Mathematics for Chemistry
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Lecture - 14

The next topic in this course is differential equations, and this will be the topic for the next 8 to 10 lectures. Now differential equations are seen almost everywhere in chemistry and physics and you would have encounter them in various areas already. But in this course what we will do is we will start from the basics of differential equations, and then we will see what are the techniques to solve the differential equations.

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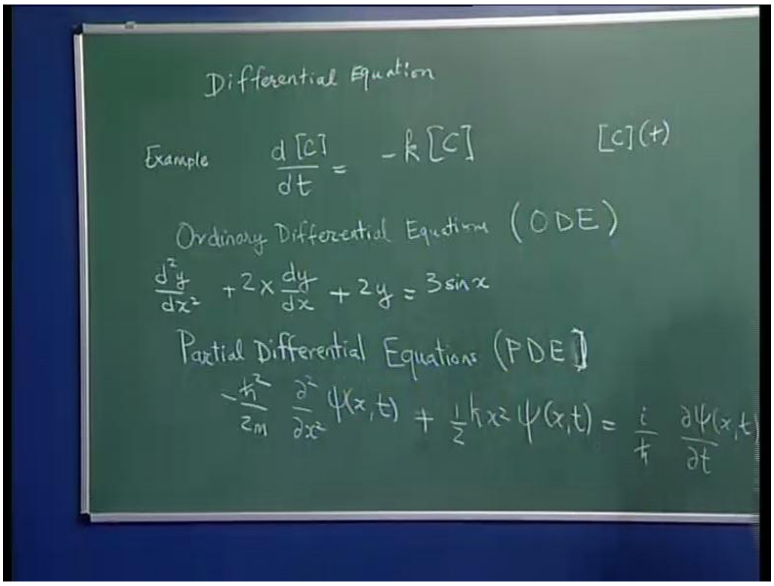

Now, a differential equation by definition is an equation that has a derivative of function in it. So, a differential equation is some equation that has one or higher derivatives and powers of derivatives in it. So, it is like an algebraic equation, but instead of just having variables you also have derivatives in it. So, for example you can have d (C) by d t is equal to minus k (C), where C could be a concentration that changes with time. So, this is an example, so this is an algebraic equation where not only C there, but also derivatives of C with respect to time. So, we say that you have see that C has a function of t and not only do you have that function, but you also have the derivative of that function appearing.

Now, there are two kinds of differential equations that are commonly encounter, the first is ordinary differential equations and we will be using the a short notation ODE, Ordinary Differential Equations and this should be contrast with what are called as Partial Differential Equations. So, we have ODE is and PDE is and these are the two types of differential equations that are commonly encountered. Now, the only difference between these two is that in an ordinary differential equation, this is a it is the normal derivatives that appear, whereas in partial differential equation the partial derivatives appear.

So, this an example of an ordinary differential equations, so another example is we can have d y by d x 2 x d y by d x plus d square y by d x square plus 2 y equal to 3 sin x. So, this is an example, this is then differential equation because it is an equation containing y, y, x and derivatives of y, with respect to x, but all the derivatives that appear are the normal derivatives and so this called an ordinary differential equation whereas, a partial differential equation do the classic example, is the time dependent Schrodinger equation you have a d square x t plus you can have a plus half is equal to i by h cross.

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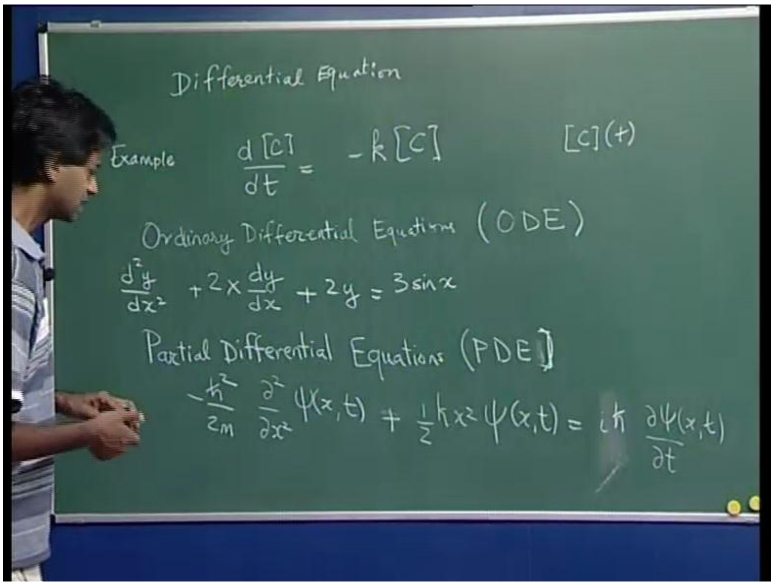

So, this is an example of a partial differential equation, you can have a other forms of partial differential equation. Other the more typically used one is one where h crosses is in the numerator i h cross. Now in this you notice that here psi is a function of x and t it is a both x and t. So, you have two independent variables x and t and psi is a dependent variable and this differential equation involves partial derivative with respect to x and partial derivative with respect to time.

So, this is called the partial differential equation. Now, if in this course you would not to be looking explicitly at both kinds of differential equations will be mostly working with ordinary differential equations, but occasionally we will refer to partial differential equation.

