Biomathematics

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Lecture No. #16
Vectors - 3

Hello. Welcome to this lecture of Biomathematics. We have been discussing about vectors, trying to understand quantities that have both magnitude and direction, and we discussed a few things about force, etcetera. So, for example, in the last lecture, we have been discussing, how the charges will move in a, in which, which direction…If you have a set of charges, and if you ask the question, what is the force on a particular charge, due to all other charges, which is a common question, where that would be nearer to understand shape of bio-molecules, because, bio- molecules have charges and they have charged, charged molecules, charged residues and charge molecules. So, essentially, an effective shape of a bio-molecules will be determined also, by its charge interaction. So, in this context, we have been discussing, how will charges feel a force, due to other charges and in which direction, which will be the direction of the force, etcetera. Today, we will continue to discuss a little more about vectors, but from a different point of view. So, today's lecture is also vectors and it will be vectors, the third session.

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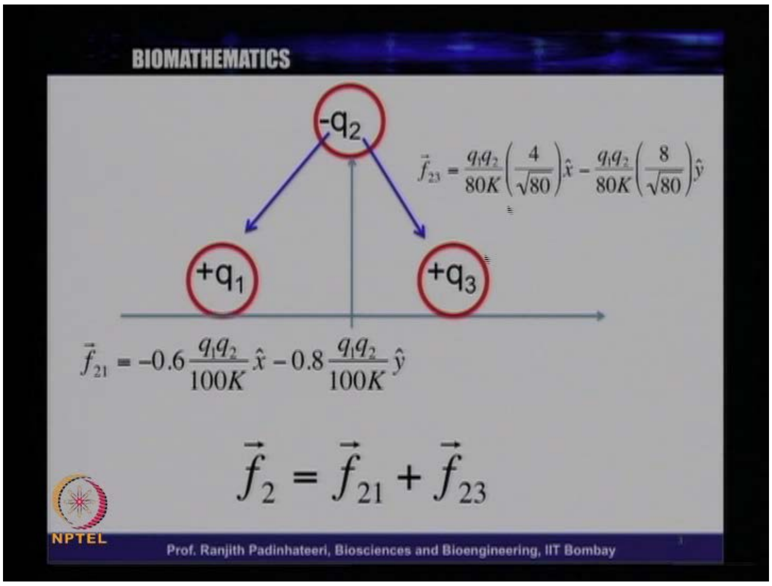

And, what we had discussed is about, basically, force. As we saw, this is our, where we stopped last time, that we said the resulting force on the second charge, is the sum of the force due to the second on the, due to the f 2 1 and f 2 3. f 2 1 is a force on the second due to the first charge and force in the second due to the third charge. We also, we also, and we said that, this is f 2 1 and this is f 2 3.

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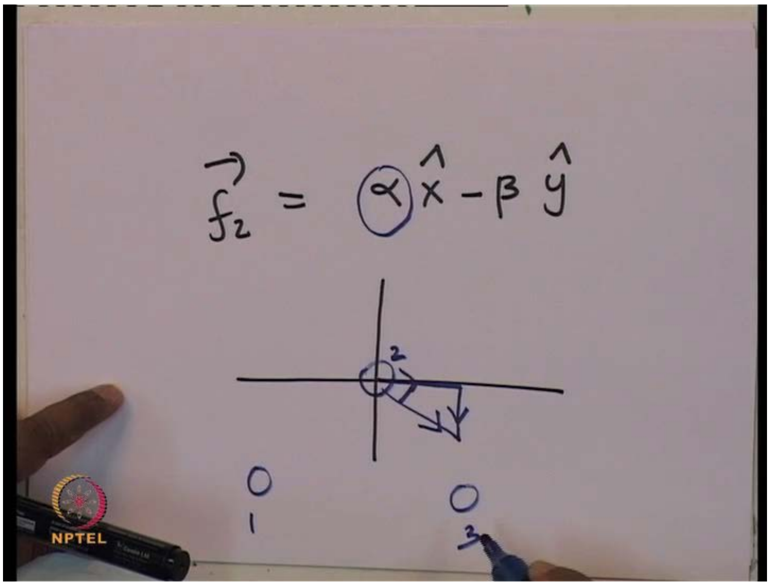

So, we also said that, essentially, we will get f 2 is equal to some alpha, which is along x and with some minus beta, which is along y. So, the force, if you look at in the x y plane, this is something along X axis, this alpha which is positive. So, you have to move along this direction, some amount of alpha and minus beta in this direction, along the minus y direction; alpha along the plus x direction, in this direction and beta along minus y direction. So, this will be the resultant direction of the force. So, this will be direction on the force, of this, due to this charge 2 and we have charge 1 and charge 3 here. So, this is the kind of thing we found out. Now, we will discuss the few…We also…

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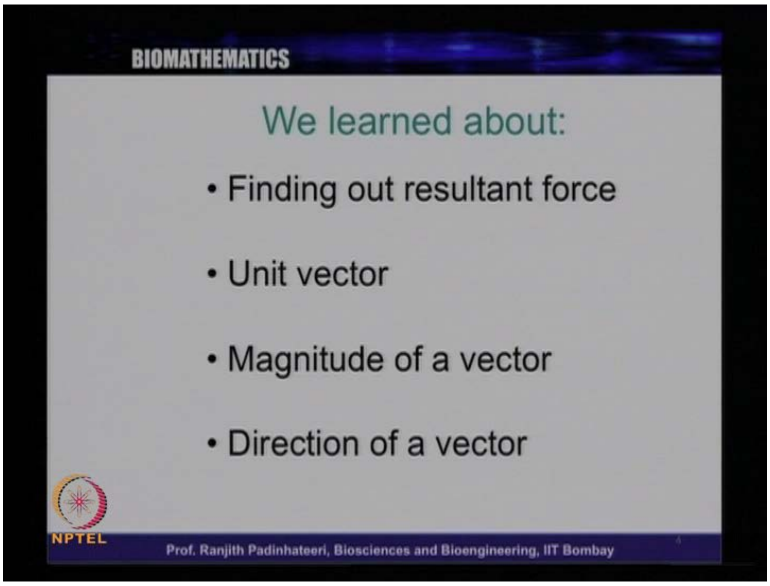

So, to ((summarize))…While we learning all this, we learnt many concepts. Those concepts are like, this concepts are here, which are finding out resultant force, idea of unit vector, how do we find the magnitude of a vector, how do we find direction of a vector; so, all these things we learnt. We also briefly discussed about addition of vectors; how we can add two vectors. So, let us generalize this to 3 dimension. So, we know that, any vector, when 3 dimension, will have three components; just like a vector in 2D has x and y component, a vector in 3D will have three components x, y and z.

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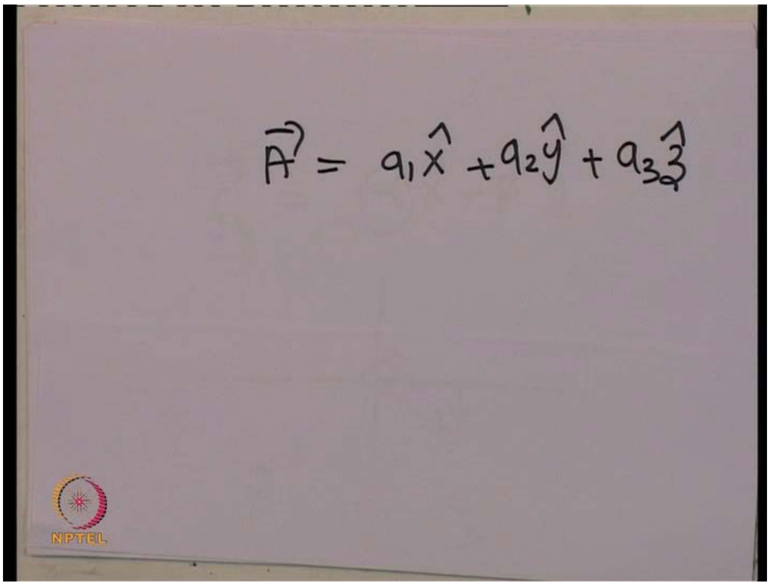

So, any vector A in 3 dimension will have three component; some component along the X axis; some component, it will have on the Y axis and some component along the Z axis. So, if you take (( )) generalize 3 D vectors, how do we add them and subtract them?

