Advanced Finite Element Analysis
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Lecture - 20

In the last class, we saw what is called as directional derivative.

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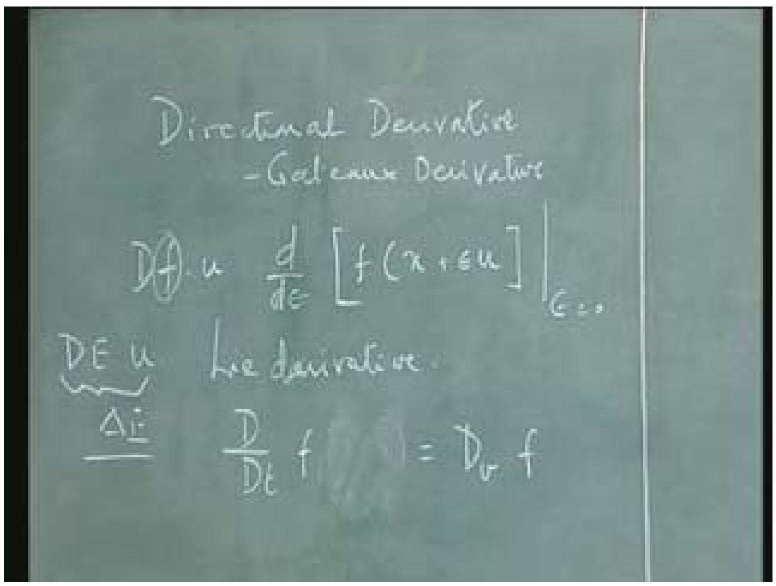

We also called this as Gateaux derivative and we said that directional derivative gives us how a particular function varies along a particular direction and that function can be anything - it can be scalar value function or vector value functions and so on and say for example, if you take a function f, then the directional derivative is the change of f along u. We said that this is very useful for us to progress with linearization and that we saw for example, directional derivative of E, DE dot u along the direction of u is nothing but an increase and that we called as delta E and so on. Please note that we had also defined Lie derivative or Lie time derivative and we said that Lie time derivative is obtained by a series of three operations; hope all of you remember what these operations are? Pull back operation, determine the material derivative and then, push forward operation.

One of the things which we stated is that the material time derivative is nothing but the derivative along the velocity vector and this is what we said. Though it is not very difficult to prove this, this proof becomes slightly more technical and so, I am not going just to prove this and I would ask you to take this. People who are interested in further proofs can refer to book by Wood on Non-linear Elasticity, if I remember right. So, I am not going to derive that further, but I just want to state that Lie derivative or Lie time derivative is nothing but the derivative taken along a particular velocity. So, when I do a pull back, do this and push forward operation, Lie derivative can be, can be understood or physically can be understood to be the derivative, when you as an observer travel along with the velocity vector.

That is going to play a role later. Though I am not going to talk much about Lie derivative further, but I will resort to some other technique to derive certain things. Instead of going to Lie derivative, I just want to, at certain point of time when I point out, it would be easier for you to understand what we mean by this. It is extensively used especially in plastic deformations, large plastic deformations and so on. Now what, what else, where else do we use directional derivative? Directional derivative is extremely useful for us to determine or for us to look at the minimisation problems.

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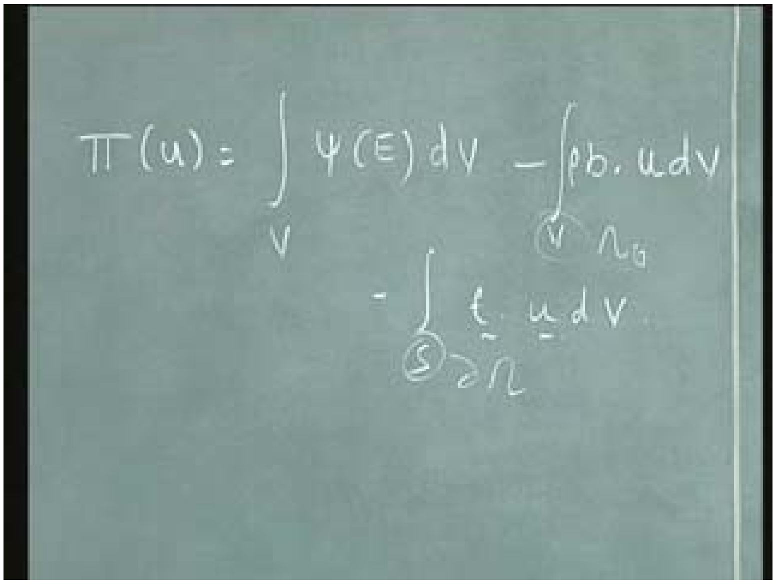