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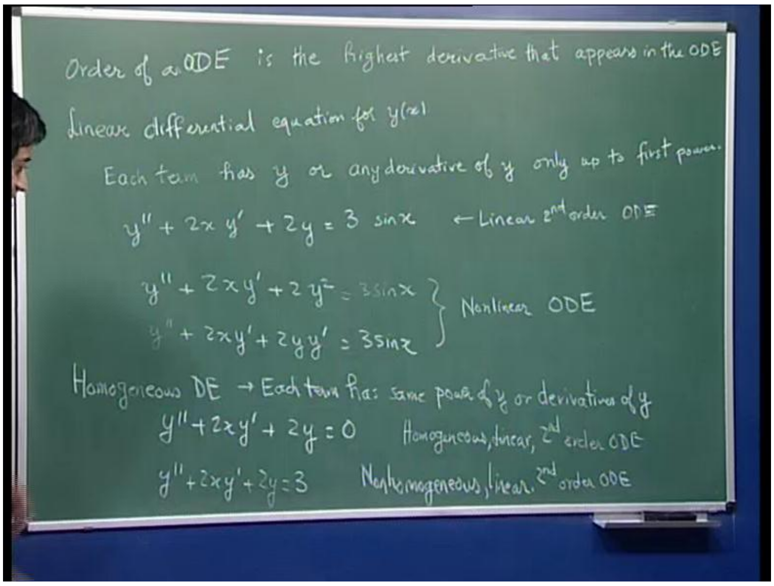

We will see how some of the methods that we are doing are used for partial differential equations. So, we want to be explicitly doing partial differential equations, separately from ordinary differential equations. Next what is a next we have the concept of the order of a differential equation and let us restrict all this two ordinary differential equations. So, all that all these saying in the next in the in the following lectures, we will be restricted to ordinary differential equations unless explicitly specified.

So, the order of a differential equation of an ODE is the highest derivative that appears in the O E D. So, you look at so suppose you ask what is the order of this differential equation? The highest derivative that appears is the first derivative. So, this is a first order differential equation and then in this case the highest derivative that appears is the second derivative. So, this is the second order derivative second order differential equation.

So, this is a first order O D E whereas, this is a second order O E D. So, that is what is meant by the order of a differential equation. Now next there is a commonly used phrase which is a differential equation or linear differential equation. So, what is a linear differential equation? A linear differential equation is one and which each term has a y or differential equation and let say for y of x so if y is a dependent variable and x is a independent variable.

Then the differential equation is said to be linear, if each term has… So, again I will make it explicit. So, if you look at this differential equation, the first term has second derivative of y, but it has only first power. So, we do not have so and the second term has first derivative of y, third term has just y. So, I write that as y double prime plus 2 x y prime plus 2 y equal to 3 sin x.

So, this is a linear differential equation because each term has a power of y that is only 1 or 0 so it has only 1 or 0 power of y secondly, So, what is an example so this would be a linear second order O D E. So, it is a linear because it has y only so each term has y or derivative of y only up to power 1 and it is second order because the highest derivative that appears is 2.

And an example of non-linear differential equation is suppose I had y double prime plus 2 x y prime plus 2 y square. Now notice that this term has y square, so this becomes non-linear. Similarly, if I had two y, y prime now this term has one y and y prime. So, effectively it has y to higher order. So, this is also a non-linear differential equation, these are non-linear O E D.

So, these are the various terminology that I used, there is one more terminology that is used and that is called homogenous differential equation. Now you can look at this equation, now each term has the same power of y. So, this term has y to first power, this term also has y to first power, this term also has y to first power, this term has no y. So, homogenous equation has each term has same power of y or derivatives of y. So, for example, if you had something like y double prime equal to 0.

So, each term has one power of y so this is a homogeneous second order O E D. So, this is a homogenous linear second order O D E. On the other hand, if you had y double prime equal to 3 and this is non homogenous it turns out to be linear second order O D E. So, the term that makes it non homogenous is this 3, because this does not have any power of y. So, each of these has one power of y, but this does not have any power of y. So, that makes it is in homogenous. So, for we have look that various forms that differential equations take and we have named follow of them.

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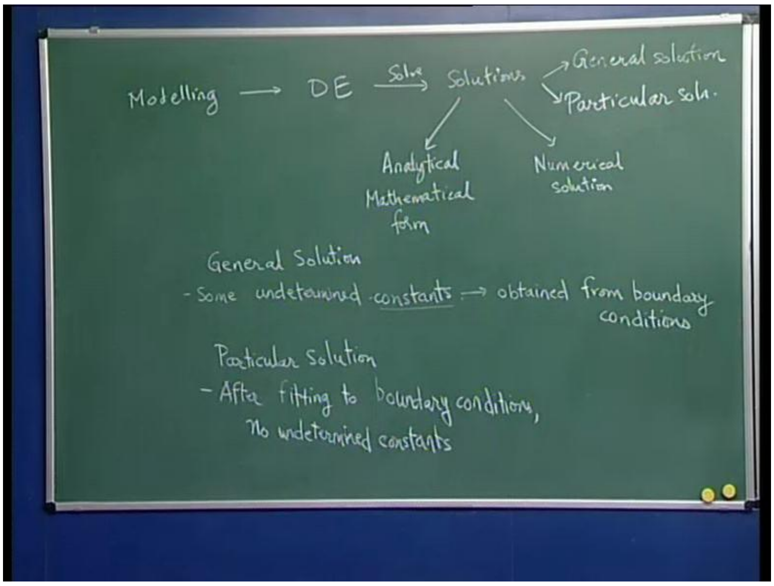

