Computational Continuum Mechanics
Dr. Sachin Singh Gautam
Department of Mechanical Engineering
Indian Institute of Technology, Guwahati

Lecture - 08
Linearization and Directional Derivative, Tensor Analysis -2

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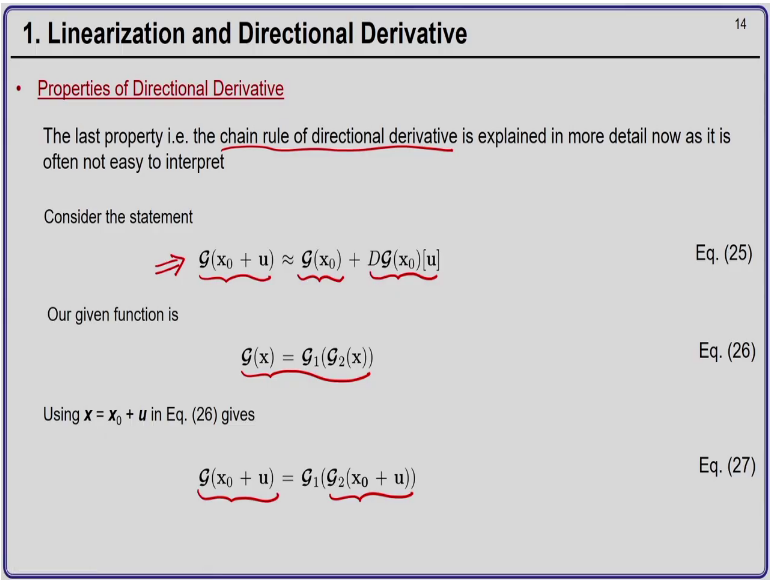

So, the last property of directional derivative that is the chain rule of directional derivative which we saw in the previous slide is now explored in more detail because it is not very easy to interpret ok. So, consider this statement given by equation 25 ok. So, the quantity G evaluated at x 0 plus u and when expanded using Taylor series can be written as the quantity evaluated at x 0 plus the directional derivative of quantity G at x 0 in the direction u ok.

So, now our given function is G equal to G 1 and G 1 is a function of G 2 and G 2 is a function of x. This is shown by equation 26 ok. So, now, using equation 25 for G 2 ok, we can write G 2 ok. So, G 2 is x 0 plus u ok, we want to get the directional derivative of G at x 0 plus u. So, using equation 25 for G 2 ok, we see G 2 is G 2 x 0 plus directional derivative of G 2 at x 0 plus u ok.

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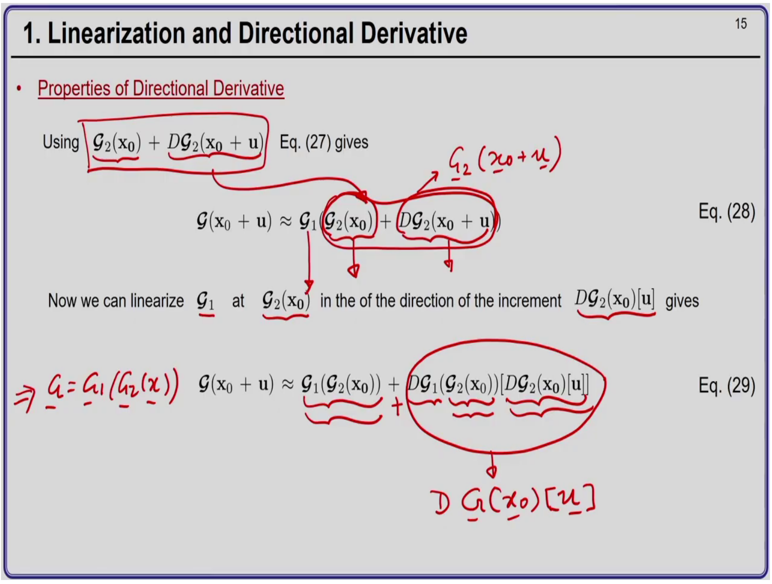

Therefore, substituting this expression over here; so, this was nothing but G 2 x 0 plus u ok. So, this is the Taylor series expansion of G 2. Now, you can imagine G 2 is say another vector. It is another vector and this term over here is the direction ok. So, now, if you have to do the Taylor series expansion of G 1 in the at the point G 2 ok, in the direction given by this second term ok; so, that would be ok.

So, it means you have to linearize G 1 and G 2 x 0 ok, in the direction of G 2 evaluated at x 0 in the direction u ok, that is the directional derivative of G 2 in the direction u ok. So, when you do this, what do you get? G 1 evaluated at G 2 plus the directional derivative of G 1 evaluated at G 2 x 0 in the direction of the directional derivative of G 2 ok.

So, now, you can see if G is G 1, G 2 x ok. Now, I am putting only one under bar because I just want to show that this is not a scalar; I mean need not be scalar, it can be vector, tensor whatever ok. So, the directional derivative of this quantity G over here ok, which is given by G 1 function of G 2 function of x is nearly G 1 evaluated at the point G 2 ok, x 0 ok.

Then, plus the directional derivative of G 1 at G 2 x 0 in the direction of the directional derivative of G 2 at x 0 in the direction u ok. So, that is what our this statement ok, that was our last property equation number 24, that is what this means ok.

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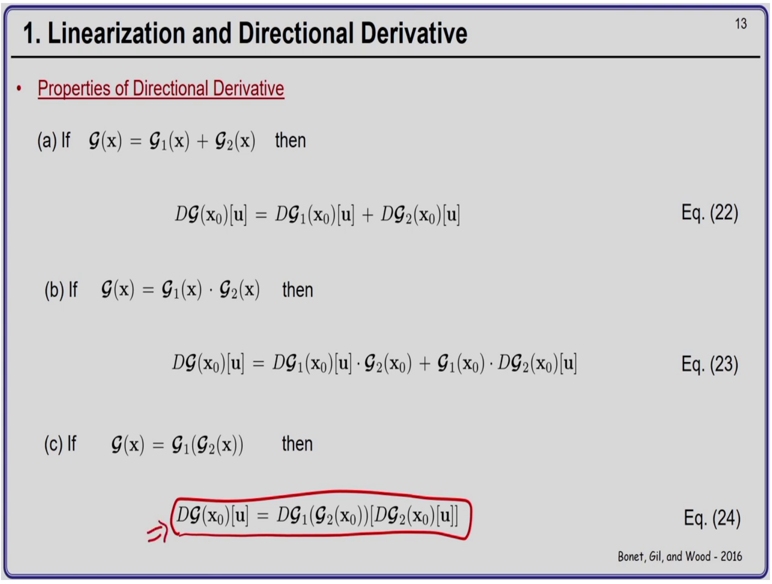

So, equation 24, this is your directional derivative and therefore, you can see this is nothing but your directional derivative of G evaluated at x 0 in the direction u ok. That is how that property equation 24 actually came ok. So, you can understand what this quantity actually means ok. So, next we move to one example ok; we look actually two examples of application of directional derivative ok.

