Mathematics for Chemistry
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Module - 02
Lecture - 04
Vector Functions, Scalar and Vector Fields, Vector Differentiation

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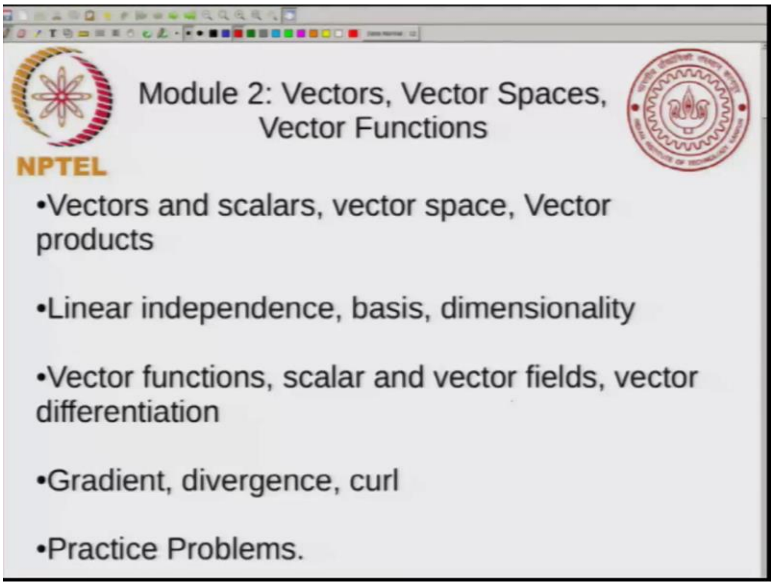

We studied various functions of vectors. We talked about scalar and vector fields. And in today's class what we will try to do is to try to differentiate the function with respect to the vector. So, and we will find out that there are 3 different ways of taking derivatives there is a gradient, divergence and curl.

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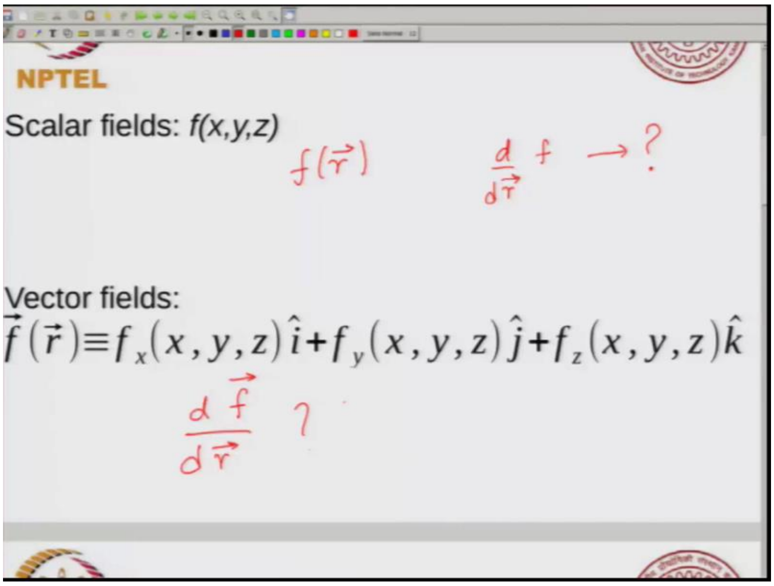

So, just to remind you; so we talked about scalar and vector fields and what we said is that is you have a function of multiple variables. So, if you have a 3-dimensional vector then this is a function of a 3-dimensional vector f of x, y, z is a function of a 3-dimensional vector you can write this as f of r. And what you want to imagine is something like a derivative of this function with respect to this vector. So, something like this. So, this is what you want to think about you want to think about something like a d f by d r where r is a vector.

Now this will be different, so it turns out that there are many ways to define this derivative and it would be different if f were part of a vector field. So, if instead of having a scalar field, you have a vector field then how would you think of differentiation with respect to this to this differentiation of the vector field with respect to a vector? So, how do you think about these? So, in doing this, we will look at 3 different definitions of quantities that look like derivatives.