Now one of the thing is you do with differential equation has to actually solve it, and that will be the main topic of the next few lectures. Before that I will talk about what are the various kinds of solutions that you can have two differential equations? Before we go into solutions of differential equations I want to mention one thing, and this is that in most cases in real scientific research problems. The hardest part is to actually set up the differential equation.

So, the process by which you set up you model your system in the form differential equation is the modeling part. So, when you model your system and that is when you get your differential equation. And this is often the hardest part in many scientific research problems and then once you get the differential equations you solve it to get the solutions. So, once you get the differential equations, then you have to solve the differential equations. And when you solve the differential equation you get solutions and these solutions are of two kinds. The first is called the general solution and the second is the particular solution. So, when you have a differential equation, you solve it you will get the general solution and the particular solution.

We will briefly discuss what this meant by general and particular solutions. Before that I want to say that, we already said that modeling your system has a differential equation is often the hardest part in any scientific problem. But, once you have the differential equation, then there are various procedures to solve it. Now in some cases you can actually get a solution in a closed mathematical form. So, this solution can be either analytical, analytical means you have a mathematical form of solution or it can be in some cases it is not possible to get an analytical solutions, you cannot write it some form of some function.

And in those cases you use the numerical solutions, where you essentially get the values of the function at various values of the independent variable. So, whenever you are not able to get an analytical solution, you go for the numerical solution. And this is one of the most commonly used techniques in all sciences in engineering. We will be in this course we will be restricting ourselves, mostly to the analytical, mostly to those cases where you can write a analytical mathematical solution.

So, when you can write this analytical mathematical solution, then we said that there are two kinds of solutions, one is called the general solution and the other is called the particular solution. So, the general solution has a property that it has some undetermined constants and these constants are obtained by from boundary conditions. And particular solution is after fitting to boundary conditions. So, after fitting to boundary conditions, it has no undetermined constants.

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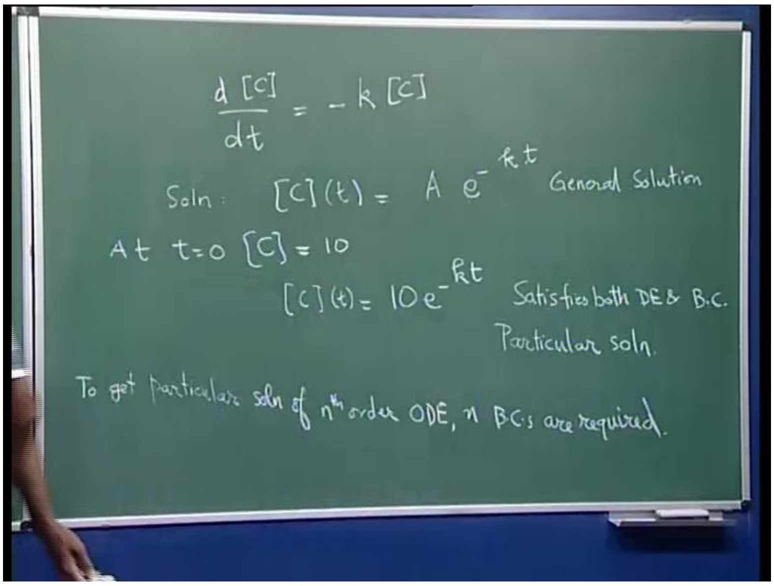

So, the general solution will typically have some undetermined constants whereas, a particular solution will have no undetermined constants. And in order to go from the general solution to the particular solutions, you have to apply the boundary conditions. So, let us take an example suppose you take d equal to minus k (C). So, this is a differential equation, this is an O D E. Solution, C as a function of t is equal to some constant e to the minus k t. So, this k is the same as this k and you can show that if you take this if you take that, now if I take this and I substitute in this d (C) by d t and I will get d (C) by d t is minus k times C.

So, this satisfies a differential equation for all values of A. So, whatever be my value of A, it will satisfy that the differential equation and this is called the general solution and A is the undetermined constant. Now suppose I say that at t equal to 0, C equal to 10. then you can show that C of t is equal to 10 times e to the minus k t. Now this is a differential equation, in this formula for C satisfies the differential equation, you can show that if I take the derivative of C.

I will get exactly minus k times C, but it also satisfies a condition and that when I put t equal to 0, then this term will go away, so C of 0 equal to 10. So, it satisfies both differential equation and boundary conditions. And this is called a particular solution. So, we have a general solution and we have a particular solution and to go from the general solution to the particular solution, we applied the boundary conditions.

Now, the question is how many boundary conditions to be need? In this case we needed one boundary conditions, is this it will be always need only one boundary conditions or other cases when we need more than one boundary condition. And the answer is quite straight forward. So, if for to get particular solution of nth order O E D n boundary conditions are needed.