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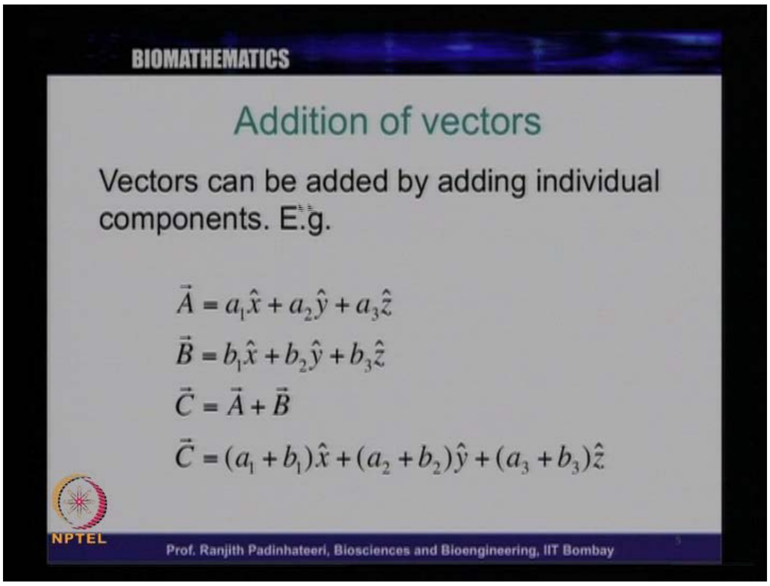

So, have a look at here. So, if we have such vector A and B, where A is a 1 x plus a 2 y plus a 3 z and B is b 1 x plus b 2 y plus b 3 z, the sum of this vectors is nothing, but the sum of the components. This is what we discussed; that is, we can just, a 1 plus b 1, which are the x components; a 2 plus b 2, they are the y components and a 3 plus b 3, they are the z components. So, these are, this is how you find the sum of two vectors. A plus B is a 1 plus b 1 x plus a 2 plus b 2 along y hat plus a 3 plus b 3 z hat; a 1 plus b 1 x hat plus a 2 plus b 2 y hat plus a 3 plus b 3 z hat. So, this are, this is the result and this is the sum of two vectors; this is how we find. So, like we said, if you want to find out f 2 1 plus f 2 3, we can find out this way. Similarly, subtraction, addition is, subtraction is like addition only.

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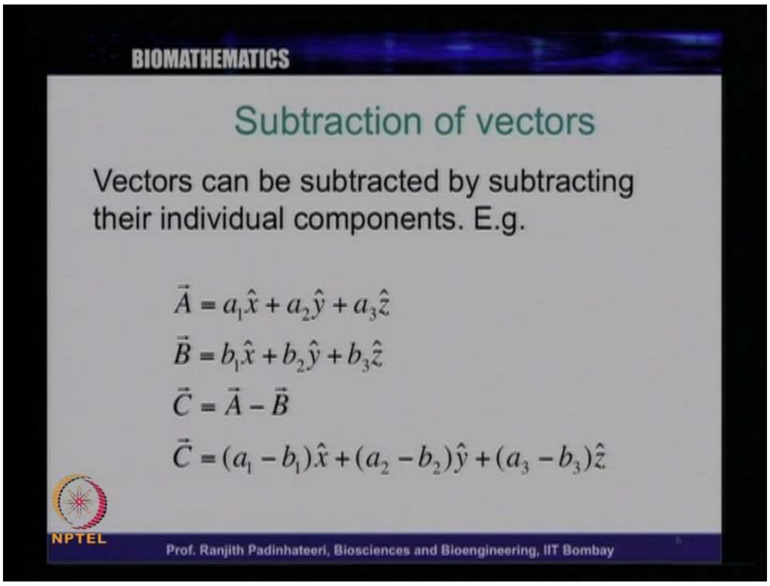

So, if you have two vectors A and B and if you want to subtract one from the other, you can do it in the following way. If you have a vector A is a 1 x plus a 2 y plus a 3 z and B is b 1 x plus b 2 y plus b 3 z, where all this, when I say x y z, they are capped; the unit vectors a 1 x unit vector plus a 2 y unit vector plus a 3 z unit vector. So, then, C is equal to A minus B, which is, you subtract the x component; that is, a 1 minus b 1 plus a 2 minus b 2 which are the y components and a 3 minus b 3 which is z component. So, this is the way we add or subtract two vectors. And, they will have, the resultant vector typically, will have, it can, it can have three components or we have, if you have vector of 3 D, you add, subtract with the 3 D, you will get another vector in 3 D; that is what you saw here basically, because what you get, the C is an another vector and the vector is obtained in this particular way. C is the, C is another vector and the C is obtained in this way. Even here, in the previous case, when you do A plus B, C is another vector. So, you can do this in a particular, in this particular way. Now…So, we learnt about subtraction of two vectors and addition of two vectors. Now, we should go and rethink a bit more about something we discussed very early, about vectors.

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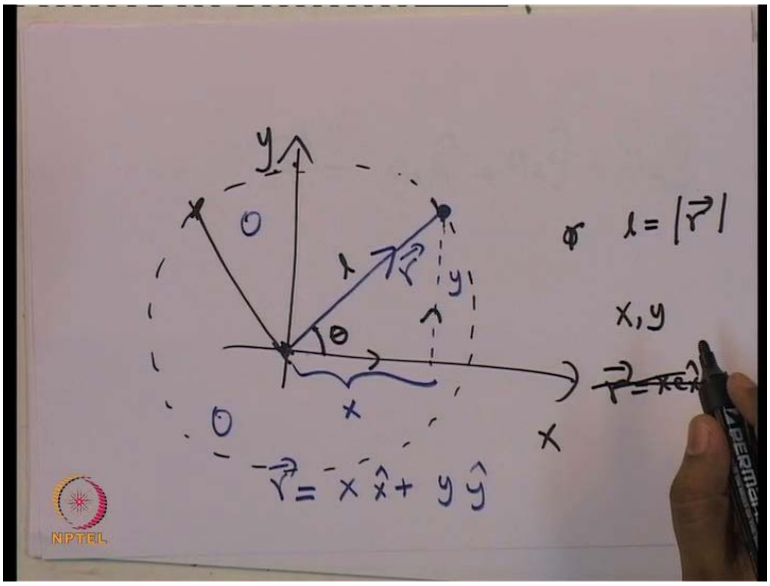

So, when I said that, if you have a 2 D plane, X axis and Y axis, any…So, this is x and this is y; any point in this x y plane, let us say, this particular point, if we want to go to this and let us say, you can imagine, for example, these are atoms of a molecule. So, let will, we can imagine some molecule, which are connected like this. Let us say, this are three atoms of a molecule; this is one atom; this is one atom; this is one atom. So, if you want to, if I want to tell this position of this particular atom, I can say that, if I start from this particular point, and if I go…So, I, the position of this point can be represented by some vector r. Now, what is r? We said that, you can go some distance along X axis and that, you will get the, and you can go some distance along X axis, and some distance along Y axis. So, if you go this much along X axis and this much along Y axis, in the direction of the Y axis, I will get this particular point. So, r is some x, along the x direction, plus some y, along the y direction.

So, this is your r vector. Now, if you think about it, to get this, exactly the same information, you can do, you can get the same information in a different way. So, have a look at here. Instead of saying that, I can go x along this, x distance along this, and y distance along this. So, this is one and this is, this, I can say one thing, I can go an angle theta, some particular angle from the X axis; and, if I go this angle theta, then, I can go a distance of r, this distance. So, let, this is the distance from here to here, in this, in this direction. So, I can specify the same point by specifying this distance and this angle. So, I can specify some distance r, which is this distance. So, this is not a vector just a distance. So, let, let me call this l. So, l is the mod of the r vector. So, this is l; this is this distance, from here to here, this distance, let us call it l. So, I can specify this l and specify this angle theta. So, that will give me, that will give me the exact position.

So, somebody, if I just specify l alone, that will not tell you this particular point; because, if I say, this is the distance, my point or this particular atom is at a distance l from the center, at this, from the starting point, there can be many points; this point also can be, there can be a many points in the, on the circle; you can draw a circle. There can be many point, that is l distance away from this. Even this point is l distance away from the center; even this point is l distance away from the center. So, there can be many points actually, along a circle, which is l distance away from this center. But, if we specify this l and this angle theta, where this is angle from the X axis, then, there is only one unique point; that is this point. So, this point or this position of this atom or this particular position, can be either represented by an x and a y, such that, r is x e x plus y e y. So, let me write this little more carefully here. So, let me write this.

