Advanced Mathematical Methods for Chemistry
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Module – 01
Lecture – 03
Vector Functions, Vector Differentiation

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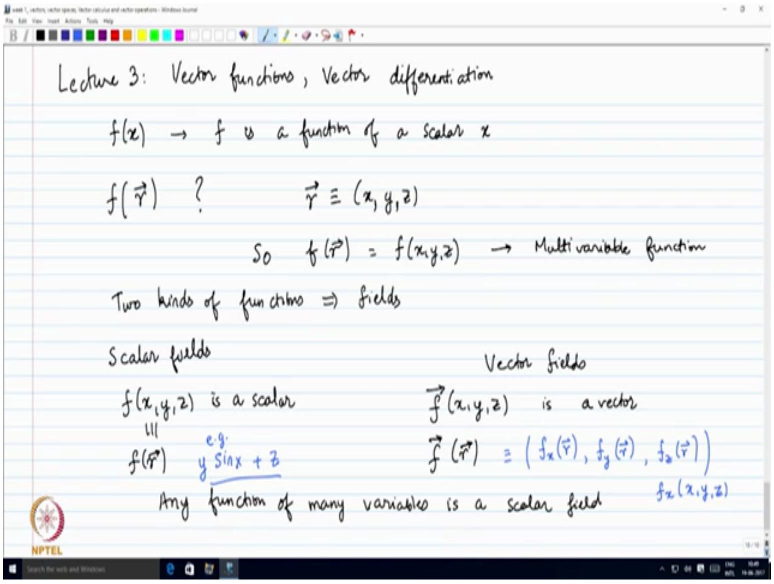

So, so far we have learnt about vectors, various operations on vectors such as addition and we learnt about vector products how to can define different kinds of vector products and we also saw how we can generalize a idea of vectors from the usual to 2 dimensionals or 3 dimensions to infinite dimensional spaces.

So, now, next today we are going to look at functions of vectors and how to take differentiation with respect to a vector. Now we will start with vector functions, now the idea here is that is the following. Suppose you have suppose you write something like f of x, what we say is that f is a function of a scalar x, a scalar x, scalar variable x a scalar means x can be any real number. So, so what we mean is x is a real number and f of x is another real number. So, what we mean is f of x is a real number. So, for any x there is there is an f of x which is a real number.

Now, the idea of vector functions is very similar. So, can you think of something like f where the argument of f is a vector for example, f of r can you think of something like this a function which is not a function of scalar x, but it is a function of a vector and the answer is yes there are there are few ways to think of these functions. So, the first thing we will say that I want to emphasize is that is that r is nothing, but x y z in 3 D. So, if you are looking at 3 d then it is just it is just 3 numbers 3 scalars x y z. So, we can just think of f of r. So, we can think of f of r as nothing, but some function of x y z. So, it is nothing, but a multivariable function. So, a function of many variables is a function of a vector.

Now, there are some more interesting things you can do we can look at 2 kinds of functions and these functions are referred to as fields. So, we can refer to we can look at 2 kinds of functions. So, functions where what are called as scalar fields of scalar functions where what you have is f of x y z is a scalar or you can think of vector fields where f is a vector and it is a function of x y z, so is a vector. So, so notice this is same as f of r vector. So, it is a scalar field now here you have f vector of r vector. So, it is a vector.

So, you can have both scalar fields and vector fields and what do these fields represent. So, so what I said is any function, function of many variables is the scalar field. So, any function of many variables is a scalar field. So, for example, you can have, you can have something like sin x, so y sin x plus z this is a scalar field. So, example is this. So, any function you can take any function you can take y square y square x z you can take x y z x y plus z any function you can take exponential any function that you take that is a function of all these variables that becomes a scalar field.

What about a vector field. So, a vector fields now since f is a vector it will have 3 components. So, I will write 3 components as f x this is the x component of f now this will be a function of r, f y which is a function of r and f z which is a function of r. So, there are 3 components to f each of them of functions of r and. So, your vector field has these 3 components each of them and each of these functions is the scalar field. So, f x of r is a scalar field, f y of r is a scalar field, f z of r is a scalar field and, so f of r is a combination of these 3 scalar fields. So, that is what forms are vector field and you can easily construct vector fields based on scalar fields. So, you have such a scalar field for each of the components.