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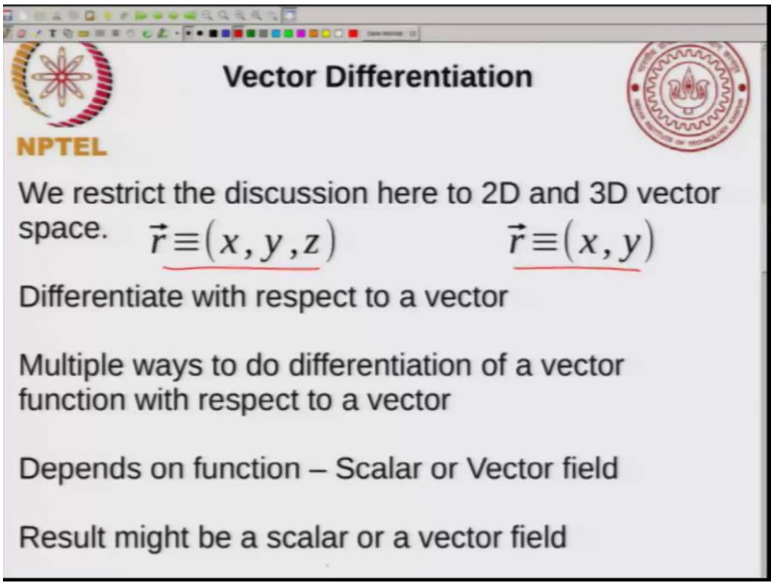

And again just to emphasize that we will restrict the discussion here to 2-dimensional and 3-dimensional vector space. So, all that I will be doing in this class will be restricted to either to 3D vector space where, r is x as a is written as x, y, z or 2D vector space where r is written as x, y. And again let us emphasize that we are going to differentiate with respect to a vector, and there are multiple ways to do this differentiation of a vector function with respect to a vector. And it depends both on the function whether it is a scalar or vector field, and it depends on what results you want, do you want the scalar as a result or do you want a vector field as a result.

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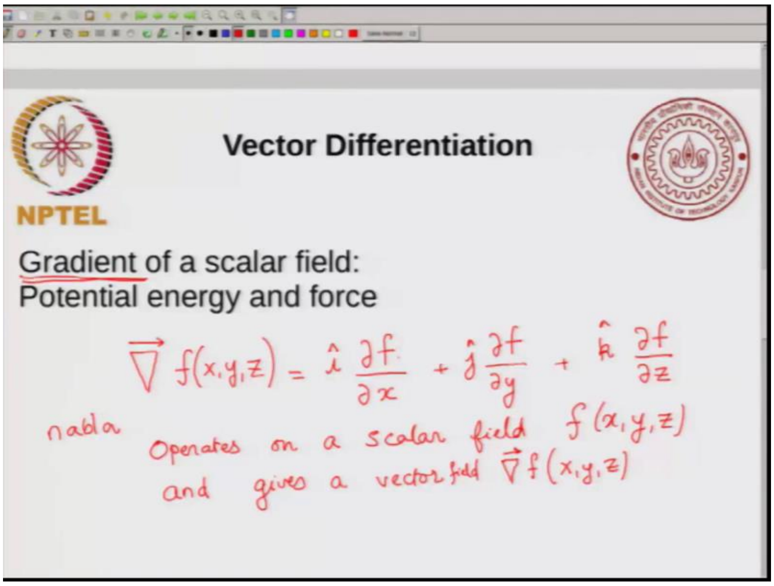