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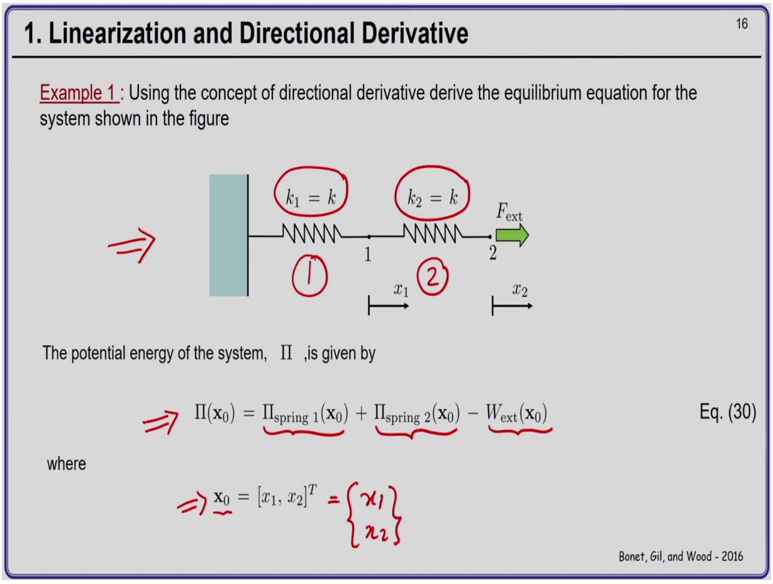

So, the first one is pretty simple ok. We just take the concept of directional derivative and we try to derive the equilibrium equation for the system as which is shown here ok. So, here what you have? You have two springs which are connected in series ok. So, the string spring stiffness of the first spring ok, there is a first spring, this is the second spring is k and the stiffness of the spring 2 is also k ok. At point 2, you have an external force which is applied ok. And say let x 1, x 2 are the displacement or the coordinates of points 1 and 2 after the equilibrium is achieved ok.

Now, we want to derive the equilibrium equation for this system using the concept of directional derivative ok. So, the first thing, we have to do is we write the total potential energy of the system ok. Now, the total potential energy of the system at equilibrium will be the potential energy of spring 1 at equilibrium position plus potential energy of spring 2 minus the work done by the external forces ok.

What are the expression for the potential energy for spring 1, spring 2 and the external work done ok? So, that we have to see next. So, remember x 0 is a vector which is x 1, x 2 ok. It is x 1, x 2 ok. So, this is not a non-linear system, this just a linear system; but to show that how directional derivative can be use to get the equilibrium equation, we have taken up this example ok.

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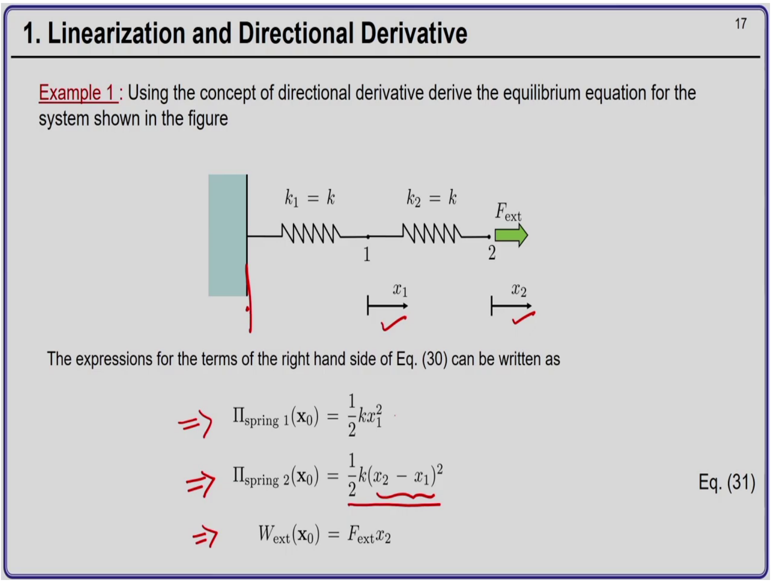

Next the expression for the potential energy for the spring 1 will be nothing but half k x square, where x is the displacement of spring 1 ok. So, what is the displacement of spring 1? It is x 1 minus this displacement at this point ok. Now, this is a fixed tend, so it does not get any displacement. The spring does not have any displacement at this point, so the potential energy of the spring will be half k x 1 square.

Now, the potential energy of spring 2 will be half k and the displacement square ok. So, the displacement of spring 2 will be x 2 minus x 1 ok. So, you have half k x 2 minus x 1 the whole square and the work done by the external forces will be F into x 2 ok. So, now, you can substitute equation 31 in equation number 30 and you can get the explicit expression for the potential energy of the system ok.

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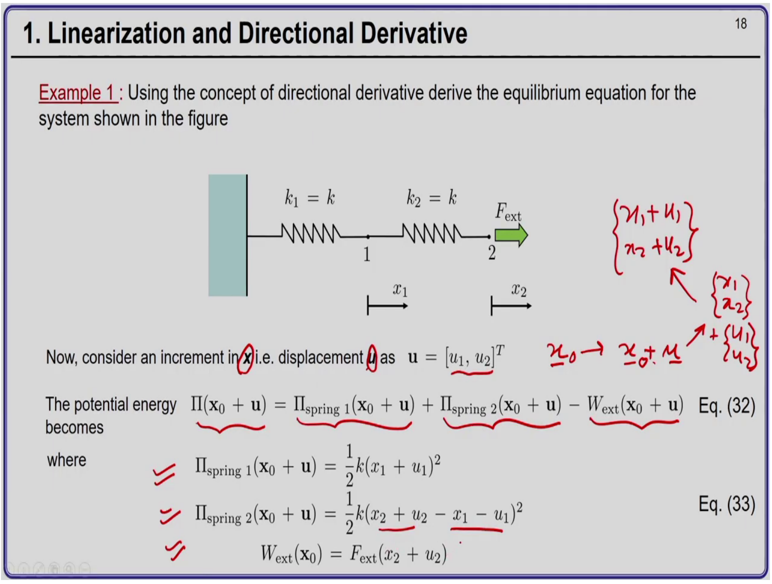

Now, you consider an increment in x ok. Now, from the equilibrium point there is a displacement u ok, where u is given by u 1, u 2 transpose ok. So, vector. So, now, from the equilibrium position, now if there is a displacement u. What will be now the change in the potential energy of the system? So, whatever happened? From x, you have gone to x plus u ok. Now, the total potential energy of the system will be evaluated at x 0 plus u ok.

So, you have potential energy of the system at x 0 plus u. The new point will be is the potential energy of spring 1 at the new point plus potential energy of spring 2 at the new point minus the work done to get to the new point by the external forces ok. Therefore, you can get the expression for the potential energy of spring 1 as half k x 1 plus u 1 whole square ok. So, if you see this expression over here, this is nothing but x 1 x 2 plus u 1, u 2. So, the resulting expression would be x 1 plus u 1, x 2 plus u 2 ok.

