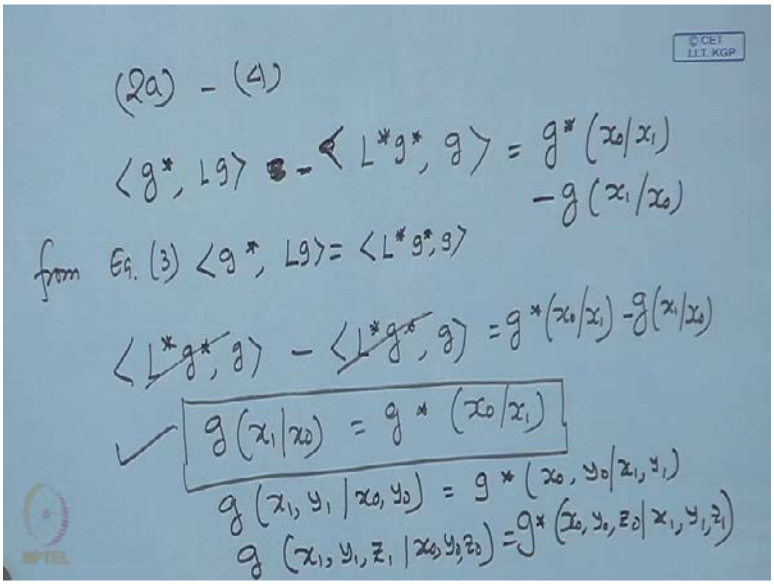

If you subtract 2 a minus 4 we will be getting as inner product of g star and L g minus inner product of L star g star and g is equal to g star x naught slash x 1 minus g x 1 slash x naught. We have already proved in equation number 3 that g star L g is nothing but inner product of L star g star and g, this is from equation 3.

Now we put it here, so this becomes L star g star comma g minus L star g star comma g is equal to g star x 0 slash x 1 minus g x 1 slash x 0. If we see the left hand side, both of this will vanish, what we get is that g of x 1 slash x naught is equal to g star x naught slash x 1; so, this is the relationship between g and g star. Same relationship is valid for three-dimensional problem, two-dimensional problem, so g x 1 y 1 slash x naught y naught, we can prove it g star x naught y naught slash x 1 y 1; for three-dimensional problem g x 1 y 1 z 1 x 0 y 0 z 0 is equal to g star x naught y naught z naught x 1 y 1 z 1.

So, that is a general relationship and this gives a relationship between g and g star, that means, you need not to solve g star separately, you can solve g first and then just change over the superscript and you will be getting an expression of g star - so you need not to solve g star separately by solving the differential equation, you solve by solving the differential equation g and then change over the superscript you will be getting an expression of g star. Then you connect g star with the original problem u, how will you do that? We will just have one demonstration.

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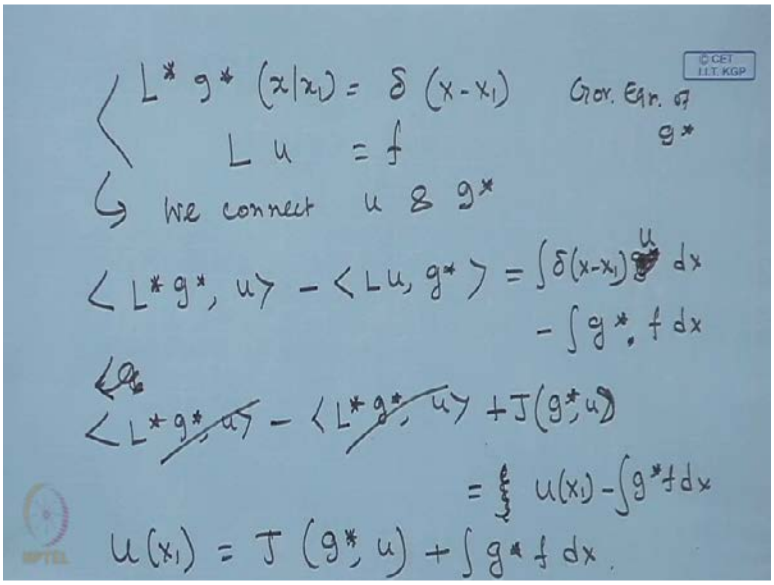

So, L star g star x slash x 1 is equal to delta x minus x 1, this is the governing equation of g star and we connect L u is equal to f - the original problem, so we connect u and g star. How we connect u and g star? We connect u and g star by taking the inner product of this equation with respect to u, by taking the inner product of this equation with respect to g star and then we will subtract.