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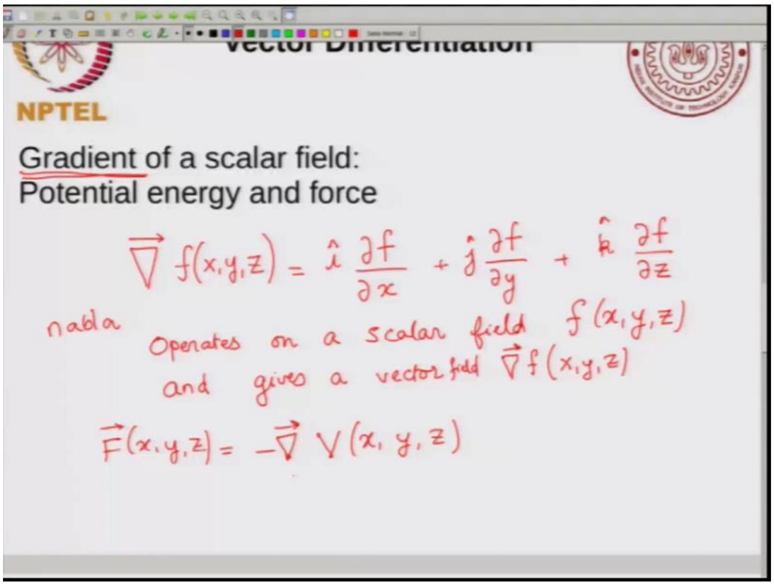

So, the first kind of vector differentiation that we will do is this gradient. Now, gradient is defined with respect to a scalar field, and it has a very natural application in potential energy and force. So, the gradient operator is shown by this symbol, it is which is called nabla, and it is a vector operator. And it is shown by this way. So, it operates on a scalar field. So, suppose you have a scale is scalar field f of x, y, z. This gives you this can be written as it gives you a vector which has as this form i partial derivative of f with respect to x plus j partial derivative of f with respect to y plus k partial derivative of f with respect to z. So, this is a definition of the gradient. So, gradient operates on a scalar field, and the result is a vector. It operates on a scalar field operates on a scalar field f of x, y, z and gives a vector a vector, and that is denoted by grad f.

And this gradient is a vector field. So, it is a vector field grad f and this depends on x, y, z. So, each of the components each of the components has a dependence on x, y, z. So, this is the definition of the gradient, and there is a very common place where you see gradients this is in potential energy and force. So, we already saw that the potential energy is a scalar field. So, you have V of x, y, z that gives you the potential energy at of at any point. And if you want to calculate the force due to this potential then the force is a vector, so force is a vector field this is written as negative gradient of the potential. So, it takes the scalar field which is the potential and converts it to a vector field, which is the force, and the operation which converts it is the negative times the gradient. So, this is a very common application, and we see this in quantum mechanics regularly.

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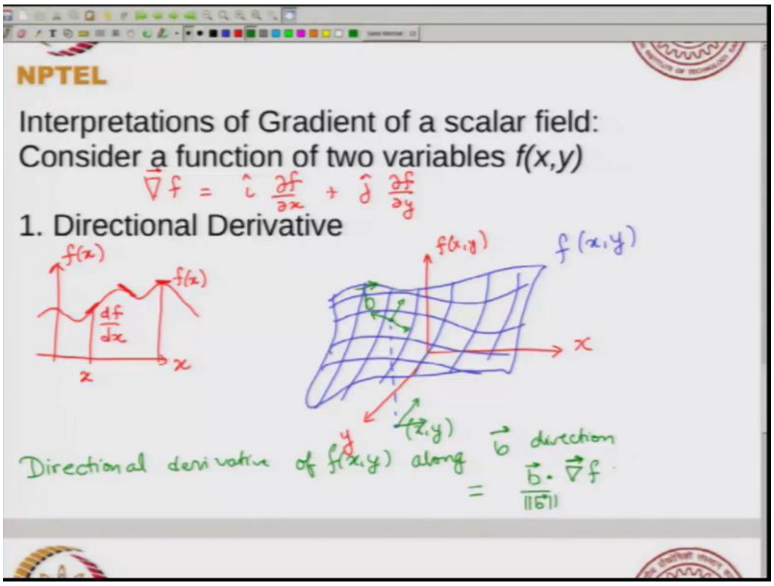