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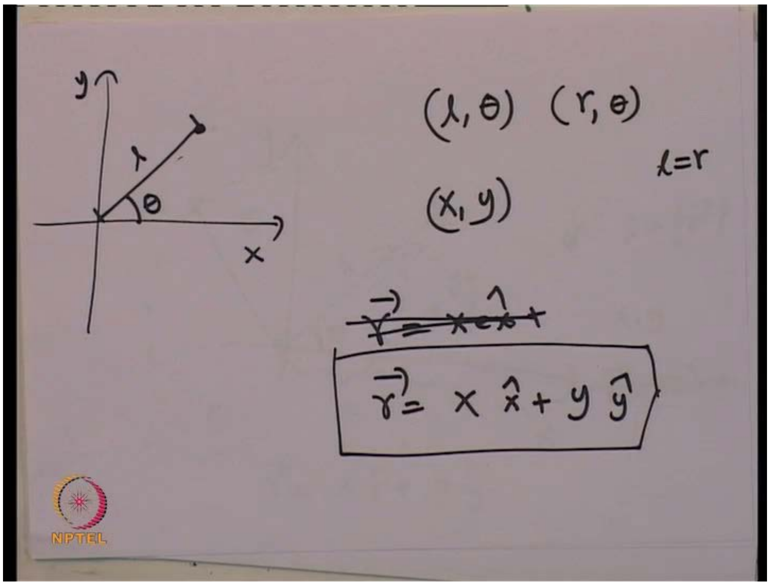

So, let us have a look at, little more carefully. So, we have X axis and Y axis and any point can be specified by specifying this distance. So, let me call this distance l and this distance, see, this angle theta. So, you can either specify an l and a theta, or, you can specify x and a y. If you specify an x and a y, this r is x e x plus, sorry; r is x x cap plus y y cap; x and y are some numbers and x cap and y cap are unit vectors. Same way, I can specify with a length and a theta. So, sometime I represent this l by r. So, or, some people write it as r and a theta; the distance r; some people write l instead of, r instead of l; some, in many text books, you would see r and theta. So, either you can, essentially, r or l, whatever you represent, it is just distance. So, either you can say this distance and say that, you can go this distance at an angle theta from the X axis or you can say that, I can go x along the X axis and y along Y axis. So, you will get this. So, now, if this is the formula for this r vector, what is the formula in terms of r and, little r and theta. So, that is the question. So, let me say, let me, let me, let me, let me explain, what I was telling in the last two minutes.

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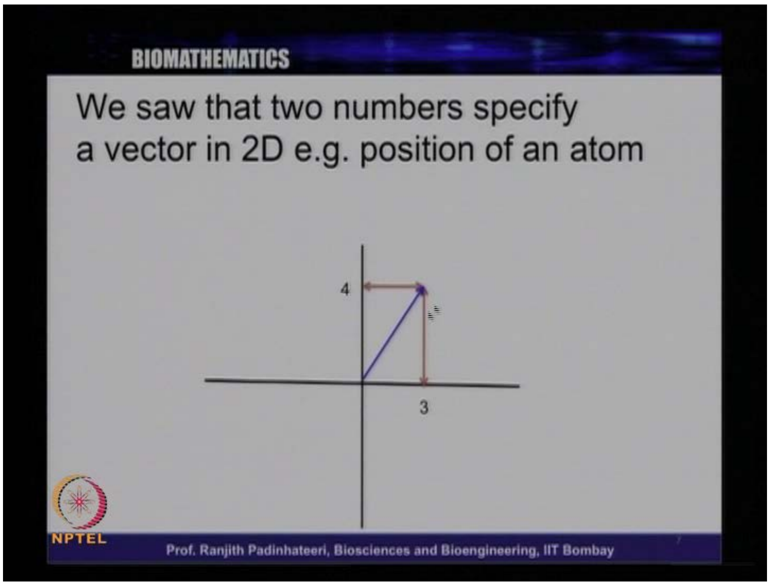

So, what I was saying is that, any point, look at here; any point, that is, the end of this blue line, this blue arrow, this point, can be represented by two numbers 3 and 4, in 2 D you can have two numbers; in 3 D, you will have three numbers. So, two numbers 3 and 4 will tell you this, uniquely tell you, this point. When I say 3, 4, in a 2 D plane, there is only one point; 3 along X axis and 4 along Y axis. When I say 23, 8, there is only two points, 23 along X axis and 8 along Y axis. So, two numbers will uniquely determine one point in a 2 D case, in a 2 dimension, in a plane. Now, as we said, how do we say, instead of saying two numbers, I can say and two distances, essentially, these are two distance, distance along X axis and distance along Y axis. Instead of saying two distances, I can say one angle and a distance.

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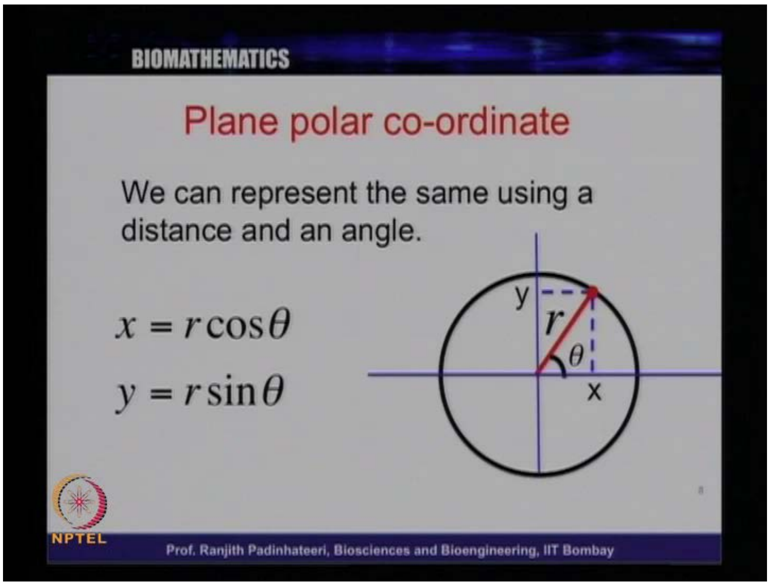

So, how do we do that? As I just said that, I can say this angle theta and this distance r. If I say this way, it turns out that, x, that is this distance, is nothing, but r cos theta and this distance y, is nothing, but r sin theta. So, if I say in this particular language that I was mentioning here…

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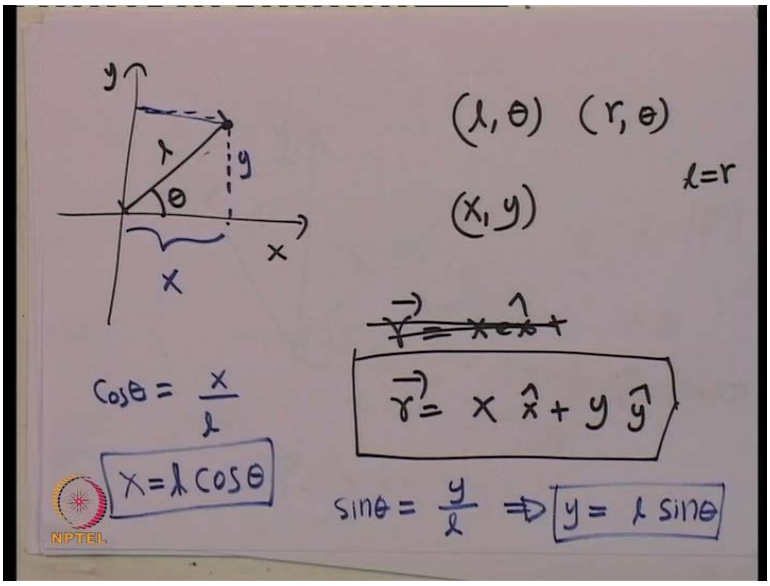

So, if you look at this particular case here, this is our point of interest and we have, this is, l is this distance. So, here this is the x. So, and you know that, cos theta is this distance, which is the y distance, this distance. So, cos theta is, the definition of the cos theta is…So, if you consider this as a, a right angled triangle, with this as a 90 degree, this is its hypotenuse. So, cos theta is always x by l; that is, the hypo, adjacent side, which is adjacent to this angle theta, which is x, divided by this hypotenuse l. So, this is the definition of cos theta. So, this would, this imply that, x is l Cos theta. In this case, you can convince that, x is l Cos theta. Similarly, you can convince yourself that, x, y is…Similarly, if you do this, you will get here that, sin theta. Sin theta is nothing, but, you can say that, sin theta is nothing, but y by l.

So, in other words, this implies that, y is l sin theta. So, here you have l Cos theta and l sin theta, where l is this distance. Just like I say in this slide here, this r, which is this distance, is essentially, x is equal to r Cos theta and y is equal to r sin theta. So, this is just simple trigonometry will tell you that, this distance is only…You know that, Cos theta is always between, for any, it is always between 0 and 1. It cannot be more than 1. It, it is, it is either 0 or any value, which is, some value between 0 and 1, including 0 and 1; it cannot be more than 1. So, if this angle theta, if there is an angle theta, this distance is always less than this distance. You also, always know that, if you have a right angled triangle, the hypotenuse is r, is basically, x square plus y square.