So, in your previous expression for potential energy, you just have to replace x 1 by x 1 plus u 1 and x 2 by x 2 plus u 2 and the potential energy for spring 1 will be half k x 1 plus u 1 the whole square plus half k x 2 plus u 2 minus x 1 minus u 1 the whole square and the work done by the external forces is F external into x 2 plus u 2 ok.

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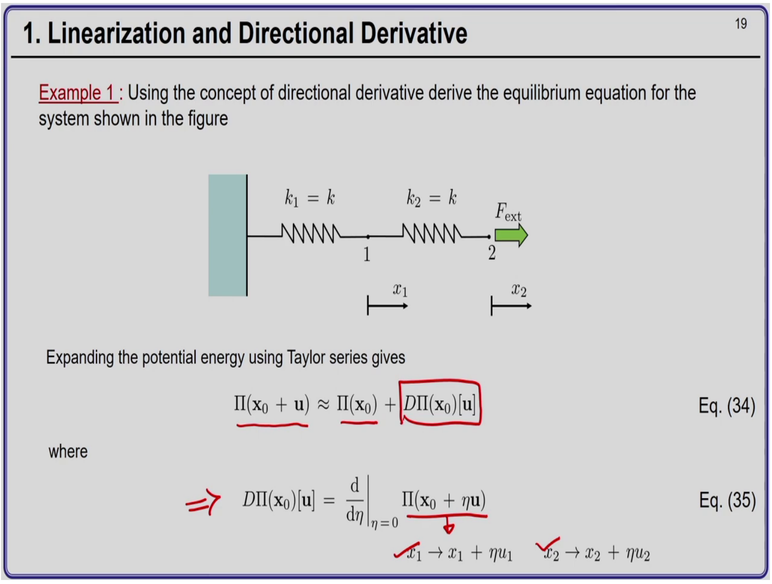

So, now, you can expand the potential energy at the current position using Taylor series and that is what you get ok. So, the potential energy at the current position x 0 plus u will be nearly equal to potential energy at x 0 plus the directional derivative of the potential energy at x 0 in the direction u ok.

Therefore, you can use the concept of directional derivative and this is a expression how you compute the directional derivative. It is given by d by d eta at eta equal to 0 pi of x 0 plus eta u ok. So, here to compute this expression x 1 has to be replaced by x 1 plus eta u 1 and x 2 has to be replaced by x 2 plus eta u 2 ok. So, if you do this, you can compute the directional derivative ok.

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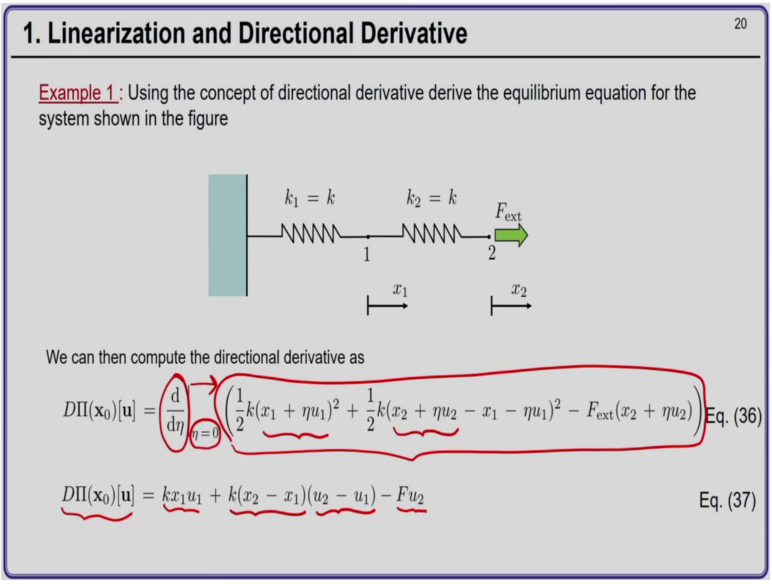

Let us see what do we get ok. So, that is what you get. You replace x 1 by x 1 plus eta u 1 x 2 plus eta u 2 and then, this is the expression for the potential energy ok, that is what you get. And now, it is very simple, you take the first take the derivative of this expression with respect to eta and then, u substitute eta equal to 0 ok.

So, this I leave it to you. If you do this, what you will find? You will find that the directional derivative of the total potential energy of the system at point x 0 in the direction u will be k x 1 u 1 plus k x 2 minus x 1 into u 2 minus u 1 minus F u 2 ok.

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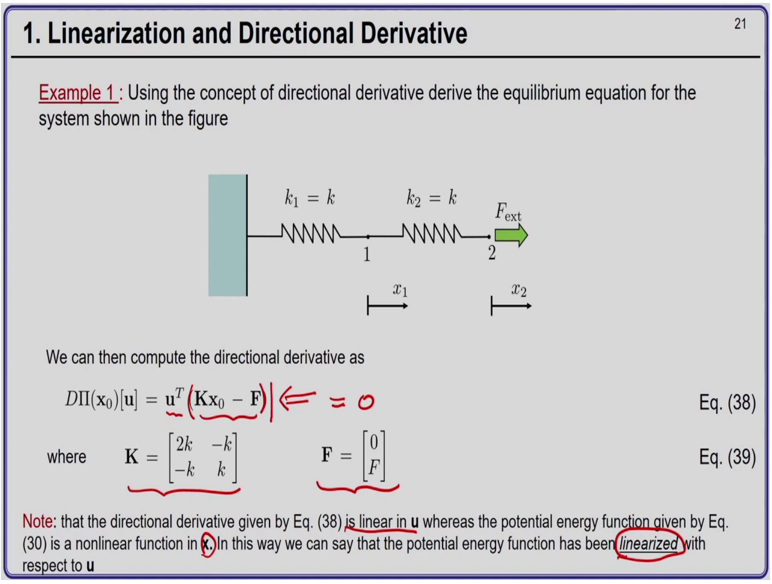

Now, this expression can be written in a matrix form. It can be put in a matrix vector multiplication form as u transpose bracket K x 0 minus F, where K is called the tangent matrix and F is called the external load vector and equation 39 gives you the expression for the tangent matrix and the force vector ok. So, that is what you get for the value of directional derivative of the potential energy computed at x 0 in the direction u ok.

Now, you note that the directional derivative which is given by equation number 38; this equation is linear in u whereas, if you see the potential energy function which was given by equation 30, it is a non-linear function in x ok. So, in this way, we can say that we have linearized the potential energy function with respect to u ok. So, this point you note equation 38 is linear in u ok.