So, now what is meant by the gradient? Now, in order to interpret the gradient, we will just consider a function of 2 variables x, y. So, suppose you have a function of 2 variables, then how do you imagine the gradient? So, the gradient of f this is given by i dou f by dou x plus j dou f by dou y. So, it is a 2-dimensional vector space, so this is what the gradient looks like. So, how do you interpret this gradient? Now, in order to do this, now there are 3 different ways you can interpret one of them is what is called a directional derivative. So, just to motivate this, let us consider suppose you have a function of one variable. So, suppose you have x then this function of one variable f of x I can just plot it like this. And if you take d f by dx, so at this point x, if you calculate d f by dx then you know that d f by dx gives you the slope of the tangent to this curve at this point.

So, just to remind again this is my function f of x, this is a plot of the function. And what I want to say is that you understand the derivative as the slope of this curve. So, the slope of the graph of the function at a point, it gives you the derivative at that point. So, suppose I want to calculate the, so you say that the derivative at this point for example, is 0 because the slope of the function here is 0. So, the derivative here will be 0. Here the derivative will be positive; here in this case, the derivative will be negative and you can you can calculate the derivative using this slope of the tangent.

Now, the gradient is in some ways extending this idea to functions of more than one variable. So, suppose you have a function of more than one variable, now it is slightly more difficult to draw, but what I will show is I will try to do this. If you have the x axis and you have the y-axis. And what I will do is I will, so imagine this is the x, y plane which is perpendicular to the plane of this paper, and I will draw the function on the third direction. Now, for every given value of x and y this function has some value. So, if you connect all those values of the function, you will get a surface, and I will show this in blue. So, this is my surface which represents f. So, this is a surface this is f of x, y. So, f of x, y represents the surface. And this is a surface that corresponds to the function.

Now, you can ask, what is a gradient at any point? So, suppose I take any point let us say this point corresponds to some point x, y. And I ask what is a gradient at this point what is a gradient tell you. So, remember in case of functions of a single variable, the derivative gave you the slope was related to the slope. Now, in this case if you sit at this on this surface and you let say you move a little bit in any direction then the function will change. So, if you change your x, y by a little bit then this function will change. So, you want to think about how this function changes as you change this point x, y.

So, suppose you ask now in this case you can go in any direction, you can go in this direction, you can go in this direction, you can go in different directions. And the rate of change of the function might be different, it might change differently in this direction, might change differently in this direction might change differently in this direction. So, suppose you have a direction given by b. So, the directional derivative of f of x, y along b direction, this is equal to b dotted into gradient of f.

So, suppose I want to know, so this is an interpretation of the gradient, so you can take the gradient, and you can relate it to a directional derivative along any direction. So, if I just take that direction and dotted to the gradient then I will get the directional derivative along that direction. So, it tells me how the function changes in that direction. So, actually this should be interpreted as a projection. So, you divide by absolute value of b. The point is that you project your gradients in different directions, you get the rate of change of the function in that direction, you get the directional derivative. So, the directional derivative means that you change x, y along a certain direction and then you see how the function changes.

See, in the case of just one variable you could only change in one direction that is the along x, but here you can change along the x-axis you can change along the y-axis you can change in some other direction. And in each case the directional derivative of f of x, y will be related to the gradient dotted into some unit vector in that direction. So, this is one interpretation of the gradient. So, in general if you have a function of many variables this function is looks like a surface. And you can look at the rate of change of that of that function in any direction is what is called the directional derivative and that is related to the gradient.