So, it is quite straight forward, if you have an nth order differential equation then you need n boundary conditions in order to get the particular solution. So, if you do not n boundary conditions then you cannot solve, you cannot get the particular solutions.

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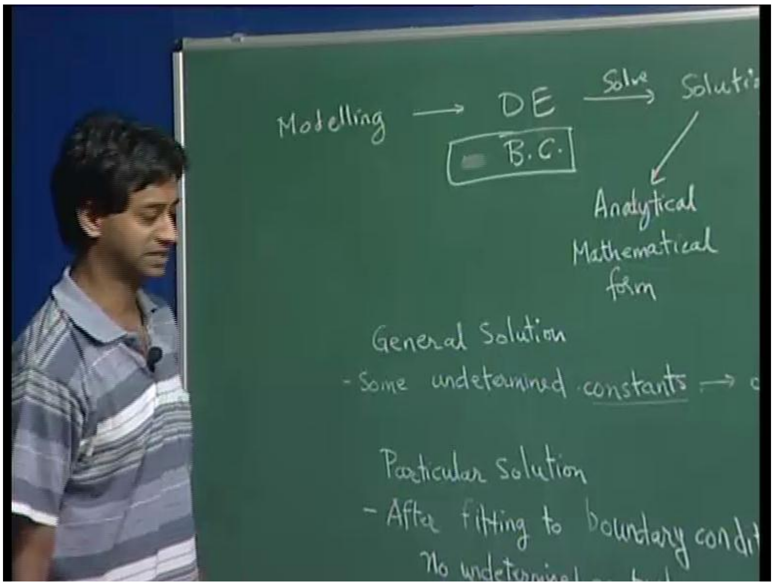

So, we have the general solution and the particular solution and then and now next what we will try to do is to try to actually solve the differential equation. We if you are so if you want to specify your problem completely, not only is that important to get the differential equation, but you should also mention the boundary conditions. So, you also need to specify the boundary conditions. So, full pledged mathematical modeling of your system will involve, both a differential equation and the boundary conditions.

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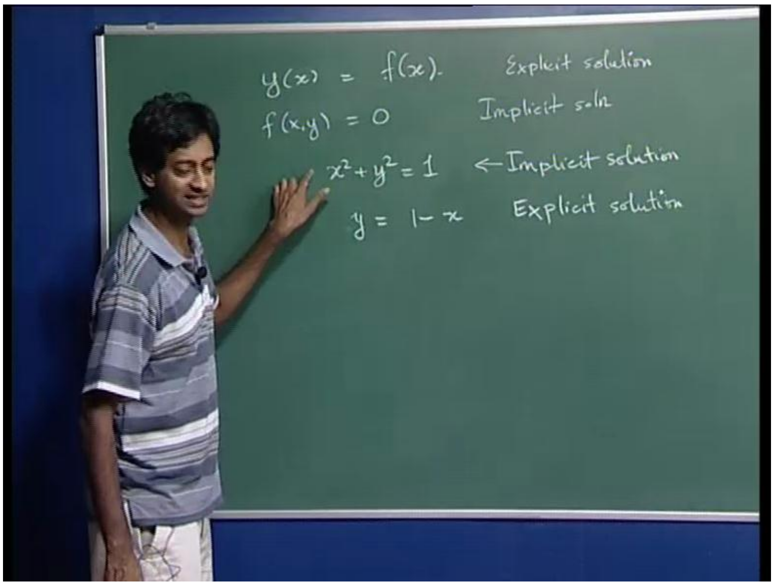

So, next let us try to look at simple ways of solving differential equations. So, now our goal is to find the solution of differential equations, before we going to that let me just briefly mention that there are you can have a solution in an explicit form. So, if you have a differential equation involving y of x, your solution can be of the form y of x equal to something.

This is called an explicit solution some function of x. So, this is explicit solution, an in some cases it is not possible to separate y and x is not to possible to let write y of x has something, you might have some function of x and y equal to 0 and this is called the implicit solution. So, for example, you might have a x square plus y square equal to 1. This is an implicit solution. So, this is some relation between y and x, it is not written as y of x is something. So, this is an example of an implicit solution or you can have an explicit solution of the form, y is equal to 1 minus x, this is explicit so in some cases it turns out that you have differential equation the solution to the differential equation can be expressed as a as some equation and involving x an y.

And in some cases you can separated into an equation where you have only y on the left and you have x on the right. So, the case is where you can separate it in this form you call this an explicit solution in this case you called it implicit solution.