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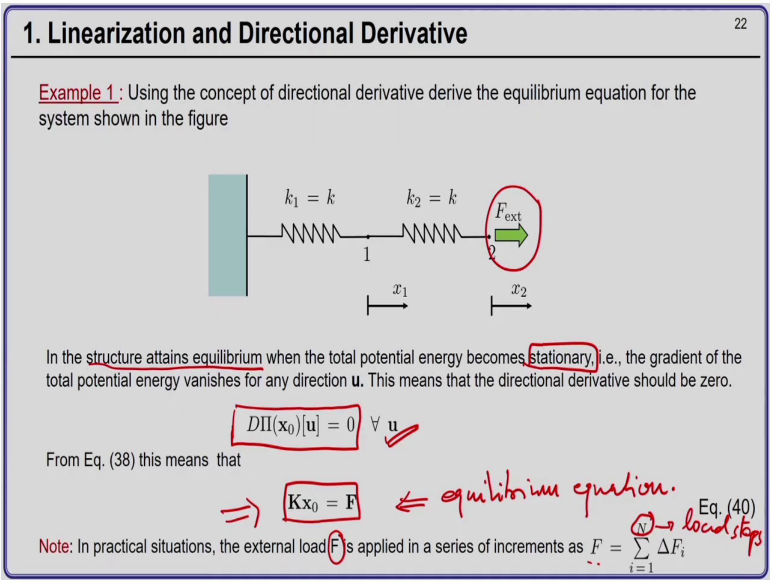

So, now the structure will attain equilibrium, when the total potential energy becomes stationary ok, that is the gradient of the total potential energy vanishes in any direction u. This means that the directional derivative should be equal to 0 at point x 0 and any direction u.

For all directions u, the directional derivative of the total potential energy evaluated at the equilibrium position should be equal to 0 ok. So, now, if you see equation number 38 and now, if you substitute this equal to 0, what do you see? u is a arbitrary direction, I mean it was up to us.

So, if u transpose K minus K x 0 minus F has to be equal to 0, what does it mean? That K x 0 should be equal to F and this is your equilibrium equation, this is your equilibrium equation ok. So, you see here how the concept of directional derivative has held us in deriving the equilibrium equation for the two spring system under the action of one external force with equal spring stiffness and the final expression is given by equation number 40 ok.

So, now, in actual practical application this external force over here ok. This will not be applied in one shot ok. What will you do is the total force will be a high magnitude, so it will be split into smaller loads ok.

So, this total load F will be applied in increments which means F will be summation from i equal to 1 to n delta F i ok. So, you will have F equal to delta f 1 plus delta f 2 all the way up to delta fn, where N is called the number of load steps ok; N is call the number of load steps ok. So, this also called the incremental approach ok.

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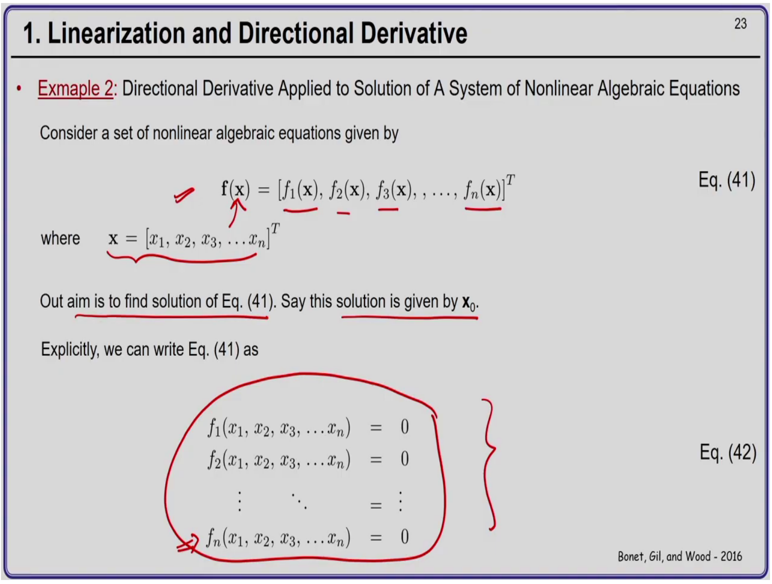

Next, we look into the application of directional derivative to the solution of a system of non-linear algebraic equations that is what we are going to get in non-linear finite element method ok, displacement base non-linear finite element method ok. So, consider you have a set of non-linear algebraic equations which is given by equation number 41 ok, where f is a vector function ok; f is a function of another vector x, where f is f 1 comma f 2 comma f 3 all the way up to f n ok.

So, there are n such functions ok. So, explicitly ok, these are these equation 41 can be written as n such equations f 1 which is a function of x 1, all the way up to x n equal to 0; f 2 function of x 1 to x n all the way equal to 0; like this the last equation is f n which is a function of x 1, x 2 all the way up to x n equal to 0 ok.

So, where the vector x is expressed as x 1, x 2, x 3 all the way up to x n. So, they are n unknowns ok. We have n equations; we have n unknowns and these are non-linear algebraic equations. So, that is what our aim is we want to find the solution of equation number 41 ok.

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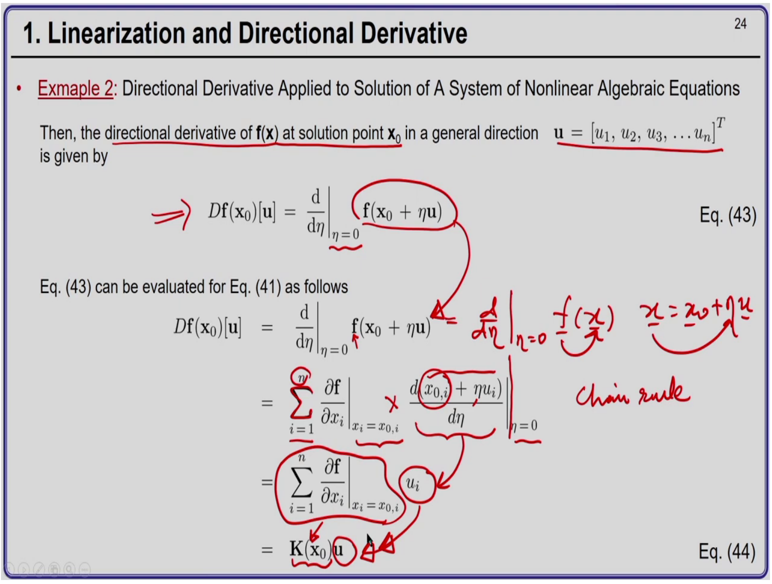

Now, let us say this solution is given by x 0 ok. So, how do we approach ok? So, what we do is we take the Taylor series expansion of the function ok, like similar and we look into the directional derivative of our function at solution point x 0 in any general direction u which is given here. And then, the directional derivative of f evaluated at the solution point x 0 in the direction u will be d by d eta of f evaluated at x 0 plus eta u at eta equal to 0 ok.