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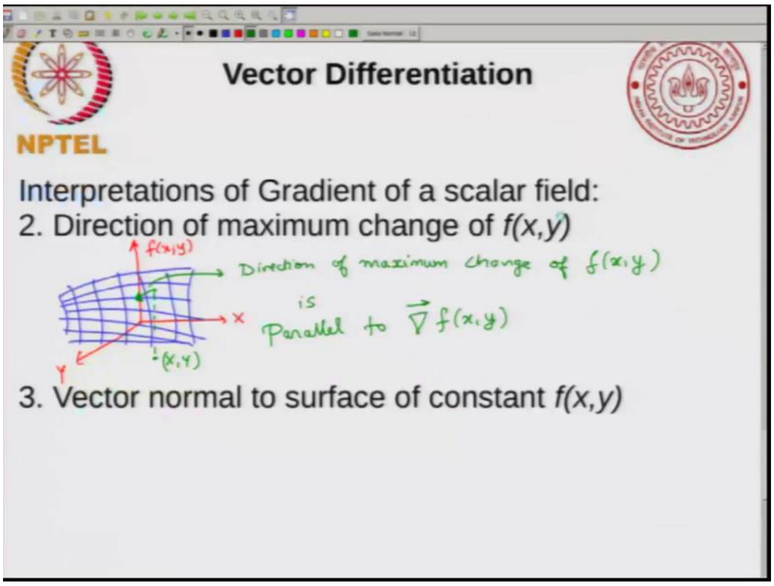

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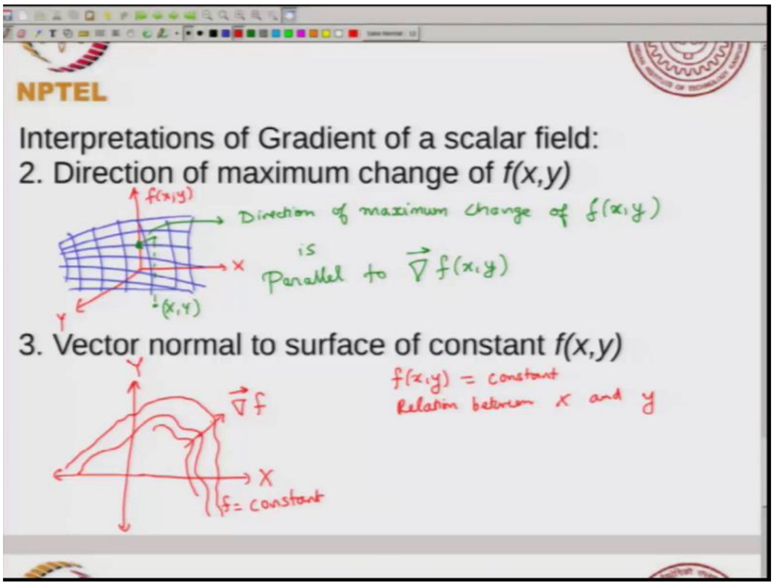

The second interpretation of the gradient of a scalar field is that it is a direction where the function f of x, y undergoes the maximum change. So, let us get back to our function. So, we had this f of x, y and you had x and y. And what we said is that this function looks like some surface. And what we said is that if you take at any point which in the x, y plane. So, this is some point and the function has some value at that point. And you look in all directions you look in all the directions and you let say you decide that the function is changing most rapidly in this direction. So, this is the direction of maximum change of, and this direction is the; is parallel to gradient of f of x y. So, this is an interpretation of the direction that the gradient points end and that is related to the direction where your function changes most rapidly. So, this function f of x, y changes most rapidly when you go along that direction.

There is another interpretation and I will just mention this briefly this is you can think of it as a vector normal to a surface of constant f of x, y. So, the again this is slightly more involved, but I will try to explain this. So, again you look at this plot. Now, suppose f of x, y equal to constant. So, suppose you put f of x, y equal to constant, now this will give you some relation between x and y. So, a surface of constant x, y f of x, y is constant then it will be some line like that I depending on what this function is it will be some graphs in the x, y plane. Now, if I change the value of this constant then I will get another graph. So, what this gradient does is it is vector that is so at any point at any point you have this surface of constant f of x, y, and the gradient is actually normal to this surface. So, this is the direction of gradient. So, this is f equal to constant. So, f equal to constant will refer to different curves, so at any point the gradient is actually perpendicular to these it takes a direction that is perpendicular to this f of x, y equal to constant surface, in this case surface refers to a curve. So, this is the other interpretation of the gradient.