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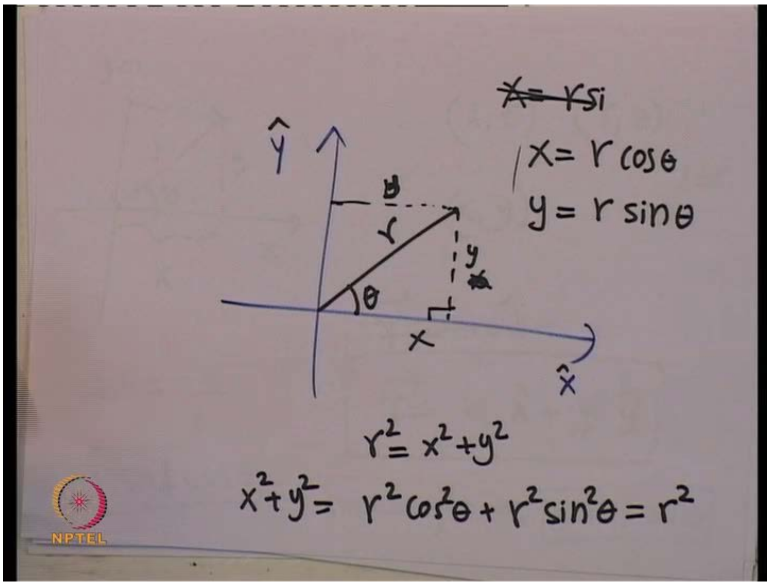

So, let us think about this. So, r. So, if you have…Let us draw this again. X and Y axis and you have a vector r; you have a distance r and this is theta and this is your x distance and this is your y distance; sorry, this is your x distance and this is your y distance, and this is, this are the X axis and Y axis. So, this is your x distance and this is your y distance and we just said that, we just said that, x equal to r sin theta, sorry, r Cos theta. So, x is equal to r Cos theta and y is equal to r sin theta. Now, let us check this using some trigonometric idea that we know. So, if we know, if we have any right angled triangle…So, this is a right angled triangle. So, this is the 90 degree, right, this is 90 degree. So, this is a right angled triangle. This line, this line and this line, this three forms the right angled triangle and we know the famous Pythagoras theorem, which says that, the r square, which is this, is x square plus y square; r square is x square plus y square.

So, now, let us do this x square plus y square, here. So, if you do this, x is r Cos theta and y is r sin theta. If you do x square plus y square, which is r square Cos square theta plus r square sin square theta. So, r square is common. So, r square into Cos square theta plus sin square theta; and we know that, Cos square theta plus sin square theta is 1. So, this is r square. So, essentially, what we knew from the Pythagoras theorem is, essentially, here. So, this is a simple trigonometric idea, that we used to get this x square plus y square is equal to r square. And, that is essentially, essentially, that is what x, this means x equal to r Cos theta, you say, y is equal to r sin theta, only mean some trigonometric identity. But, this has an interesting application. That x component, that is what this x is, this x component is r Cos theta and y component is r sin theta.

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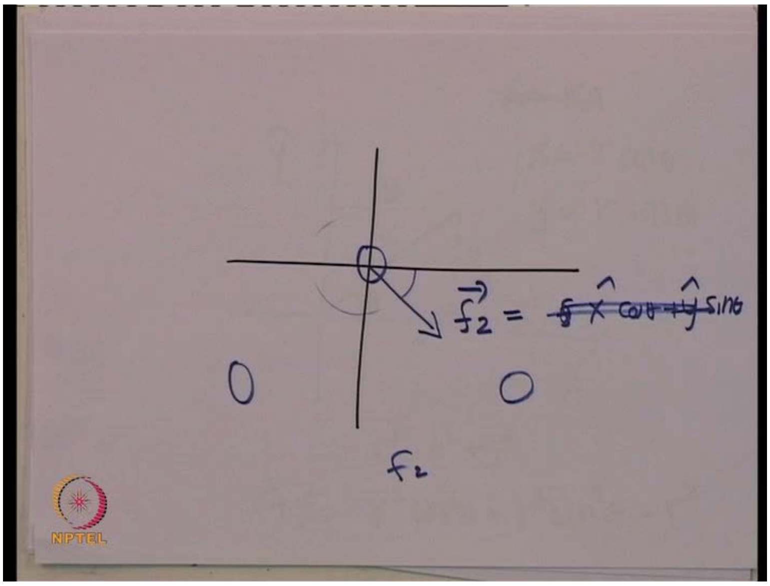

So, this has interesting consequences, like, we were discussing charges. So, if we had one charge here and two charges here, and if we say that, the force is in this particular direction, and if we know that particular angle...So, let us say, we know this particular angle. So, let us say, either you know this angle or you know this whole angle. If you know this particular angle, we can calculate the x component and y component, in the manner that we specified. So, this is, this is interesting con… So, one exercise will be, for you to check the x component and y component you got for the force in the previous day, can they be represented as a Cos theta and a sin theta? So, that is something which you would want to check. So, when I say, the vector f 2, that is, we yesterday's force, this (( )) can be written as some kind of x Cos theta plus y sin theta, where x and y…So, x, sorry, this can be written in terms of Cos theta and sin theta.

So, f 2 can be written in the cos…So, we were, after today's lecture, you would be able to write this, in a position, you will be in a position to write this force, in terms of Cos thetas and sin thetas. So, we have taken the first step. We have understood, how x component and y component can be written in terms of Cos theta and sin theta. And, how does this r square now depends on. r square is essentially…How do we calculate r square? That is something that we want to check. So, now, before, check… So, what, if something is r square…r square is nothing, but r into r; r times r is r square. So, to understand that, you would need a bit about, to you need to understand about product of two vectors. So, that is what the next idea that you will learn, that product of two vectors.

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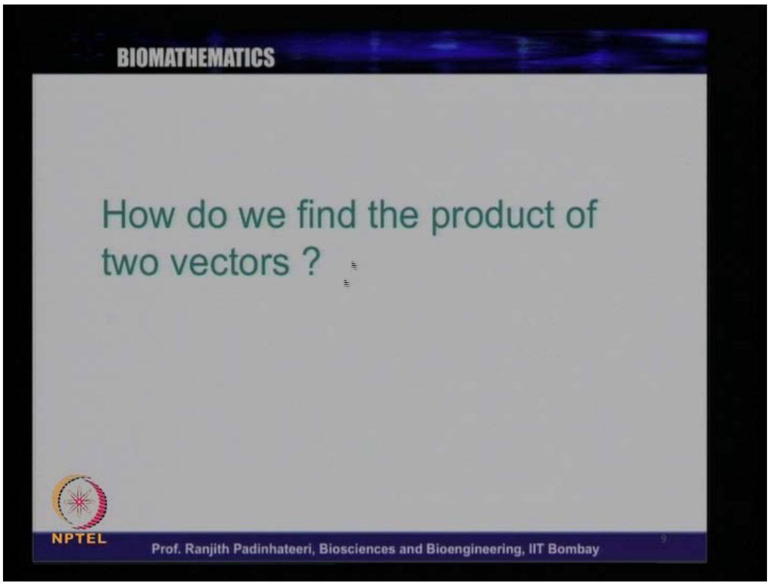

So, the question we get, we want to ask is, how do we find the product of two vectors? Now, you know that, vector has a magnitude and direction. And, we also show that, if you add two vectors, or, if you subtract two vectors, you always get another vector. Then, the question is, if we find the product of two vectors, will we get a vector or not? So, this is some question we can ask. If you find the product of two vectors, will we end up with a, another vector or a scalar? So, let us think about it. So, let us think about…Have a look at here. So, you have a pen here and if I apply a force on this pen, the pen moves. So, force is a vector. Force is a vector. The position of this pen is a vector.

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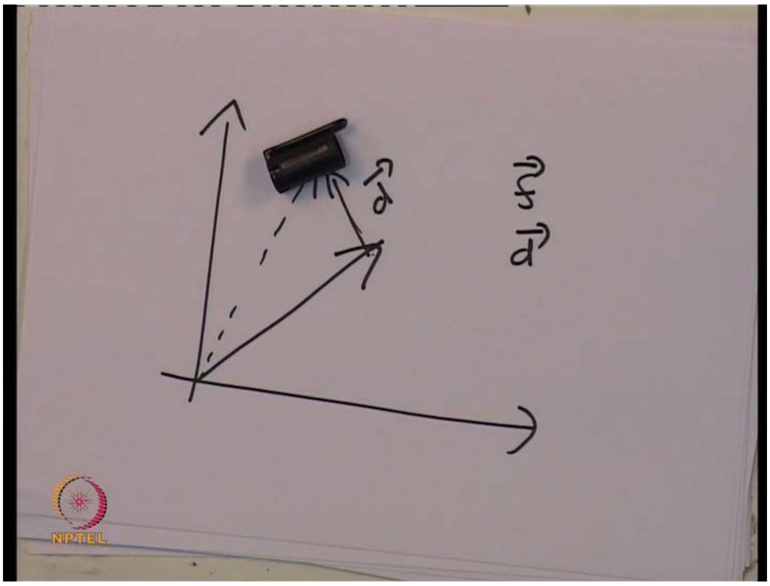

You can always represent an X axis and a Y axis and the position of this, position of this can be represented by a vector. This particular vector represent the position of this particular, the top of this pen. Now, I can apply a force to change this position. I change the position from here to here. So, I, I introduced a displacement. So, I change the position from here to…I change the position. Now, the new position is this. So, essentially, the way this, this, this top, this particular thing moved by certain distance. So, this is a displacement. So, this distance d is a vector. It moved in a particular direction. Something which was here previously, moved from here to here. So, when this is moved, I, I applied a force. I applied a force f, such that, it moved in this particular direction.