So, this becomes inner product between L star g star u minus inner product of L u and g star is equal to delta x minus x 1 g star dx minus g star multiplied by f dx. If you open up this equation as we have done earlier, this becomes u L star g star is nothing but L u or you can do it in the other way, L star g star comma u is nothing but L star g star comma u, this is nothing but inner product of L u and g star, is nothing but inner product of g star and L u and we write it down as L star g star comma u plus bilinear concomitant g star and u is equal to, it should be multiplied by u, so u of u integral delta x minus x 1 d x is u of x 1 minus integral g star f d x.

Now, these two will vanish, the bilinear concomitant term will be present if u is having some of the non-homogeneous boundary condition, so let us put it down in this way - u of x 1 is equal to J g star and u plus integration g star f dx.

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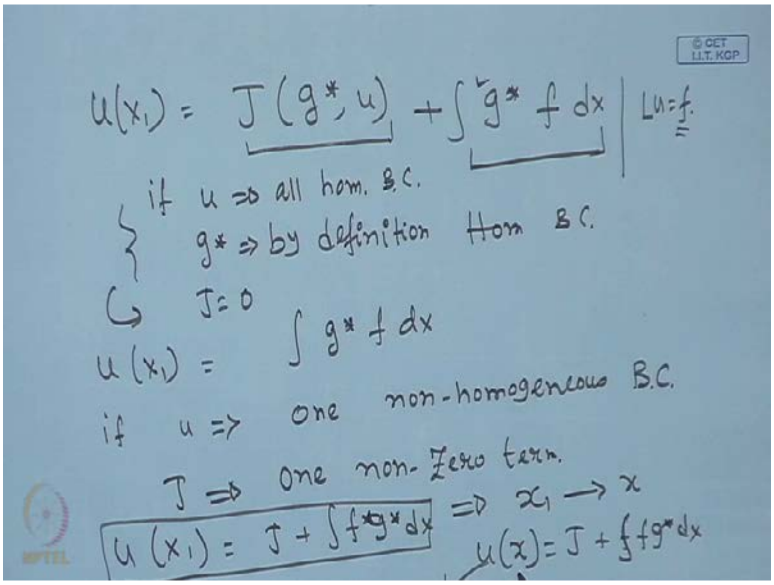

So, let us explain it more clearly, u of x 1 is equal to inner product of g star and u plus integral g star f dx. Let us look into the original problem, remember the original problem was L u is equal to f.

In this equation if you remember the steps, first we solve the Green's function by constructing the Causal Green's function, once we get the causal Green's function we change over the subscript and get the expression of adjoint Green's function by the derivation we have done just few minutes back that, g of x 1 slash x naught is equal to g star of x naught slash x 1. By changing the subscript, we will be solving an actual problem after sometime, so while changing the subscript one can get an expression of g star from expression of g itself, you need not to solve g star from the differential equation.

The expression of g star is known to you, the function f is a known function, so this function here we carry out this integral and you can carry out this integral quite analytically. On the other hand, let us look into the bilinear concomitant term, bilinear concomitant term corresponding to homogeneous boundary conditions will vanish; for the non-homogeneous term one or two terms will be present depending on the number of non-homogeneity.

If u has all homogeneous boundary conditions, g star by definition has homogenous boundary condition, in that case J will be equal to 0 and you will be getting solution as u of x 1 g star f dx. If u is having one non-homogeneous boundary condition then your J will be having one non-zero term.

In that case J will be not equal to 0 and u x 1 will be J plus integral f g star dx. If u has two non-homogeneous boundary conditions, then J will be having two non-zero terms. Once you get that you will see that right hand side will be entirely a function of x 1, then change the running variable x 1 to x, you will be getting an expression of u x as J plus f integral f g star dx - we change the running variable from x 1 to x and you get the complete solution.