So, essentially there are 3 ways to interpret the gradient, you can think of it as the directional derivative. So, it tells you how this function changes in a certain direction or you can think of it as the direction where the change of function is maximum that is actually parallel to the direction of the gradient. And then you can also think of the direction of a gradient as perpendicular to this surface where surface of constant f of x, y. So, these are the 3 interpretations of the gradient.

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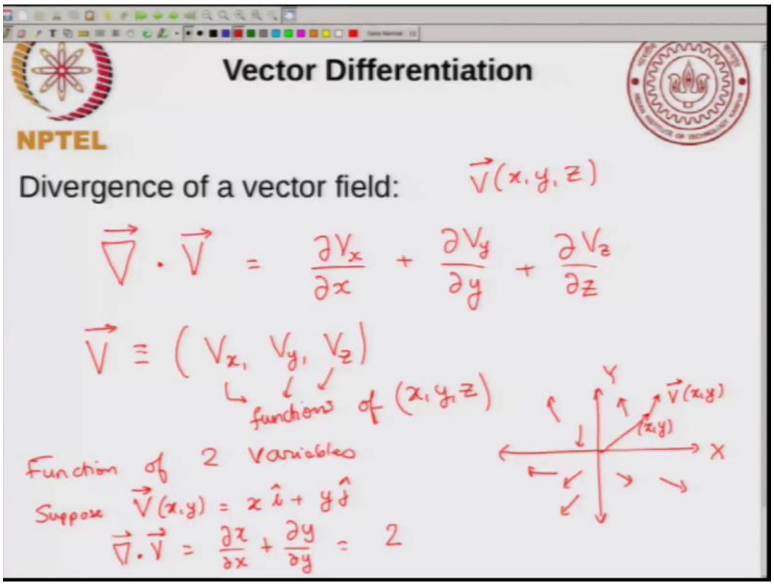

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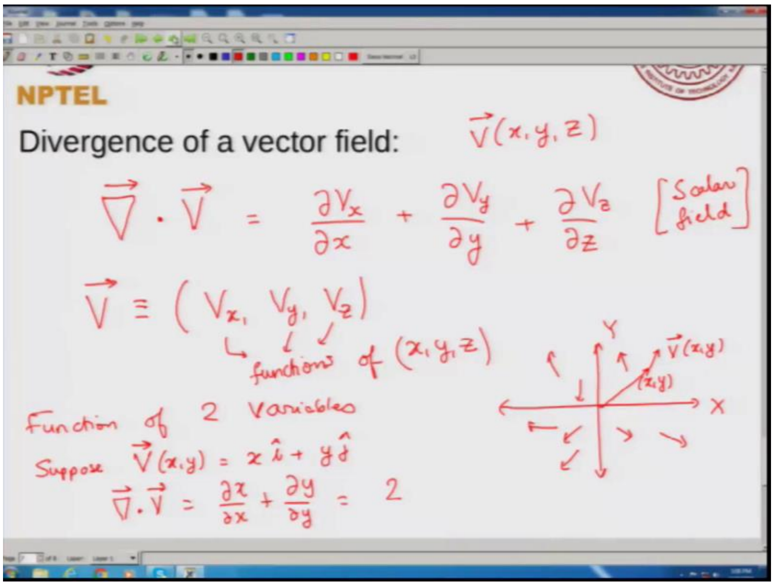

Now, the next object that we will define is called the divergence. And the divergence is defined with respect to a vector field. So, suppose you had vector field, I will just say V of x, y, z then the divergence of a vector field is denoted by the nabla dotted, this is a dot product into V. And this is equal to dou V by dou x - dou V x by dou x plus dou V y by dou y plus dou V z by dou z. And just to remind you my vector field V is equivalent to V x, V y, V z, so these are the comprehends of the vector field, and remember each of these has function of x, y, z, so that is the vector field.