So, now can we simplify equation 43 for our given set of non-linear algebraic equations? So, let us see how you can do that ok. So, the first we can write the expression for directional derivative and then, this f for here is nothing but what is given by equation number 42 in the previous slides ok. See you have these n equations ok. So, using chain rule you can write ok. So, using chain rule, you can write summation over i equal to 1 to n del f by del xi evaluated at the equilibrium or at the solution point into d by d eta of x 0 plus eta u i ok. This evaluated at eta 0. This is your using chain rule because f depends on x 0 plus eta u ok.

So, you can write this as d by d eta of eta equal to 0 to look it more closely, let us say this is x ok, where x is x 0 plus eta u. So, f is a function of x and x is a function of eta. So, if you have to take del f by del eta, it would be del f by del x into del x del eta that is what we have done in the second step. Now, here if you see this expression, the first term is independent of eta and the second term only has eta. So, if you take this derivative, you only get u i ok.

So, the from the second term, you only get ui; eta equal to 0 have no meaning here. Because once you take the derivative with respect to eta, there is no eta left into the final expression ok. So, then what do you get? You get summation del f by del xi into ui. This you can write as a matrix K evaluated at x 0 into a vector u ok. So, this term over here ok. So, this term over here is nothing but your matrix K and the second term over here is nothing but your vector u ok.

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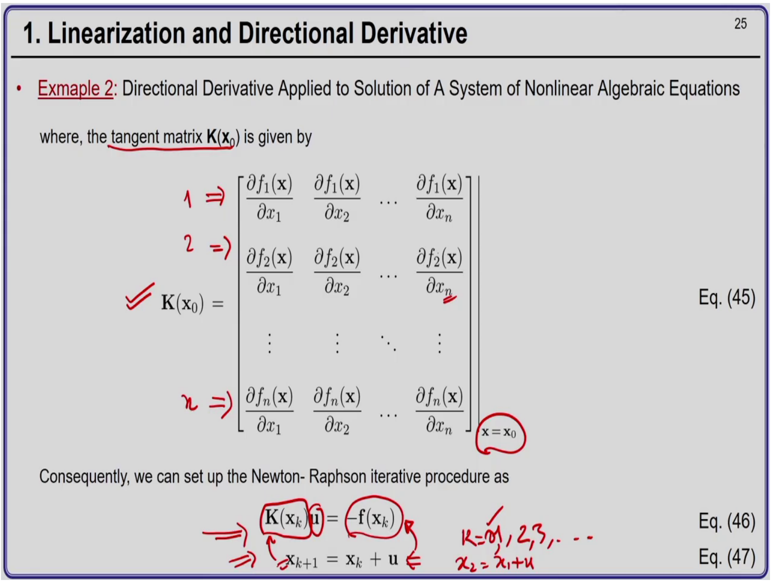

Now, this matrix K is also called the tangent matrix ok. So, in traditional linear finite element, sometimes the term stiffness matrix is used; but in the context of non-linear finite element or non-linear algebraic equation, it is the term tangent matrix which is commonly used ok.

Now, what is K ok? K is the first row, if you see is del f 1 by del x 1 ok; second is del f 1 by del x 2 all the way up to del f 1 by del x n. So, this is your first row. The second row is del f 2 by del x 1, del f 2 by x 2 all the way up to del f 2 by del xn like this the last row, the nth row ok.

So, this was your first row; this is your second row; the nth row will be del fn by del x 1, del fn by del x 2 all the way up to the del fn by del x n evaluated at x equal to x 0 ok. So, once you know this tangent matrix ok, you can set up the Newton Raphson iterative procedure ok.

So, how do you start? You have some initial guess say we have some initial guess; so, here K. So, we have some initial guess x 0 and then, we want to find out the solution of our system of equation. So, what we will do? We will start with finding the tangent matrix at x 0 and then, using this equation number 46, we will find out the increment u ok.

Now, because K was 0 ok; so, K was 0. So, x 1 will be; x 1 will be x 0 plus u. Now, once you have x 1, you can recompute the tangent matrix at x 1, you can recompute your given non-linear algebraic equation at x 1 and then, you can then, recompute u. And, then you can get x 2 as x 1 plus u and like this you will keep on doing and there is certain stoppage criteria ok, we will see.

Today, we will going to see the algorithm ok. The next one is the algorithm, once a stopping criteria is met, you will say that particular value of x, where this stopping criteria is met is your solution ok.

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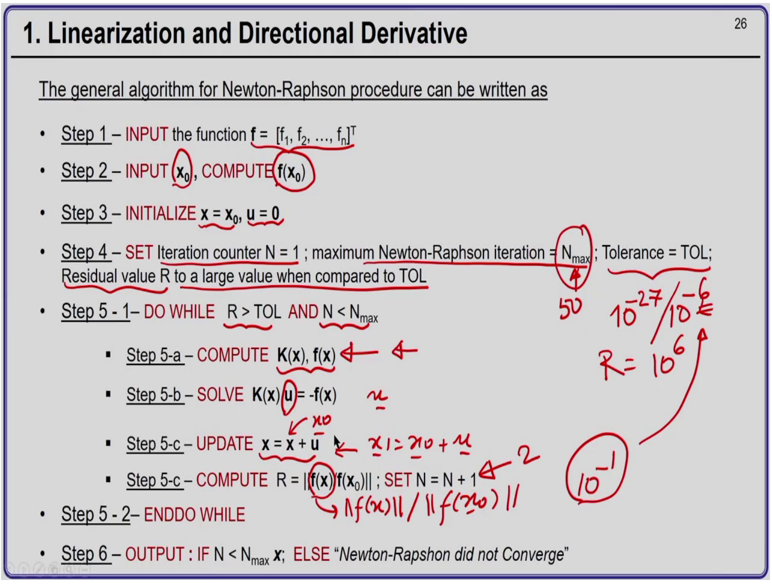

So, for the given second example that we have seen, this is the general algorithm for the Newton Raphson, Newton Raphson procedure ok. So, it requires a number of steps to be performed in a certain way. So, we look how we have to proceed if you want to find out the solution of a system of non-linear algebraic equations ok.

The first thing you have to input in your computer program is the function ok. So, your function has to be known ok. You know the function in terms of x 1, x 2 all the way up to x n ok. Now, you want to find out the solution ok.

So, let us say you have some guess ok. So, let us say you have some initial guess x 0 ok. So, you can compute the value of the function at this point x 0 ok. So, you input your initial guess and then, you compute the function all the functions at this point ok. Now, let us say our solution will initialize to x 0 because right.

Now, we do not know the solution. So, we will say that let our initial guess be the solution and let the increment u be equal to 0 ok. Now, we set the iteration counter. Iteration counter means the Newton Raphson iteration counter to be 1 and also, the maximum number of Newton Raphson iteration that we want to do ok, let us say it is N subscript max ok.

So, this is also we need to define ok. So, this is essential because we do not want our Newton Raphson iteration to go on indefinitely ok. At certain point, if the Newton Raphson procedure does not result in our solution, then we will have to stop.

Because otherwise in computer, it will keep on going there are situation, where Newton Raphson will be stuck and will not go anywhere. At that point, you have to do something extra ok. Toward the end of this course, we will see ok; arc length method and line search method, these are two techniques that you can use ok.