So, that way one will be getting the complete solution from the Green's function method and complete non-homogeneous partial differential equation. The vital clue of all these steps is obtaining or formulation or getting the expression of Causal Green's function; once you get the expression of Causal Green's function you can get the expression of adjoint Green's function, then the connection of the adjoint Green's function with the original problem becomes very simple. Now, let us look into the different steps of how one can get the causal Green's function.

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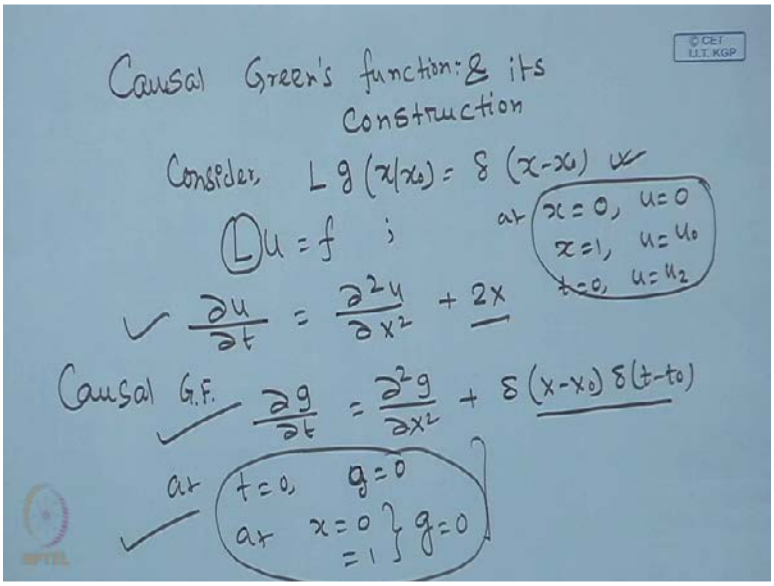

Construction of Causal Green's function - consider L g x slash x naught is equal to delta x minus x naught. How you will be getting this if you have the original problem L u is equal to f? I will just take up an example, let us say del u del t is equal to del square u del x square plus 2 x, so f is 2 x. Then causal Green's function will be del g del t is equal to del square g del x square plus the non-homogeneous term has to be replaced by a Dirac delta function, it will be x minus x naught delta t minus t naught. Why will there be two terms here? Because, you have a two-dimensional problem, t and x are independent variables, so at the location x minus x naught and t minus t naught we apply the Dirac delta function.

Suppose the boundary condition is, let us say, at x is equal to 0 and 1, x is equal to 0, u is equal to 0; and at x is equal to 1 u is equal to u naught; at t is equal to 0 u is equal to u 2. Then, in the Causal Green's function we force all the boundary and initial conditions to be homogenous, at t is equal to 0 we have g is equal to 0 at x is equal to 0 and 1 we have g is equal to 0, so we force all the boundary conditions to be homogenous and we will be constructing the Causal Green's function.

This is how a Causal Green's function is obtained from an original problem. So, there are two characteristics one has to remember for the construction of Causal Green's function: first one, the non-homogeneous term of the governing equation must vanish - that is number one; the L of original problem and L of operator of the Causal Green's functions are identical, non-homogeneous term has to be replaced by the Dirac delta function or unit step function. The initial and boundary condition of the original problem has to be replaced by the homogenous conditions in the same form; if at x is equal to 1 you had del u del x is equal to 0 in the Causal Green's function, also you should have at x is equal to 1 del g del x is equal to 0.

We take the corresponding form of the boundary conditions, but make them homogeneous. So the idea is, in the case of construction of Causal Green's function we make the operator same - number one, number two is the non-homogeneous term in the governing equation must be replaced by a Dirac delta function, and number three is that, form of the boundary condition remains same but in case of Causal Green's function all the boundary conditions are forced to be equal to 0.

So I stop it here in this class; in the next class I will take up this problem forward and we will be solving a Causal Green's function from given an operator L u is equal to f.

Thank you very much.