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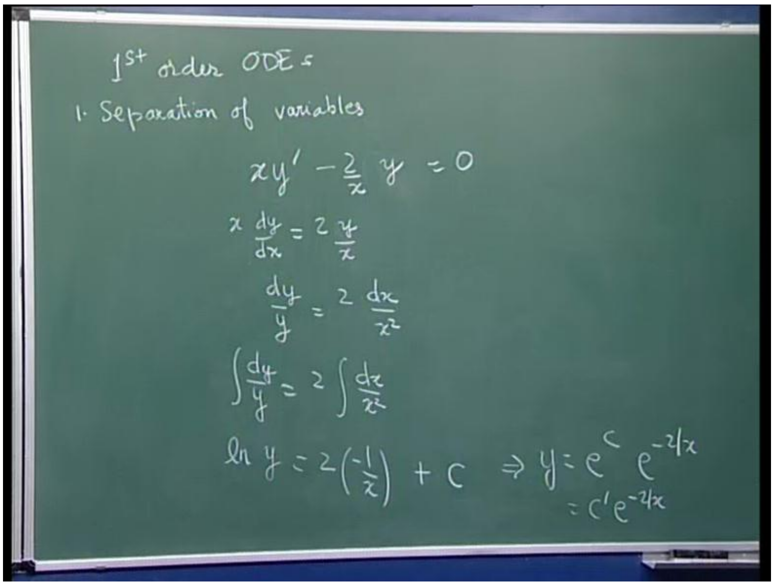

So, it means that y and x are related, but you cannot separate it in this form. Now let us go and look at ways to solve. So, to solve differential equations, we will start with first order O E Ds. so a first order O E D means the highest derivative, that appears in your equation is one so you cannot have a second derivative appearing in a first order differential equation. So, how do you go about solving first order differential equation?

Now the first thing you will try to do is, what is called as separation of variables. So, I will illustrate this with an example, so for example, if you have x y prime minus 2 x y equal to 0. So, you have a differential equation of this form. Now what we will do is you will say that this is x times d y by d x is equal to 2 x y and then what we will say is that we will make this 2 times, this make it is slightly more complicated. We will say 2 by x y equal to 0. So, then we will say is equal to 2 y by x.

Then what you do is you take the all the terms involving y to one side and take all the terms involving x to the other. So, it is a d y by y is equal to twice d x divided by x square. And then the next step is two integrate both sides now this involves only y, this involves only x. So, we can carry out this integrals. So, when you integrate both sides you will get integral x square so integral d y by y is natural log of y and this is twice, this is d x by x square is minus 1 by x.

And you can have some constants of integration. So, adding any constant will not change the if I had any constant, I take a derivative, the derivative of the constant is 0. So, I can always add a constant and this is your undetermined constants. So, the solution can be written in this form and if you can write this as y is equal to e raise to C minus 2 by x and C is arbitrary. So, e to the C is also arbitrary, so you can write this as C prime e to the minus 2 by x. So, this is a general solution. So, the general solution has been found and based on the boundary conditions have the problem, you can solve, you can get the particular solution. So, the strategy here was to separate the variables.

So, you put you bring all the terms involving y on one side, all the terms involving x on the other and once you would once you have done that you can integrate both sides and you can write the solution. So, this is the first thing that you would to try whenever you have differential equation, whenever you have any differential equation, first order differential equation you try to separate the variables .

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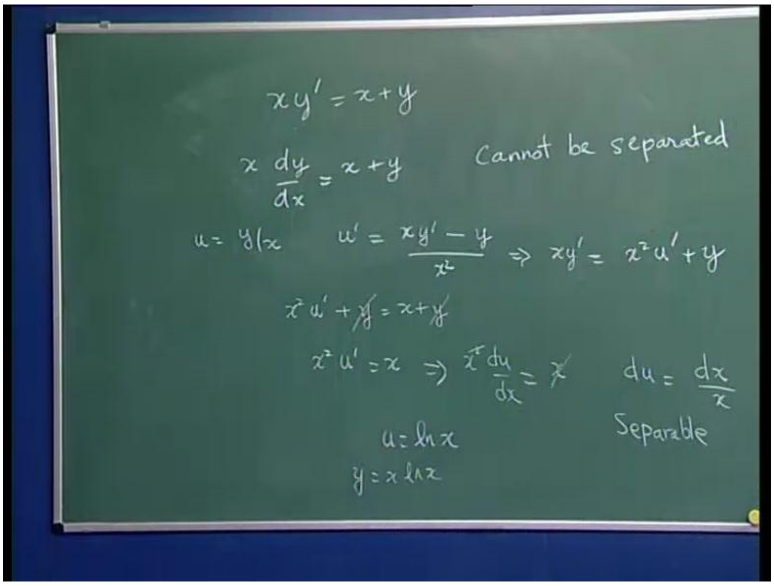

And in this case fairly straight forward. Now in some cases you can do a change of variables and that can bring the equations to separable form, so for example, if you have x times y prime equal to x plus y. So, if you look at this differential equation then it does not look as that so it can be written in separate form. So, if you try to bring the y terms on this side, you want to be able to separate it into terms that involve only x and terms that terms involve only y.

So, this cannot be separated. So, we cannot separate x and y in this case. So, then what is the strategy to do and in this case it turns out that you set u is equal to y by x. So, suppose I set u equal to y by x, then I immediately I can write u prime is equal to y prime x y prime minus y divided by x square. So, u prime is this and this is equal to. So, then that implies x y prime is equal to x square u prime minus y or plus y.

Now if I substitute for x y prime here, what I see is that x square u prime plus y equal to x plus y cancel the y is. So, I get x square u prime is equal to x. So, this implies x square d u by d x is equal to x and cancel the x and what I get is d u is equal to d x divided by x so I was able to bring to a separable form. So, this is separable.