So, you have a force which is a vector; you have a displacement, which is a vector. Now, the product of force and displacement, we know is energy. So, what is energy? Energy is, is it a vector or is it a Scalar? It a, as you know, energy is a scalar. Energy has no particular direction. So, since energy is a scalar, it is clear, or it occurs to us, they (( )) that, the product can be a scalar. So, a product between two vectors can be a scalar. So, it turns out, the realities that you can have, the product of two vectors can some time be a scalar, sometime be a vector. So, you have two situations, two possibilities. The product can be either, it can be either a vector or a scalar.

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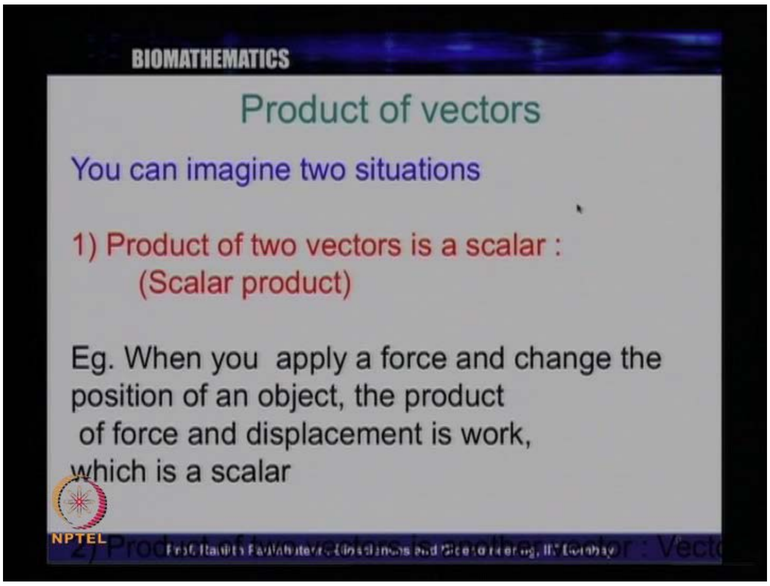

So, have a look at here. So, what I, you can imagine two situations. Product of two vectors is a scalar; that is one situation; that is, we just discussed. Example, when you apply a force and change the position of an object, for example, the product of a force and displacement is work and the energy is, the work is a scalar, or, the energy is a scalar. So, the product of force and displacement is an example for a, something called a scalar product, where the product is a scalar. You can also…Now, what is the example that you have, where you have the product is a vector? So, again, if I look at here, I can apply a force and then, move this in a particular way, in a…So, the, you know, something can rotate in a particular way.

So, let us say, this, this, this way of rotating, this is, we can say, what we are rotate, say, generating this, we, this is a counter clockwise rotation; something is rotating in a counter clockwise. I can also apply a force. I can apply something and rotate it in a clockwise direction. So, what you have to apply to do this rotation is called a torque; you to apply a torque. So, torque is some quantity, which is a vector, which is again the product of the force you apply and this distance. So, the product of this force and this particular distance, if I try to rotate it here, or, try to rotate it, apply a force here, or, if I apply a force here, the torque is different. I can rotate, I can rotate it more, by applying a force here. So, the torque is essentially, a product of force into the distance, from this particular pivot, from where it is rotating.

So, any time, like, all of you might have seen, when you try to open a door, the handle, the force you apply on the handle is making it to rotate. So, the essentially, what you are applying is a torque. So, the torque is again, force to rotate something. So, the torque is essentially, a vector, which is also a product of two vectors, we will see that. Another example, which is biologically very...So, the torque, which, when you are opening the door, the torque is something that we see in everyday life. Another such example, which is biologically relevant will be, one example will be, let us say, if you want to twist a DNA. So, DNA, you know that, their proteins twists the DNA and they get supercoiled and so on and so forth. So, if you want to twist a DNA, you have to apply again, a torque.

So, proteins apply a torque on DNA. So, the torque has a particular direction. So, this is some quantity, which is product of two vectors, but is again, a vector. So, two vectors and the product is the vector, is a torque. Again, in bacterial flagella, you know that, the flagella, flagellar motor can either rotate clockwise or counter clockwise. This is another example, where things, you have to apply a torque, which is again, product of two vectors. You can also holding something right, if you want to hold something, this muscles will have to apply some force, apply some torque; otherwise, if there is a heavy object, which will try to fall under gravity.

And, if you have to hold them, this muscles, or if you want to, if you do this, if you want to push, pull this up here, essentially, you are applying a torque. So, there is particular direction for this. So, all this are some vectors. We will, we will, we will explain this a little more carefully. But what I am trying to say is that, there are objects which are product of two vectors, but they have directions. Such objects are, they…One example of such object is torque, which is, you are, you are very familiar, when you are opening a door; or, even in the Biology, when you, when you talk about super-coiling, there is some direction associated with it and the, you have to apply some torque to supercoil the DNA and such torque has direction. So, essentially, we will discuss them, but then, what we want to understand is, how do we find this product of two vectors. If you are given two vectors, how exactly will you find the direction of these two vectors? So, that is the question that we are interested to ask.

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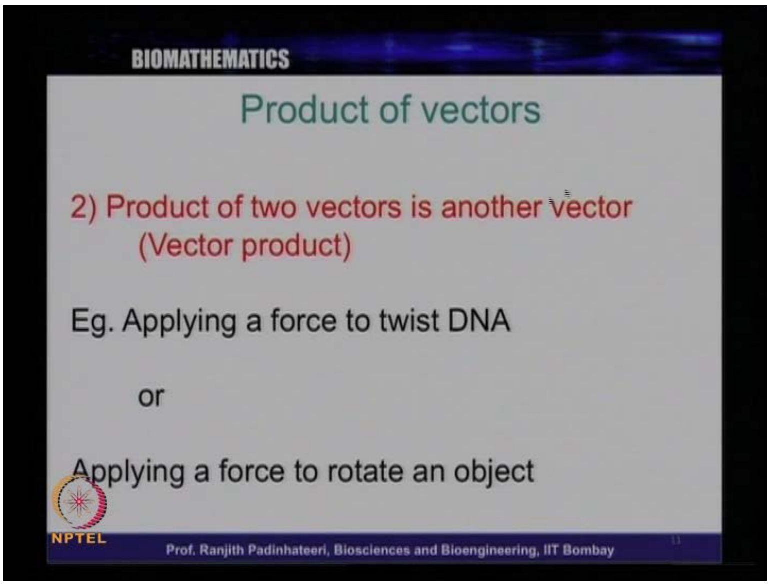

So, let us say, the product of two vectors. The second point I wanted to make is that, the product of two vectors is another vector, and, that is, example is, applying a force to twist DNA; applying a force to rotate an object. So, these are examples, where you have force and some displacement, essentially, distance, essentially, giving to a torque or a twist.

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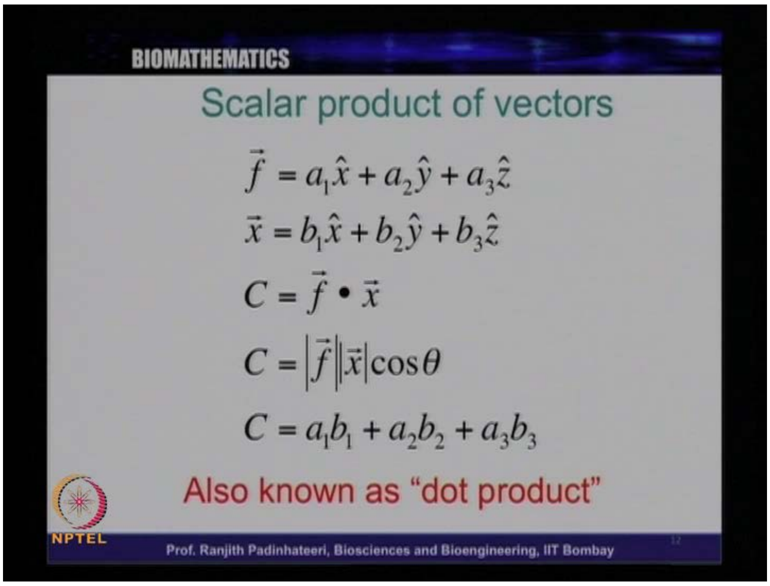