But right now, we just set the maximum number of Newton Raphson iteration that is N max and also, let us say we set a tolerance which is given by TOL ok. Tolerances is its use for a stopping criteria ok, when are the value of the stopping criteria becomes less than this value TOL, then we say that our Newton Raphson iterations have converge.

And then, let us say we have say a residual value R and this has to be set to be set to a very large value as compared to our tolerance TOL ok. So, normally you may set tolerance to be 10 raised to power minus 27, a very small number or somebody might say 10 raised to power minus 6, it depends ok. You might set a very small number or you may set like 10 raised to power minus 6.

And then, you may set R to be 10 raised to power 6 ok, it is a very large number as compared to tolerance ok. Now, you start a loop while loop and you see whether your value of R is more than tolerance and the number of Newton Raphson iterations is less than the maximum number of Newton Raphson iterations ok. If both the criterias are met, then what you do?

You go and compute your tangent matrix and the system of non-linear expression non-linear algebraic equations at this point ok, at x and then, you solve for u and then, you update x as x plus u. Remember at N equal to 1 this x was x 0 your initial guess ok. So, in a way for N equal to 1, what you are doing?

You are finding x 1 as x 0 plus u ok. Now, once you have evaluated the new value of x, you can recompute your function and then what you can do? You can take the norm of the function ok, thereby the norm of the function at initial guess ok. Now, this value of R ok, if you are approaching correctly will now become a small value ok.

It is very unlikely that within the first Newton Raphson iteration, this value of R will become less than tolerance which is 10 raised to power minus 6; but in a way, it will become a small value say 10 raised to power minus 1 ok. And then, what you do?

You increment the number of Newton Raphson iteration and because your R right now say is 10 raised to power minus 1 which is more than 10 raised to power minus 6 and you are in say N max is said to be 50. So, N now is 2 ok. So, now, because 2 is less than 50, you go to next Newton Raphson iteration ok. Now, again what we will do? You will compute K, the tangent matrix at x 1 and the force vector at x 1, you will recompute u and then, what you will do?

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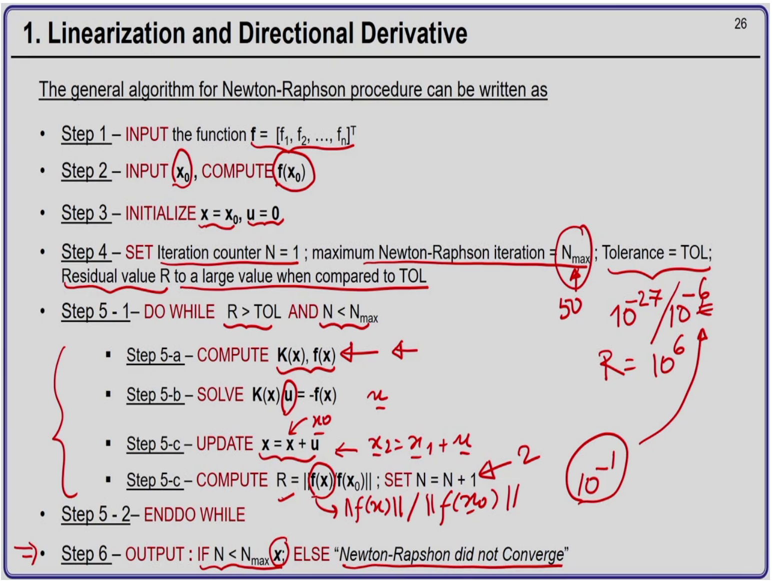

You will get x 2 as x 1 plus u and then again, you check compute the value of R and increment the iteration counter and you keep on doing this till you come out of this do while loop. So, once you come out of this do while loop which is step 6, your output will be if the number of Newton Raphson iterations are less than the maximum number of Newton Raphson iteration that you had.

Then your solution will be x, otherwise you will say that you are Newton Raphson iteration did not converge ok. Once it did not converge, it does not mean that there was some problem. It might mean actually that there are some other issues convergence issues, which you can go back and handle using arc length method line search ok; all these kinds of methods can be applied ok. But here for our second problem for a given system of non-linear algebraic equation, the following algorithm should work ok.

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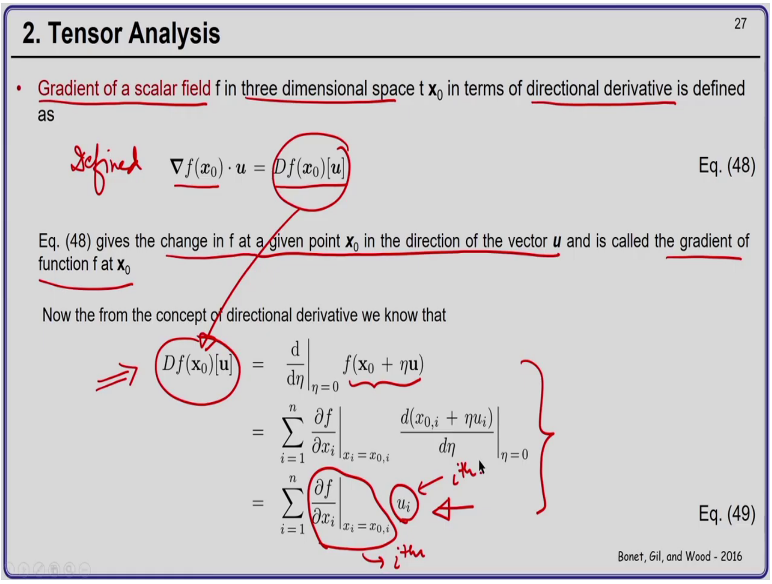

So, with this general algorithm, we come to our second topic which is tensor analysis ok. So, this is the last topic, before we go to some worked out examples ok. So, till now, what we have seen is our vectors or tensors, where a quantity which was fixed in space.

Now, we will have quantity which varies in space that is it is a field ok, we want to carry out certain operations on these fields ok. We will have scalar fields, we will have vector fields, we will have tensor fields. Scalar fields like temperature, vector fields like velocity, tensor fields like stress tensor ok.

So, now the first quantity of our interest is gradient of a scalar field f in three-dimension. So, we will restrict our self to three-dimension and we want to compute the gradient of this scalar field f at point x 0 in the direction u and then, we will do this in terms of the directional derivative ok. So, the gradient of a scalar field f at x 0 in the direction u is defined as that is how it defines ok. It is defined as del f evaluated at x 0 dot u is nothing but the directional derivative of the scalar field f at x 0 in the direction u ok.

So, what does it mean ok? So, equation number 48 will give you the change in scalar field at x point x 0 in the direction of the vector u and this is called the gradient of the function f at x 0 ok. So, you know how to compute the directional derivative ok?