Now, remember that you all you have f x depends on x y z, f y also depends on x y z, f z also depends on x y z so. So, now we have seen how to define functions of vectors, now one of the things that we that we do often when we are dealing with functions is to plot them now you are used to plotting functions of a single variable. Now if you want to plot functions of 2 variables then it becomes a little more complicated.

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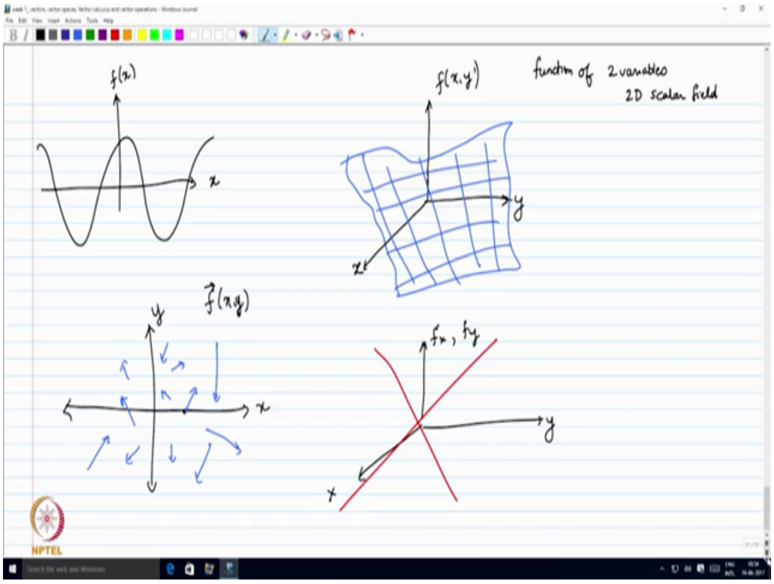

So, if you had only 1 variable x then you plot f of x and you can show it as a, you can show the graph of f of x, suppose it is a sin function or something then you will have a graph like this, this. So, f of x will have some graph. So, you can show graph that represents f of x.

Now if you have a function of 2 variables then what you need to do is you need to your vector space your space of variables is 2 dimensions and then and then you have a function of those 2 variables. So, you need 3 dimensions to judge just to show this and you can think of you can imagine showing this in this form.

So, suppose you take this as the x axis this as the y axis and you show the function in the third axis you show f of x y in the third axis. So, this is a function of 2 variables, variables or a 2 dimensional scalar field, now what will this look like? So, this will look like, for each point x y, each point x y there is a function there is a value of this function. So, the value of function you are showing in this dimension. So, this f of x y will basically be some sort of surface some sort of surface in this I reached it by accident so will be some sort of a surface in this.

So, let us just get back to this we will draw. So, if you have your x y axis then this function will look like some sort of surface. So, for each value of x y there is a certain value of this function and it will be some surface. So, if you connect all the values you will get some sort of surface. So, this is what your f of x y will look and now it might have some curvature, it might have various properties.

Now what about functions of 3 variables? Well that is a little difficult to show how you row you it is very hard to show that because you need a 4th dimension to show it, you have 3 variables x y z and at each for each value of x y z you have some value of the function.

Now, what about a vector field let us say a vector field of 2 variables? So, suppose you have x y and now you have a vector field. So, a vector field, now again you need the vector field has 2 components. So, in principle you need 4 dimensions to show this, but you can do you can do this in a slightly better way and what you can do is to is to in instead of trying to show this. So, you need both f x and f y and that is not possible to show. So, instead of that what you do is the following. So, you do not do this instead and very convenient way to represent the vector field is the following.