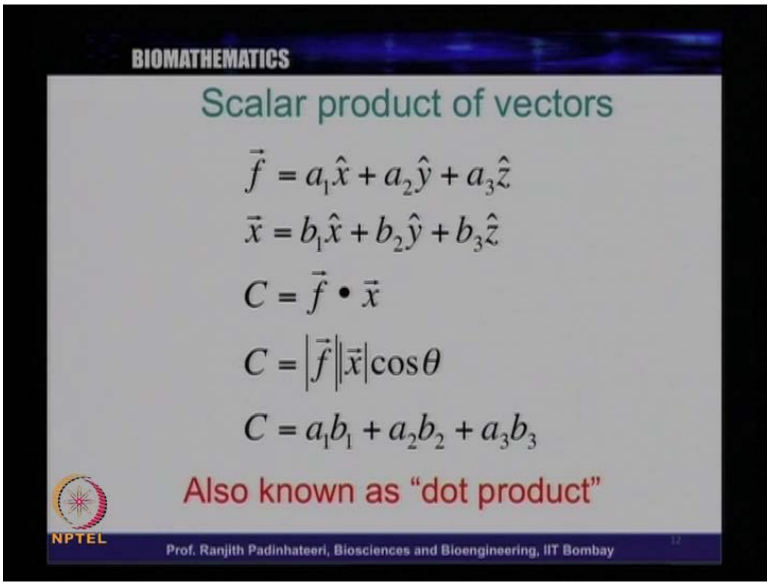

So, now, how do we find this scalar product? This scalar product is defined in this particular way. So, let us say, you have a vector f, which is some x component a 1, some y component a 2, some z component a 3 and some distance x, which is some x component b 1, some other x component b 2, some other x component, some, some x component b 1, some y component b 2, some z component b 3; then, the product, the scalar product, which is written as f dot x… So, this is sometimes is also known as dot product, because this is represented typically, by a dot in between this. And, this is nothing, but the magnitude of f times, the magnitude of x times, the Cos of the theta between f and x. You have two vectors, you can always define an angle between these two vectors. So, this f into x into Cos theta. So, this is what it is. So, let us have a look at carefully, how exactly this is defined. So, we said that, I have some object here. So, we had discussed this. So, this is some object here. If I apply a force, in this particular direction…

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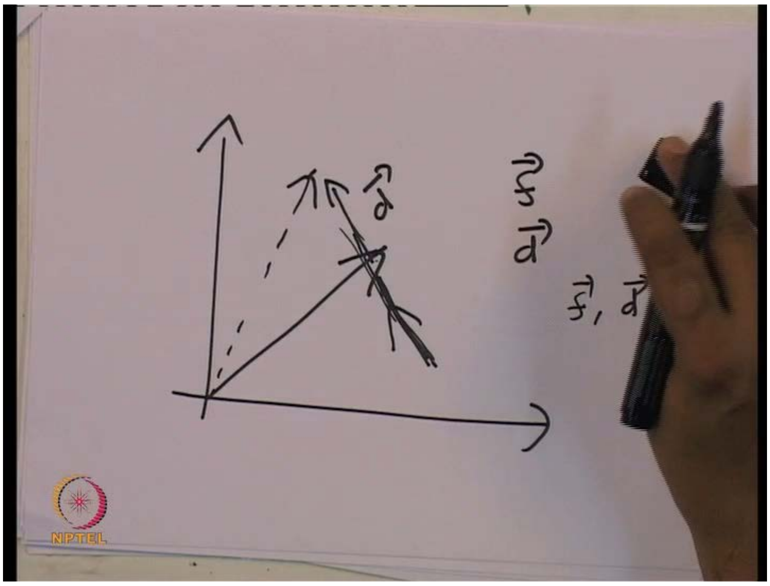

So, my force is in this particular direction. Let us say, I am applying a force in this particular direction and it is moving in the same direction as, moving in the same direction. So, the angle between the force and the distance…So, you have force and you have a distance. So, let me, let me explain this again here.

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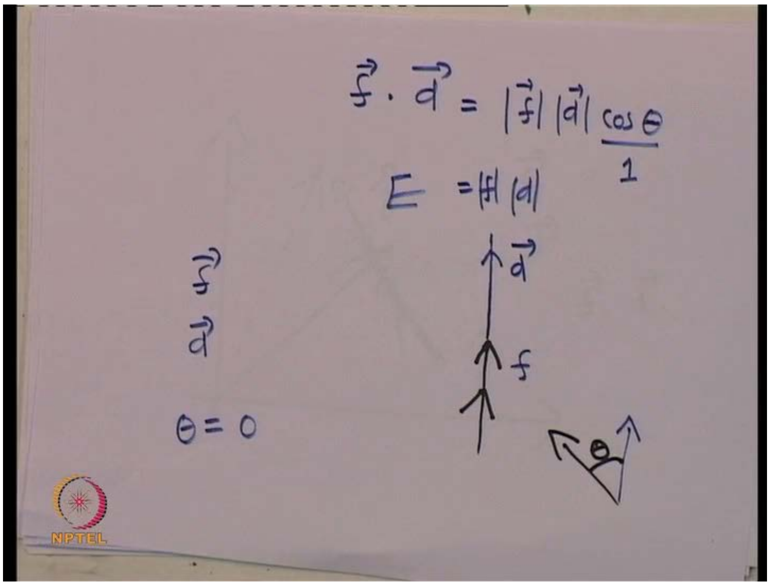

You have, you have something here, an object here, and you want to apply a force in this particular direction to move it. So, this is your direction of the force. So, let me, apply this force in this particular direction. So, applied this force and made it to move. So, I made it to move, in this particular direction. So, this is the direction in which it moved. So, this is the d. So, the force which is a, d, they are in the same direction. So, the angle between the force and...So, you have vector, force and the d, which is this displacement vector…So, the d, the distance, the angle between f and d, is 0. So, the theta, in this case is 0; no angle. They are going in the same direction. Then, the f dot d…So, let me, let us write f dot d, this is the product. This is mod of f, mod of d, into Cos of theta, which is angle; here, the theta is 0.

So, Cos theta is 1, when theta is 0. So, Cos theta will become…So, this will be just mod f mod d. So, this is the typical energy that we talk about. f into d, when we say, we are talking about, you are applying a force and it is moving in the same direction as you apply the force. You need, need not move, if I apply a force in this direction, it can move in some other direction. I can apply a force in this direction and the object can move in this particular direction. So, then, there is an angle between this. So, then, the work done is mod f mod d Cos theta. In the last class, we discussed how do we find the mod of a vector.

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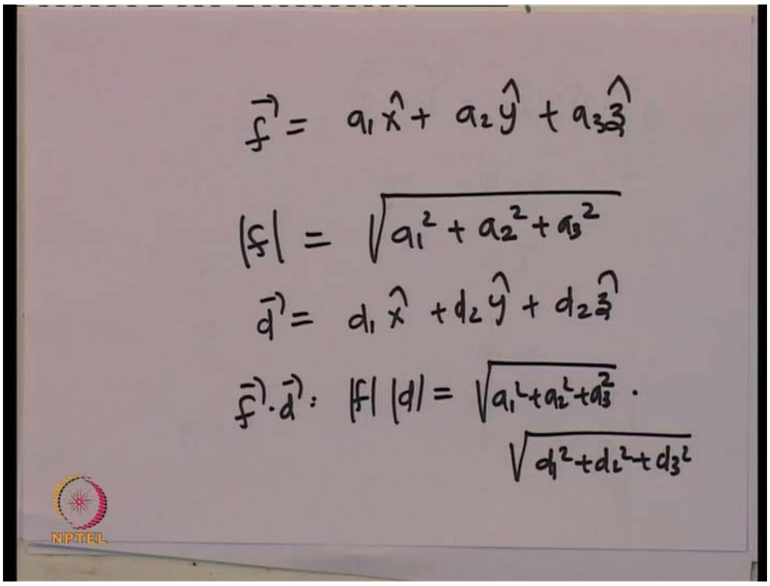

So, if we have any vector f, which is a 1 along X axis and a 2 along Y axis and a 3 along Z axis, the modulus of this, we said is, root of a 1 square plus a 2 square plus a 3 square; this is what mod of this. We also said that, similarly, if you have a vector d, which is d 1 x plus d 2 y plus d 2 z, then, f dot d is mod f, mod, dot d, mod d, if they are in the same direction. So, this is basically, root of a 1 square plus a 2 square plus a 3 square into root of d 1 square plus d 2 square plus d 3 square. This is how you find out the energy. So, this is basically the energy. This is the scalar product. Now, if there is an angle, you have to take the angle also, into account. So, you will get f d Cos theta. We just…So, now, let us take a simple example. Let us take an example f dot f itself.