So, this term over here ok, this is here. So, the directional derivative of f at x 0 in the direction u will be d by d eta eat at 0 evaluated eta equal to 0 f of x 0 plus eta u ok. If you carry out as we did for the system of non-linear equation, you will get equation number 49 which is summation from i equal to 1 to n del f by del xi evaluated at x 0 into u i ok. So, the first term is an ith term and the second term, we will also an ith term ok.

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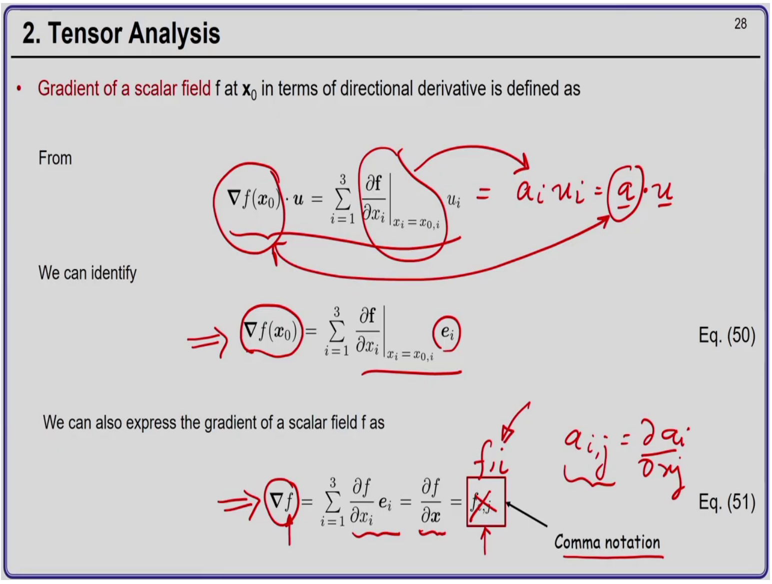

So, you can see the gradient f at x 0 in the direction u is nothing but del f by del xi into u i ok. From this, you can recognize ok, we can find out that the del x 0 is nothing but del f by del xi e i because this is nothing but say a i this term ok, I can write this is a vector this is a i into u i which is nothing but vector a dotted with vector u and comparing the left hand side with the right hand side, I can identify gradient of f at x 0 is nothing but this vector a.

This vector a is nothing but del f by del xi evaluated at x 0 ok. So, the gradient of f evaluated at point x 0 is nothing but del f by del x i e i or for a generic point x, this can be expressed as gradient of f is nothing but del f by del x i e i or in direct notation, I can write del f by del vector x ok.

So, more conveniently in indicial notation, I can write this as f i comma j and this is called the comma notation ok. So, you can see the gradient of a scalar field is in indicial notation is given by f i comma j because there is a comma; whenever there is a comma, it means the quantity before the comma is being differentiated with respect to the quantities after comma.

In general, after comma, it is always the position x ok. So, whenever you see they say a i comma j, it means del a i by del x j ok. So, rather than writing this big expression, we can use a comma notation to shorten our expression ok.

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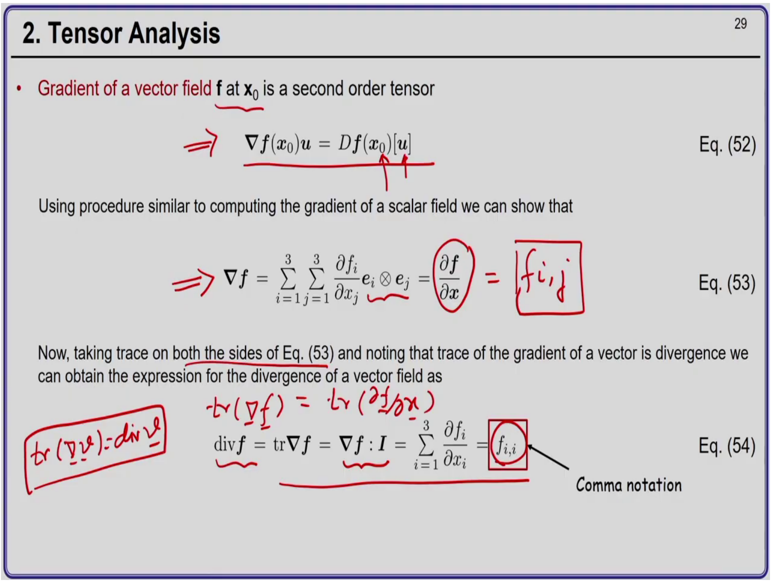

So, moving now from scalar to vector field for example, let us say we have velocity field ok. So, vector field for example, f at x 0 will be a second order tensor. If you had seen closely equation 51, the scalar field f was a something which was free of indice, but now you have one index which comes ok, sorry this comma notation this will be f comma i ok.

So, you see you started with a scalar and you ended up with a vector. Similarly, when you start with a vector, you will end up with a quantity which is one order higher ok. So, after vector, vector is one index. So, we end up with the second order tensor which has two index and gradient of a vector field f at x 0 is defined as the directional derivative of the vector field evaluated at x 0 in the direction u.

And if you follow the procedure, what is similar for these scalar field, we can show that the gradient of a vector field is nothing but double summation over i and j going from 1 to 3 del f i by del x j e i tensor product e j or in direct notation, we have del f by del x and this incidentally is f i comma j this is nothing but f i comma j.

Now, one interesting thing notice is if you take trace on both the sides of equation number 53 ok, now if you take the trace on both the sides, what do find? You find that ok, so trace of gradient of a vector is nothing but divergence of the vector ok. This is a identity that we use.

So, trace of gradient of the vector field f nothing but trace of del f by del x ok. So, trace of gradient is nothing but divergence and this is nothing but gradient of f into double contracted with the second order identity tensor and in direct notation ok, this is divergence of f and indicial notation you have f i comma i ok. So, in comma notation, you have f i comma i.

So, divergence of a vector field is f i comma i or any one of these mentioned over here ok. See question number 54 will be used later on when we go to our constitute relation ok. It will be used a lot.

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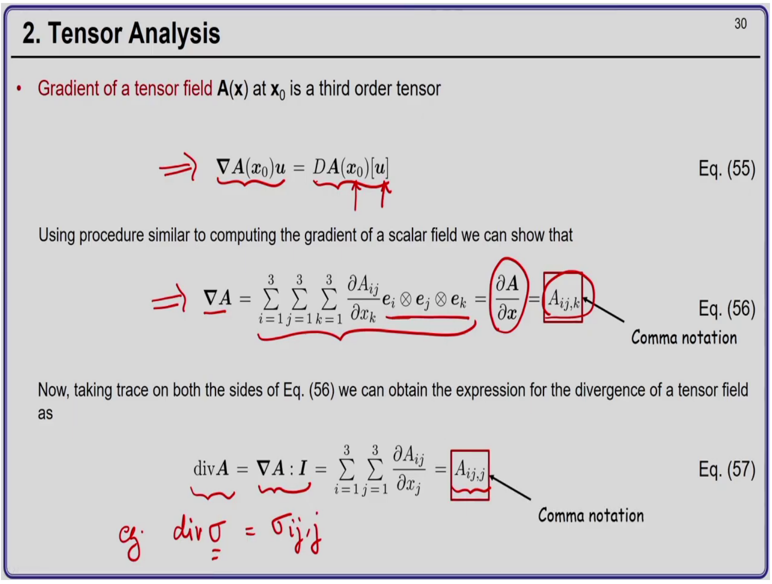

Next, we move to the gradient of a tensor field ok. So, now, we have a tensor field for example, stress ok. Stress is a tensor field, it is varying over the entire domain of the body; stress occurs in the entire domain of the body, so it is a field ok. So, now, how do you take the gradient of a tensor field ok?