So, suppose you had x and y axis, x and y, now a vector field means for any given value of x and y there is a vector. So, now, a vector has both a magnitude in a direction it has both an x and y component. So, if you want to show f vector of x y then all you have to do is to you take any point x y. So, let us say you take this point x y I will show it in blue and you will have some vector, you take some other point you have some vector. So, it has both a magnitude and a direction some other point you might have a vector like this.

So, you can sort of represent this vector field by taking a large number of points and showing where the vectors go you can show both the length and the direction of these vectors. So, some can be larger some can be smaller. So, this would be an example of a vector field. So, the length of these vectors is proportional to the magnitude of the function and their direction is the die the direction of this function. So, what I want to say that in for a 2 dimensional vector or scalar field there are ways to show it graphically, but for 3 dimensional scalar or vector fields there is no convenient way to show it graphically and you can just represent it and try to imagine what it looks like.

So, we have defined functions of vectors now the next thing we want to do is to start doing things with this function.

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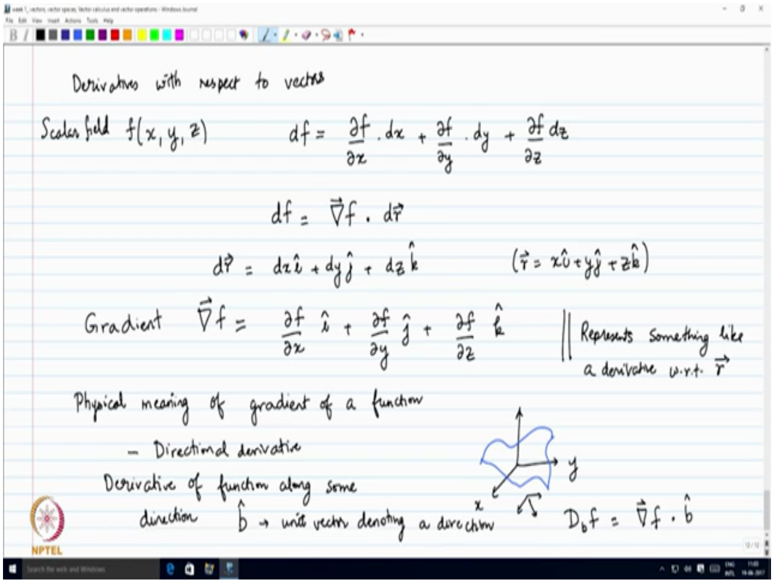

So, one of the things we do with functions is to take derivatives what about derivatives with respect to vectors. So, suppose you have a function of a vector you can always take a derivative of that function with respect to the vector. Now it turns out that there are a few different ways to take derivatives, now let me motivate one kind of derivative which you will see which you will probably see the most often and then and then and then we will go to the other 2 derivatives.

So, now what we said is that suppose you had a scalar field. So, scalar field is nothing, but a function of the vector. So, it is a scalar function of many variables. So, now, f of x y z is a scalar field now what you see is that this is just a function of many variables. So, suppose I write d f the total change in f. So, this I can write it in terms of partial derivatives. So, I can write this as partial derivative of f with respect to x times d x plus partial derivative of f with respect to y times d y plus partial derivative of f with respect to z d z. So, this is the chain rule for a function of many variables right. This is how we take the derivate; this is how you write the differential element of f the differential change in f.

Now, we look at this we look at this expression and we immediately notice that I can write this expression in the following form, I can write this as d f equal to I will write a notation so I will call something as gradient of f I am denoted by this a this triangle inverted triangle and I will write dot into d r where d r is basically d x i plus d y j plus d z k which if you remember we had r equal to x i plus y j plus z k. So, d r is nothing, but a differential element of half.

So, you are taking a d r vector. So, it is a vector differential it is just you can just write it in this form now and the quantity grad f this is called the gradient. So, notice the components of d r or d x, d y and d z, and d x is multiplying d f by d x, d y is multiplying d f by d y, d z is multiplying d f by d z. So, gradient f has components d f by d x d f by d y and d f by d z. So, I can write this as d f by d x into I plus d f by d y to j plus d f by d z into k. So, now, you can see that this expression the differential change in f is given by a gradient dotted into the differential element d r, d r is a vector gradient of f is a vector and their dot product gives you the differential change in f. So, that is the change in f when due to change in x, change in y and change in z.