So, I take this function. So, V x is a function of x, y, z, I take the derivative with respect to x. V y is also a function of x, y, z, I take a derivative with respect to y. And I take the derivative of V z with respect to z. I add all those 3 what I get is called the divergence of the vector field. Now, again if you want to think about vector fields what you really have to do is to is to imagine, suppose you consider a function of 2 variables then what does the vector field look like. So, you have x and y and what the vector fields say it is that at any point here, you have a vector field this is my V, this is x y. So, at this point x, y, you have a vector V of x y. Similarly, at some other point you have V. So, at every point in space you have a vector which is what tells you the vector field.

So, a vector field looks like, you can you can think of it as a collection of vectors. So, collection of arrows pointing in different directions based on the direction of the vector field. So, what the divergence is actually related to the properties of this vector field. So, if you see that around some point, there is a net inflow or outflow of arrows then the divergence will be nonzero; if there is no net inflow or outflow of arrows then the divergence will be 0.

So, suppose we had V of x y is equal to x i plus y j, then you can immediately calculate the divergence of v del dot v is equal to, so what you will get is dx by dx plus dy by dy is equal to 2. And the divergence is nonzero. Now if you imagine looking at this vector field what you will see is that at every point the arrow will point radially outwards, so the divergence is nonzero.

Now, so the divergence of a vector field is actually a scalar field. In this particular case, that we considered we just got 2 a number, but in general it is a scalar field because the each of these quantities each of the V x, V y, and V, z they depend on x, y, z, so each of these terms in the divergence depends on x, y, z. So, the divergence of a vector field is actually a scalar field. So, this is a scalar field.

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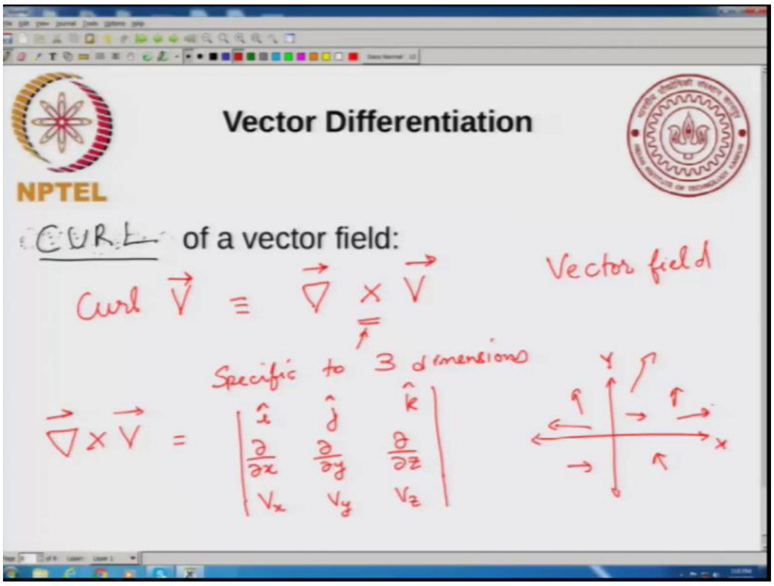

Now, see the other kind of derivative you can think of is you can think, suppose I had a vector field and I operate it and I take a derivative and can I take a derivative and get a vector and this is referred to as a curl of the vector field. So, the curl of a vector field V is denoted by nabla cross v. So, this is the vector field and obviously, since it is a cross it is specific to 3 dimensions. So, the definition of curl is specific to 3 dimensions. And you can write del cross V is equal to you can write it in this form i j k d by dx d by dy d by dz just like a dot product just like the usual cross product V x, V y, V z. And usually curl if you have a vector field then the curl actually tells you the about the rotational properties. So, if you have a vector field that looks like various arrows pointing in different directions. So, if this is my x, y axis and this is the vector field that I have then the curl refers to the rotational properties of this vector field. We would not talk too much about curl, but I just wanted to emphasize that there are different ways of taking derivatives with respect to a vector.

So, in the next class what I will try to do is try to work out some problems, where we apply all these concepts of vectors, vector functions, vector derivatives, vector products etcetera.