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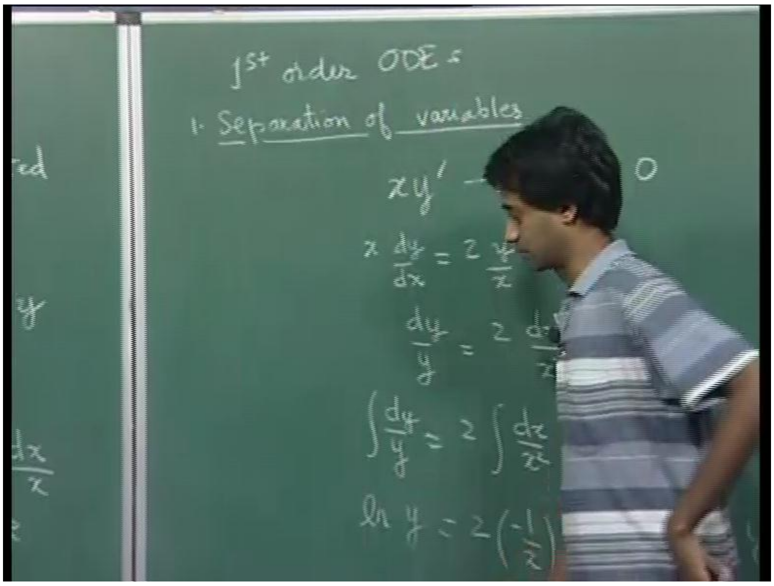

So, we started from something that did not look separable the simple transformation of variables, we came to separable form and once you separated it I can easily solve this. So, the solution will be u is equal to natural log of x and once I know u then I substitute for u, so y is equal to x natural log of x. So, by transforming variables from y to u we were able to separate the equations and we were able to solve them. So, there core of this strategy is to separate the variables. And if you cannot separated in a very simple way you try to transform variables and you try to make it separable. So, this separation of variables is going to be the core strategy for solving first order differential equations.

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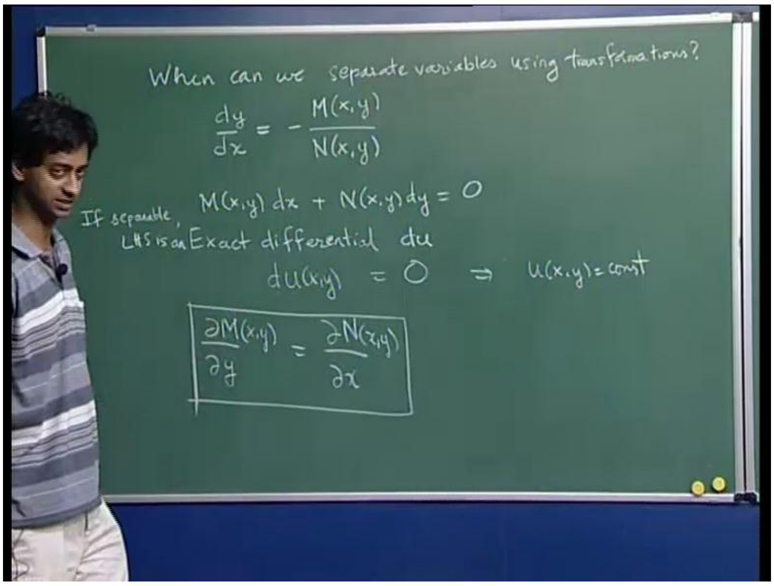

So, we saw that the first strategy to solve first order differential equations is to separate the variables. And when we are not able to separate it in terms of the variables given we try to transform the variables. So, we can write it in separable form. Now, the question remains when can we separate variables by using transformations. In other words suppose you are given a differential equation is, there a way of knowing just by looking at the differential equation. Whether there exists a transformation that allows you to separate variables.

So, the question we are asking is, is it always possible to find a transformation which allows you to a separate variables in your differential equation? So, here we are really asking about a is it always possible to find such a transformation. The answer is no, it is not always possible in some cases, you cannot find a transformation that will allow you to separate variables. And what is the condition for existence of such a transformation. So, when can we separate variables using transformation?

To answer this question we will write the differential equation in a slightly different form. So, this is a first order differential equation so it involves d y by d x somewhere so you have d y by d x is equal to let we call it some M which is a function of x and y divided by N which is the function of x and y and just for convenience we will put a minus sign. So, suppose I can write my differential equation in this form. So, it just express whatever my derivative this is a function of both x and y. So, the this is also a function of x and y. So, you express your differential equation in this form. Then I can rewrite this as M of (x,y) d x plus N of (x,y) d y equal to 0. So, alternatively I can write my differential equation in this form.

Now, when you write a differential equation in this form. Now you can ask what is the condition that there exists this transformation that allows you to separate variables? And by writing it in this form, we can motivate that such a transformation exists. If there exists a transformation, then this whole left hand side should be equal to should be an exact differential and should be equal to some d u. So, the whole left hand side should equal some differential of some function u of (x,y).

So, it should be an exact differential and so d u is equal to 0. So, if you believe that you can find the transformations that allow you to separate variables, then the left hand side should be an exact differential and it should be able to write this. And this implies that the solution is u of (x,y) equal to constant. That will be the solution to the differential equation. So, if this exists, if separable then left hand side is an exact differential and that is d u and d u of (x,y) equal to 0 becomes, the equation and this is the solution.