So, the change in x y and z causes a change in the function f which is related to the gradient of f. So, the gradient is one way of, this is one way of this represents something like a derivative, derivative a with respect to r. So, it is almost like saying I make this change in r I make this differential change in r and how what is the change in f that I see not exactly that there are few more conditions, but this is one derivative that is very important.

Now the gradient, gradient is the physical meaning of the gradient of gradient of a function. So, what does what is the physical meaning of the gradient to the function? So, now, actually as I said it represents something like a derivative now if you want to understand it better we introduce the idea of what is called a directional derivative. So, what that means, is the following that suppose you have a function of many variables and you change the variables that is change x y. So, for example, if you had a function of, if you had this function of x y, x y and you had this function f of x y.

Now, you can ask how does f change as you change x y, now you can change x y in different directions you can change x y in along this direction, you can change x y along this direction, you can change along the x y along this direction, you can change x y along different directions and you can define something called a directional derivative. So, directional derivative represents the derivative of function along some direction. So, if we take a direction that is denoted by a unit vector b hat. So, this is a unit vector denoting a direction.

So, now, if you had a unit vector denoting a direction then the gradient or the directional derivative the directional derivative of f, so I will just a denote this D b of f. So, the directional derivative along the direction along the unit vector b this is nothing, but gradient of f dotted into b hat. So, the gradient of a function allows you to calculate the derivative value of the function along any direction. So, you can go, so instead of instead of just see you can change along x y, you can change in any direction and you can see how the function changes and the gradient dotted into a unit vector that direction will give you the directional derivative of that function that is how fast the function changes in that direction.

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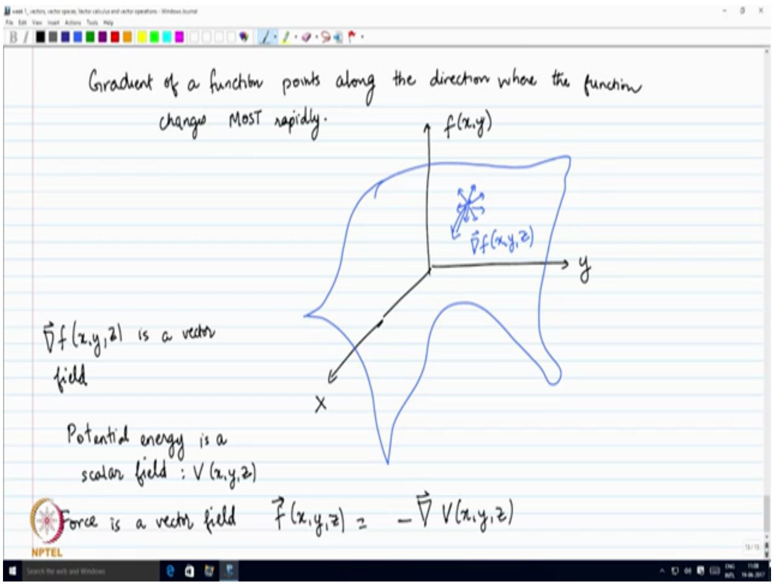

So, this directional derivative is a very important interpretation of the gradient. The other interpretation of the gradient is the following it is a gradient of a function points along the direction where the function changes most rapidly and again the, again I will go back to our picture of our graphical picture which suppose you had a, suppose you had a x y and I am showing this function f in this axis

Now it might be that you know your f might be some surface that I am just showing like this, this is my f and suppose you take any point and you go in various directions. So, you go in this direction, this direction, this direction we go in various directions and you look at the direction where the function changes the fastest let us say the slope is maximum along this directions. So, if you go in one direction then the change of the function rate of change of function is the fastest. So, the gradient will point along that direction. So, grad f at the point x y z will point along the direction of the maximum gradient ok. So, this is another physical interpretation of the gradient.