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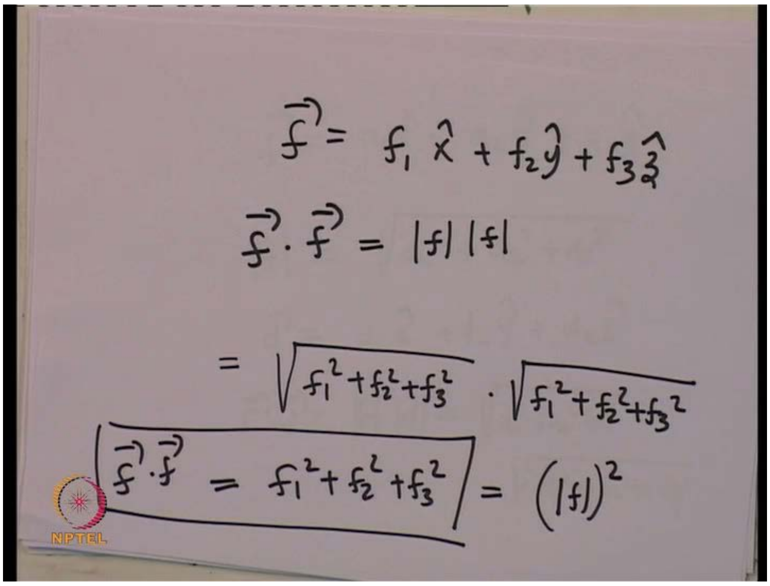

So, we, let us say, f is some vector. Let us call this f 1 along X axis, plus f 2 along Y axis plus, f 3 along Z axis. Now, let us say, f dot f. What is f dot f? This is like finding square. So, this is mod f, again mod f; and, the Cos of angle between, if you have same vectors, there is no angle, because f is the same direction as f. There is f and f, they are the same thing. So, the direction is the same. So, Cos theta is 1. So, just f times f. So, now, what is mod f? mod f is root of f 1 square plus f 2 square plus f 3 square, into same thing, f 1 square plus f 2 square plus f 3 square. So, this is square root, square root goes away and you will get f 1 square plus f 2 square plus f 3 square. So, f dot f is f 1 square plus f 2 square plus f 3 square. So, this is an interesting result, that will be useful. If square f of vector is f 1 square plus f 2 square, but this is, this is how you find the square of a vector.

So, when you say f square, or any, any square of a vector, you will have this particular form. So, you know this is nothing, but mod f square, mod f into mod f. So, you know mod f is square root of f 1 square, f 2 square, f 3 square and square of this is this. Now, let us have a look at another one. So, let us again, go back to 2 dimension, so that, everything is simple.

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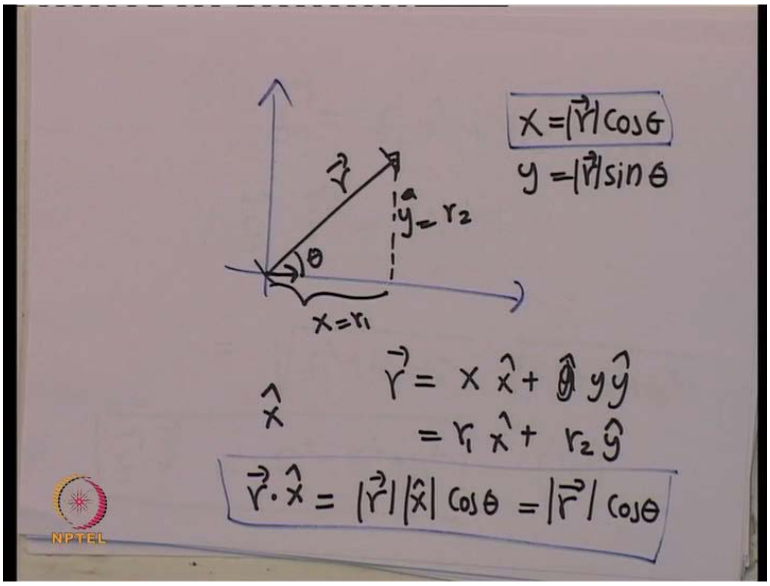

So, let us think of a vector in 2 D. So, you have a vector in 2 D, which is this vector and this has some x component and some y component. So, this is the x component and this is the y component. Now, we already learnt that, this can be represented as x is equal to r Cos theta and y is equal to r sin theta; we already learnt this, where this is the angle theta. Now, this is the, a unit vector in this direction… So, let us say, a small vector, a unit vector in this direction can be represented as x cap; x cap is a unit vector in this direction. And, we, let us call this vector r. So, x is this distance. This distance is modulus of r, r vector; modulus of r vector is this particular distance. So, you know that, this distance times Cos theta and this distance times sin theta is x and y. Now, let me also, we can also define r as x component along X axis and y component along, y along Y axis.

So, or let me write this, r 1 along X axis and r 2 along Y axis; this is r 1. So, x you can write r 1 if you want, and this distance, this distance y, you can call it r 2. Now, if we find r vector dot x cap, what is this? What is r 1, r vector dot x cap? It turns out that, if you do this, according to our definition, this mod r vector mod x cap vector into Cos of this angle, between, theta is angle between this x and this r…Now, mod of x is, x cap is 1. So, this is r cap, r times, the modulus of the r vector times Cos theta. So, have a look at this. So, r dot, r dot x cap, r vector dot x cap is nothing, but mod r Cos theta, which is the same thing that we described here. So, this r Cos theta, is nothing, but mod r dot X axis. If you do this, you will get r Cos theta.

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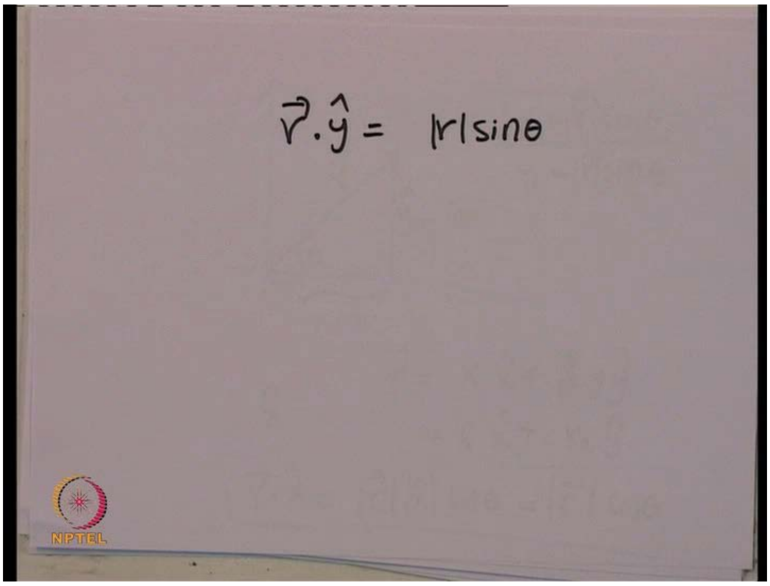

Similarly, just viewing this, you can also see that, you can also see that, r vector dot y cap is mod r sin theta. You can use simple trigonometry that you already know, and find out the dot Product between the r vector and the y, y, unit vector along y. So, this is all related to each other. So, this is one thing that you should know about the dot product. And, another kind of thing that you…There are a few things that you can deduce from this, which we will come to, we will come, we will discuss this later, a few things that we can use, the way we can use the dot product in Biology.

Of course, when you are calculating energy is a big example; because force and displacements are very common. You might have heard of something called molecular dynamic simulations. Molecular dynamic simulations are something that is extensively used in Biology to understand protein folding or dynamics of proteins or dynamics of bio- molecules. So, when we set up, when somebody set up, sets up molecular dynamic simulation, they have to get exact idea about vectors, positions and the energy. So, they have to calculate the force. In the molecular dynamics simulation, what they are essentially doing is, solving a set of differential equations to get the positions.

So, they have to use the idea of, all these idea of calculating the force between the charges that we discussed. They have to calculate the position of each atoms. So, they are represented by vectors; they will have x component, y component and z component. So, the position of each atoms are represented by vectors and the forces, there are each charge, each atom or each amino acid is, each atom in an amino acid will be feeling force from, due to all other atoms. So, basically, you have to calculate the resultant force due to all other atoms to do this molecular dynamic simulations. So, we have to calculate the resultant force that we discussed; you have to calculate the position vectors. And then, you have to calculate the energy. So, energy is nothing, but the force times d, f dot d, just we discussed.

So, you have to also use actually, the idea of a scalar product. So, everything that we learnt so far, that is the idea of vectors, so, finding the resultant force and position vectors and the dot product to calculate the energy, etcetera, has to be used, if you want to really do a molecular dynamic simulation, for example; or, if you want to do theoretically, any calculation of protein folding or any calculation of dynamics of bio-molecules. If you want to do it, do those calculations, you basically have to understand, whatever we have been discussing so far. Now, what about the next one, which is vector product. So, what is the definition of a vector product?