So, gradient of a tensor field will be a third order tensor ok. So, it is defined as this gradient of a tensor field A evaluated at x 0 in the direction u is directional derivative of tensor field A evaluated at x 0 in the direction u ok. So, you can show that gradient of A is given by this expression over here ok.

So, now, there are three base vector. So, it is a third order tensor ok. In direct notation you have del A by del x or in indicial notation, you have A ij comma k that is your comma notation ok.

Now, you can take the trace on both the sides as you did for vector field and you can show that divergence of a tensor field is gradient of the tensor field contracted with the second order tensor or in indicial notation this is A ij comma j ok. So, if you have to take example divergence of stress; stress is the second order tensor. This will be nothing but sigma ij comma j ok, that is your comma notation.

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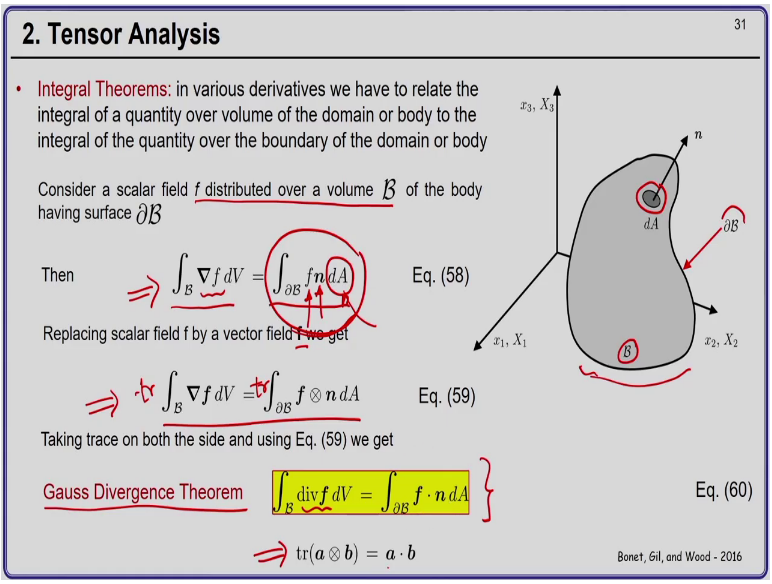

So, the last point to see is the integral theorems ok. So, now, in many of the derivations in continuum mechanics, you have to deal with quantities which are integrated over the domain ok, domain of the body or the volume of the body and you have to relate them to the integral of the quantity over the surface ok. So, how do you do that? So, now, consider you have this body as shown over here ok, you have a body B and the surface of the body is denoted by del B ok.

Now, consider you have a scalar field f which is distributed over the volume B ok, may be like a temperature. Temperature will be distributed over the body; different points of the body may have different temperature ok.

So, you have say for example, temperature field now you want to compute the integral of the gradient of the scalar field over the volume. And, this will be equal to the integral over the surface of the scalar field multiplied by normal to a point on the surface and then, integrated over the entire surface ok, where n is the normal to this infinitesimal area dA.

So, what do you do? You just if you want to compute the gradient of these scalar field over the entire volume of the body then this will be same as the integral of this scalar field multiplied by the normal to a infinitesimal area dA integrated over the entire area of the body ok.

So now, we can extend this to vector field f an equation 58, then become what is shown here in equation 59. So, the gradient of a vector field integrated over the entire volume of the body will be equal to the vector field tensor product normal to the infinitesimal area dA integrated over the entire area of which is bounding this volume B ok.

Now, if you take the trace on both the sides, if you take the trace on both the sides ok, if you take trace on both the sides, what do you get trace of gradient of f is nothing but divergence of f ok. So, integral of divergence of f over the entire volume will be nothing but trace of f tensor product n, I am using this property the trace of a tensor product b nothing but a dot b.

So, we will have integral over the surface f dot n dA and this is nothing but the celebrated Gauss divergence theorem. This will be used very extensively in our coming lectures. So, you need to always remember this theorem that divergence of a vector field over a volume integrated over a volume will be equal to the vector field dotted with n integrated over the entire area ok.

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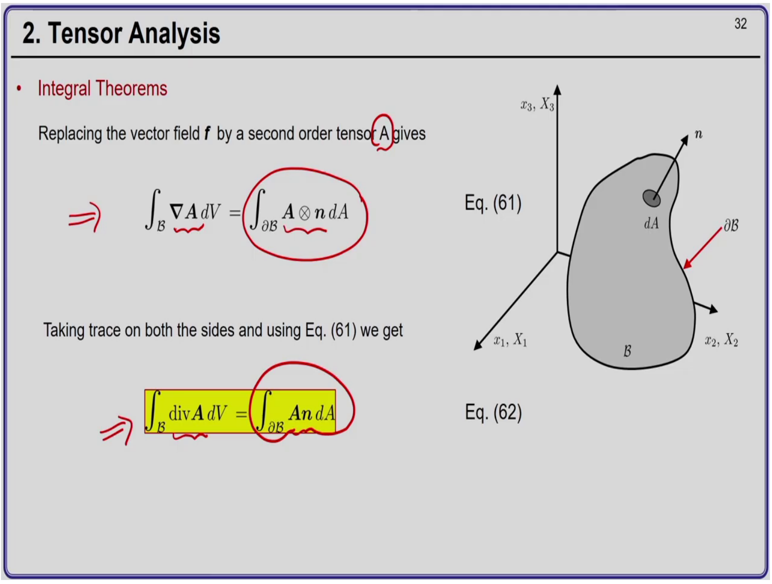

Now, we can extend this to second order tensor ok. So, instead of a vector field, now if you have a second order tensor field A, then what do you get? The gradient of the tensor field A integrated over the entire volume will be A tensor product n integrated over the entire surface ok.

Now, again, if you take the trace on both the sides, you will get divergence of A integrated over the entire volume will be equal to A n integrated over the entire surface ok. So, that is how you can connect the volume integrals to the surface integrals ok. So, with this we have covered all the essential elements of tensors ok, all the mathematical requirements for this course have been dealt with.

So, next we will see some worked out examples ok. We will see how to take the directional derivative of determent of a tensor, second order tensor; how to take the directional derivative of inverse of a tensor and some other expressions ok, before we move on to our next topic which will be kinematics.

So, next job is to move to worked out examples that will look next ok.