So, to summarize the gradient of a function gradient of a scalar field is a vector field who which has 2 interpretations. So, the gradient at any gradient at any point dotted into a unit vector in some directions gives the directional derivative along the direction. And secondly, the gradient at any point points in the direction where the change of function is maximum. So, this way of taking derivative of the function is actually fairly useful and in mechanics a very useful application of the gradient is the following that the potential energy is a scalar field.

So, you could have V of x y z; that means, your potential energy depends on where you are in space and the force is a vector field n, the force at any point. So, if you are at any point in space you will have a force which is a vector field and this vector field force is a function of x y z is nothing, but the negative gradient of the potential. So, this is this is true in general. So, in general if you have a potential energy then that is a scalar field and a it is a function of the position and in general if you have a system which is not homogeneous then the potential energy will be different everywhere and the force will be different depending on where you are and the force is nothing, but the negative gradient of the potential. So, this is probably the most important application of gradients in physics and chemistry and we will see some applications of this.

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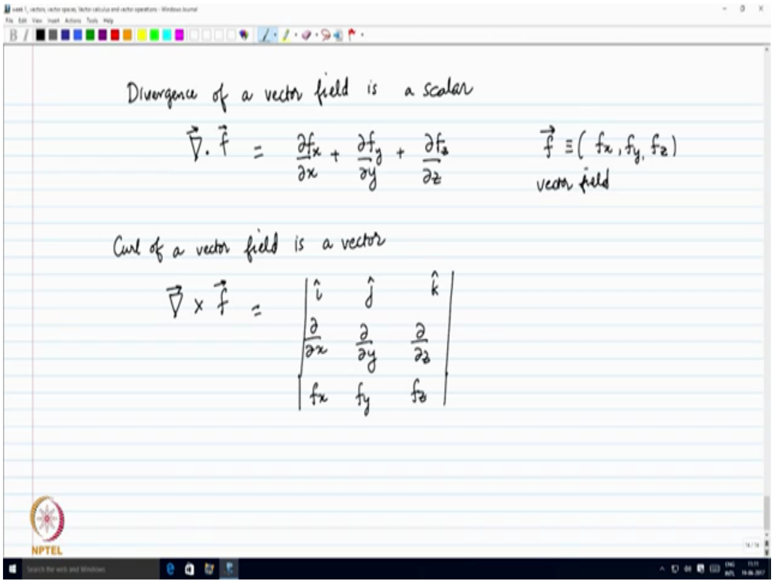

Now, as I said before there are other ways to take derivatives and let us talk about some other derivatives. There are 2 other well known derivatives - one is called the divergence. So, divergence of a vector field, this is denoted by del dot f, and just this notation basically the gradient. So, the components of the gradient are dou. So, it is dou f by dou x plus dou f by dou, dou f x by dou x plus dou f y by dou y plus dou f z by dou z where f is a vector that has 3 components f x, f y, f z. So, it is a vector field. So, f is a vector field. So, f x, f y and f z are all components of x y z. So, if you have a vector field you can define the divergence of the vector field in this way.

There is a third way you can take a vector field curl of a vector field. So, this is and here what is done if you take a it is denoted by del cross f which is; which I can write in the following form I can write it as i j k this is again since it is a cross product it is specific to 3 dimensions d by d x, d by d y, d by d z and then you have f x, f y, f z which are the components of f. So, you can you can write the curl of the vector field in this form.

So, these are all different ways of taking derivatives here the curl of a vector field. So, divergence is a scalar. So, divergence of a vector field is a scalar curl of a vector field is a vector. So, gradient divergence and curl they represent 3 ways of taking vectors gradient we took of a scalar field to get a vector field, divergence you take of a vector field to get a scalar field and curl you take of a vector field to get a another vector field. So, these are I just wanted to show you different ways you can take derivatives, there are lot of interesting relations involving these quantities which I will not go into, but at least I thought you should be familiar with these quantities.

So, in the next class what I will try to do is show you some ways in which you can integrate vectors. So, we saw taking derivatives with respect to vectors now next we can think of integrating over vector arguments.

Thank you.