This is if it is separable and now you go back to your earlier notes an exact differentials and you will say that if this has to be an exact differential. Then dou M by dou y should be equal to dou N by dou x. So, this is the condition for exact, this is the condition that your left hand side is an exact differential. So, once you have this condition then you know that the this is an exact differentials. So, therefore, you should be able to separate variables by finding a suitable transformation. So, this is the condition for existence of such a transformation.

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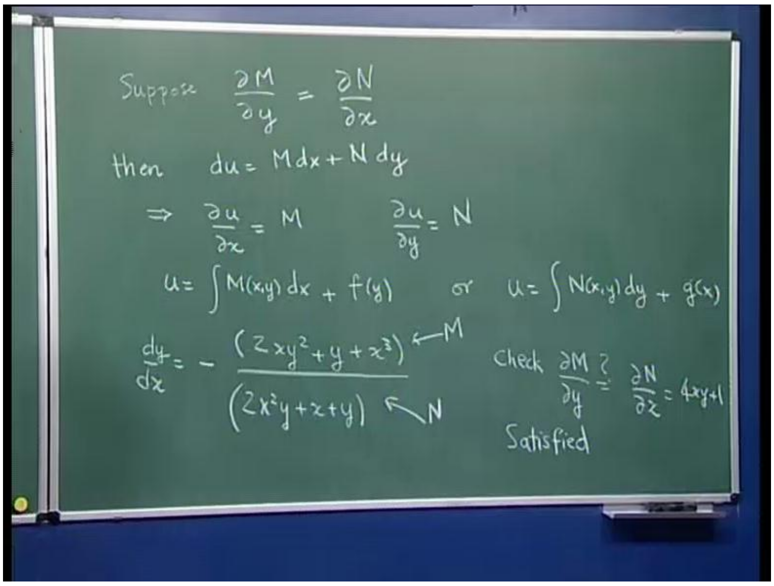

Now, when I given a differential equation, you write it in this form, then you see a derivative of M with respect to y is equal to derivative of M with respect to x. If that is satisfied then you know that there this is an exact differential. And once you know that it is an exact differential, then we can go ahead and try to calculate what is this u is. So, suppose, dou M by dou y I am omitting the dependence on x and y dou x.

So, I am not bothering to write this, but it is understood that these are functions of x and y. So, suppose you have this condition then d u equal to M d x plus N d y. this implies partial of u with respect x equal to M partial of u in order to solve this what we will say is that u is equal to integral M, M is a function of x and y d x.

So, you integrate with respect to x and you have some constant, but this constant is a function of y. So, if you had u written in this form and you take the partial of u with respect to x, that will give you this term will give you M this term will give you 0. So, your partial of u with respect x will be 1 or you can write u is equal to integral N of (x,y) d y plus some function of x. So, notice that the constant of integration when you doing partial derivatives the constant of integration depends on the other variable. So, if I have a partial derivative with respect to x ,the constant of integration can be any function of y.

If I have a partial derivative with respect to the constant of integration can be any function of x, so this is the strategy or for solving this differential equation of first order. So, let us try to take an example. So, for example, you solve d y by d x equal to minus divided by so try to solve this differential equation. In order to do this we immediately notice that, M is this so this is M and this is N. So, that is a first thing we notice we notice what M and N are next we want to check for this condition. So, check dou M by dou y equal to dou N by dou x.

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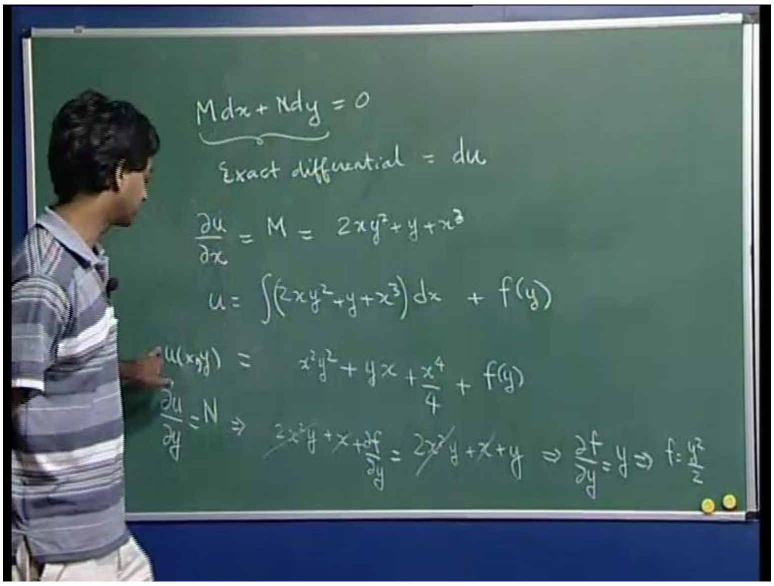

So, check for that and you can see that dou M by dou y will give me 4 x y plus 1. So, 2 x into 2 y that is 4 x y plus 1 and in this case dou N by dou x will give me 4 x y plus 1. So, you can show that both of these are equal to 4 x y plus 1, so this is satisfied. So, we can see that partial derivative of M with respect to y is equal to partial derivative of N with respect to x.