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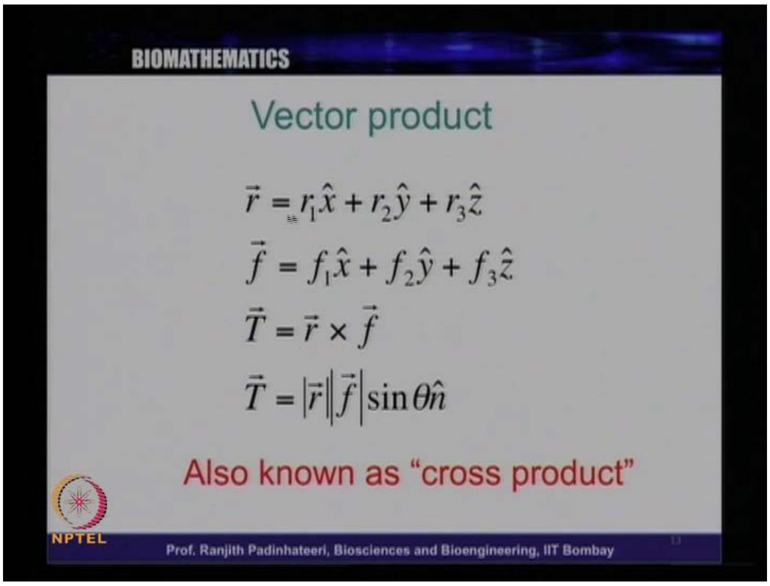

So, the definition of a vector product is basically, if you have a vector r, which is r 1 x plus r 2 y plus r 2 z, and f is f 1 x plus f 2 y plus f 3 z, you can define the torque T as r cross f. So, this is called cross product; this is because, the r and f are vectors, and the resulting torque, is also a vector. Why is this resulting torque a vector? Because, now, how, what is the answer? So, this is basically, mod r mod f sin theta which is the angle of theta between this; and n is the unit vector, which is the, representing the direction along which the torque will act. So, what is the direction of the n, that we will discuss later. But, n will represent, is a unit vector, that represents the direction of this torque.

So, essentially, the answer r cross f is a, is basically, r cross f is basically a vector, and this kind of products are known as scalar products, sorry, this kind of products are known as vector products, where the resultant, the result is essentially, a vector; r cross f is a vector. So, you can, we can think of simple thing that we do every day, that is, again go back to opening and closing the door. You can apply, if you apply in a particular direction the force, you will open the door. If you apply the force in another direction, you will close the door. So, for this particular torque, there is plus or minus sign, if you wish. So, or in other words, if you look at here, if you look at, if you look at this particular case of applying, this is the distance r.

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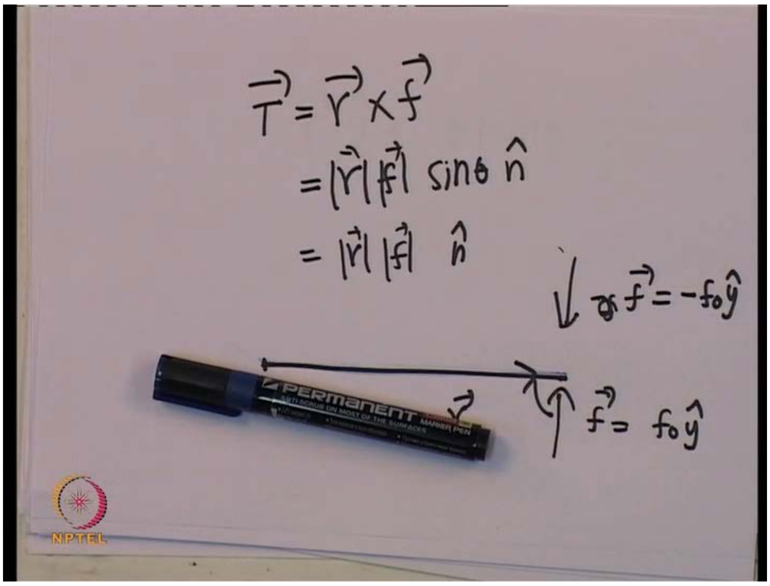

So, I can call this as the distance r. So, let, let me keep this here. So, this distance, let me call this r, this is my r vector. So, this vector is my r vector. Then, what I am doing is, I am applying a force here. So, if I apply a force in this direction, the torque, so, this will rotate in this particular direction; if I apply a force in this direction, it will rotate in this direction. So, this will be counter clockwise rotation and this will be a clockwise rotation. So, there is a direction of the force. This is, it can, if we call this plus f and if we call this minus f; this is a force you are applying in the y direction. So, let me call this y direction. So, f is some f 0, along the y direction. Here, I am applying the force, which is along the minus y direction. So, minus f 0 y. So, I can either represent along plus y direction or minus y direction. So, depending on that, the torque which is defined as T here, is basically, the r, which is always in the same direction, cross f. So, f sometime, with that, that direction, or the other direction. So, depending on that, the direction of the torque will change. So, we said that, r f sin theta.

So, we know that, the theta, which is this angle, this angle is 90 degree here. So, when 90 degree, theta is, sin theta is 1. So, it is essentially, r f and there is a unit vector n. So, the answer is r f n; the modulus of r, modulus of f, n. Now, what is n? So, it turns out that, n will be always in the direction perpendicular to the direction of the force, and the, in the, and the r. If f and r are in the 2 D plane, the n will be in this perpendicular direction. So, this is one way, where you want to know about this scalar product. So, we will, we will, vector product and we will come back to this and tell you this in little more detail, whenever we need it, to use it for dealing with some examples. But for the moment, you just understand that, this is the case. And, one more idea, which I want to say today briefly, and which we will, we will elaborate in the coming classes is, something called gradient.

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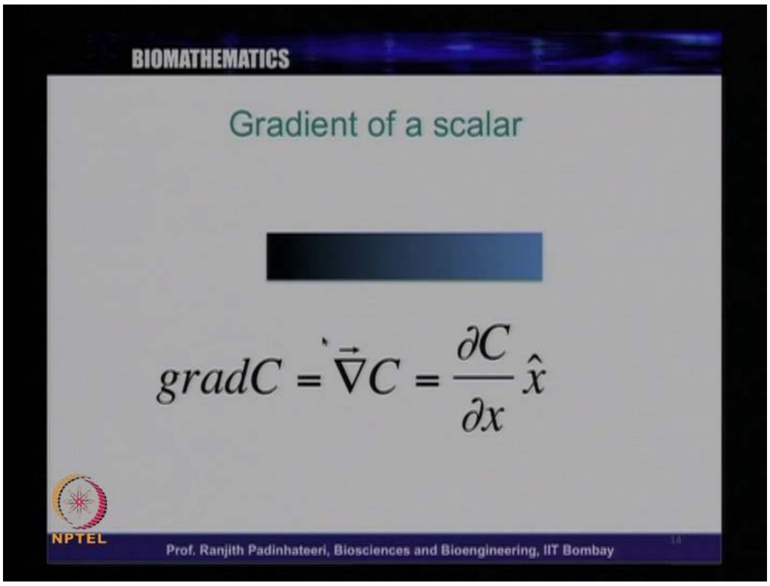

So, have a look at here, that is brief. If, imagine this is a concentration of some protein and the concentration of the protein is more here and is less here. It is dark here and this is not so dark here. So, the concentration is changing in this direction. But, if you look at here, in this direction is not changing; in this x direction the concentration is changing. So, to represent that, this direction for the concentration is changing, we can introduce something called gradient. So, the gradient is some vector called dell. So, and concentration is a scalar. So, gradient of a concentration can be represented by derivative of C, with respect to x, with an x cap. So, this is some definition, which we will come back later and try and help you understand in the coming classes. But so far, today, we learnt a few things and we will stop with this today.

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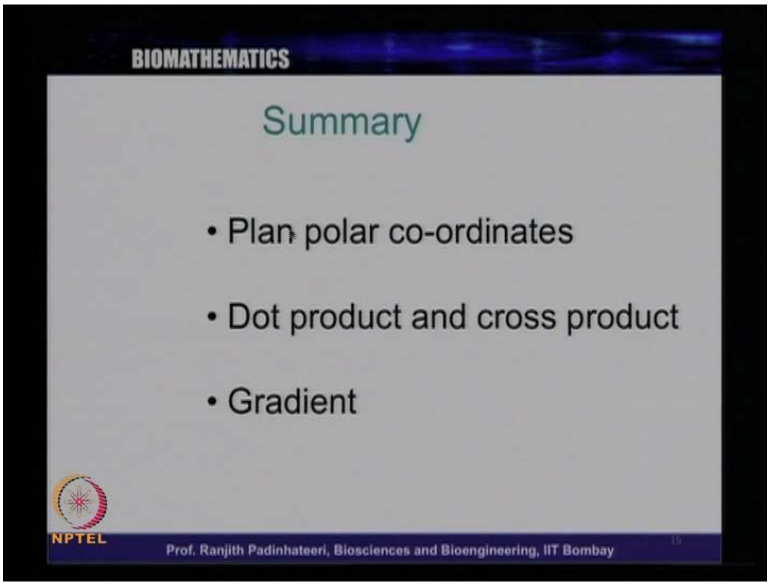

So, to summarize what we learnt today, we learnt about plane polar coordinates; see there is an error in what I wrote here. So, it is essentially, plane we talk talked about something called plane polar coordinates. This is basically, this is basically, have a look at the slide, and the plane polar coordinates is r and theta. You can represent any vector by a distance and an angle theta. So, that is called plane polar coordinates. And, we also learnt about dot product and cross product, two way of finding the products of vectors. We also learnt about the gradient. We briefly mentioned about the gradient and we will discuss this in the coming, one more class. In the coming class about vectors, we will discuss about that gradient and how will that lead to diffusion equation, etcetera. So, with this, I will stop today’s class. These are the ideas that we learnt, and we will continue the discussion in the next lecture. Bye.