So, we have seen that, this differential equation is satisfies the conditions of separability. So, in other words M d x plus N d y equal to 0 and this is an exact differential and we called this equal to d u. Now we have to solve for u. So, we know. So, we say that partial of u with respect to x should be equal to M is equal to, M is two x y square plus y plus x cube. So, this is 2 x y square plus y plus x cube. So, when we integrate this you will get u is equal to integral 2 x y square plus y plus x cube d x plus a function of y. So, when I integrate with respect to x I keep y as a constant. So, this will give me integral x square y. Sorry, they would not be an integral sign. So, the first term will give me 2 x integral of 2 x is x square, y square is a constant. So, constant for integration over x, second term is y times x, third term is x cube integral of x cube is x 4 by 4 plus some function of y.

So, u of (x,y) is this, now how do you determine f (y). So, in order to determine in f of f (y) in order to determine f (y), we use the condition that dou u by dou y has to be equal to N. And if I take this as my u then this implies dou u by dou y is 2 x square y plus x differential of this, with respect to y is 0 plus f prime. So, dou f by dou y is equal to N, N is nothing but 2 x square y plus x plus y.

Now I can cancel this, I can cancel this, I can cancel this, I can cancel this. So, I am left with dou f by dou y equal to y and this implies f equal to y square by 2. So, we have f equal to y square by 2, So, now if we substitute in u of (x,y).

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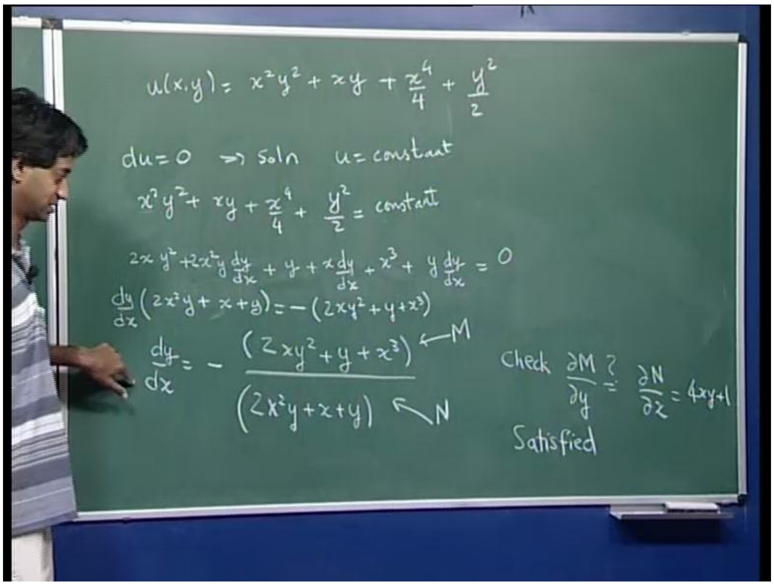

So, we get u of (x,y) is equal to x square y square plus x y plus x 4 by 4 plus y square by 2. So, we get that u of (x,y) is equal to this. Now the differential equation is d u equal to 0. So, differential equation is d u equal to 0. So, implies solution u equal to constant. So, in other words the solution can be written as x square y square plus x y plus x 4 by 4 plus y square by 2 equal to constant. So, this is an implicit solution to this differential equation. It is a solution, because it does not contain any derivatives of y appearing.

So, satisfies our differential equation like this, we came to this kind of solution and it is a general solution because that has this constant of integration. And the has an exercise you can verify that, this indeed satisfies this differential equation by taking the derivative with respect to x. You take the derivative with respect to x and both sides. Then you will get so when I take the derivative with respect to x, then I will have two terms here.

So, the first term will be 2 x y, y square, the second term will be x square into 2 y d y by d x. This again we will have 2 terms as y plus x d y by d x, this will have only one term that is x cube. And the last term will have y d y by d x, and this will be equal to zero because right hand side has no power of x or no term containing x. And you will get this form and if you rearrange it, if you take all the terms involving d y by d x and you take all the other terms on the left, you will get exactly this equation.

So, you can verify that this satisfies the original differential equation so this is indeed a solution of this differential equation. So, this is always whenever you get a solution to a differential equation, you should substitute back on the original differential equation and sees that indeed that satisfies a differential equation. So, in other words I take all the terms involving d y by d x times 2 x square y plus x plus y is equal to minus 2 x y square plus y plus x cube.

So, we came back to this and we can see that this was indeed the original differential equation that we started with. So, what we have here? So, this implies this and therefore, this is a solution of this differential equation. So, this is the general strategy for solving first order differential equation. So, we try to separate them and when we are not able to separate them. When we are able to not able to separate them, we look for exact differentials and if this exact differential exists. So, if we check that d M by d y is equal to d N by d x.

Then it is an exact differential and then we can solve it using this separation of variables. So, the next step is what happens if a differential, if a first order differential equation cannot be expressed in terms of this exact differentials. What do you do if you cannot write it in terms of exact differentials? And that will that what we will discuss in the next class and how to go beyond exact differentials.