For example, all of you know that we had a potential, you call this as a functional and so on. This potential, which say for example, you can write it as a pi u, consists of two terms. The first term is the strain energy term and the strain energy term is say, written in terms of, the large deformation case in terms of, E. When I write that in the terms of E, obviously I have capital V to it and that is the first term in the expression; you know it from your earlier studies and I have two more terms that come into picture. One is the, this is the potential loss due to the external loads. One of them is say, the body forces that act, so, that will be say, depending upon how you define the body forces, whether you can put rho b or b, whether it is per unit volume or density; but, many times it is defined in terms of unit volume, because density also may undergo a change, so, minus integral S t dot u dV. Note that many times you define this as omega or omega$_0$ and this as dow omega so on. These are the symbols that are usually used in many text books.

Now, what is our idea here? I have to find out the minimum; minimisation problem is one which looks at you or which stares at you, when you look at this kind of a functional. Now, what is this minimisation problem? How can you define this problem? What do you mean by minimum?

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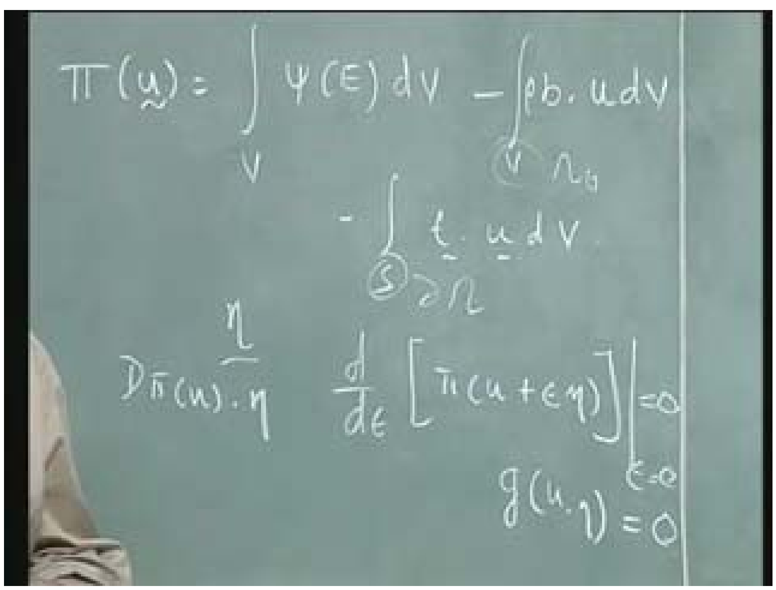

What it means is that whatever be the direction I take from say, the minimum u, if you want to call it, you can call it as u naught; whatever be the direction, the ensuing difference D, D of, let me call this as D of pi u dot eta is equal to zero. This is because you cannot, u is not one variable, so, I cannot write it as just dow pi by dow u; I cannot write it like that and that is equal to zero. What we actually mean is that whatever be the direction or in other words, I have to take the directional derivative, directional derivative of pi, which means that I have to write this as d by d epsilon pi of say, u plus epsilon eta at epsilon is equal to zero. This is the directional derivative or Gateaux derivative that is, that has to be equal to zero. So, that is equal to zero. How do you write this? Usually this function is written as, please note that this is not, before I proceed, this is not Newton-Raphson method. The next step is the Newton-Raphson method. Usually this function is written as, in most of the text books as, g. In other words, this g, which is now say, a function of u comma eta that is equal to zero. When I linearize this g, then only do I get the Newton-Raphson scheme. Is that clear? Then only, you will get Newton-Raphson scheme.

Let us see now, how this directional derivative gives rise to, what is that we will get? Gives rise to, no, from here we go to virtual work principle. The next step here is the virtual work principle. So, let us see how we get to the virtual work principle. It is very simple, let us take the first term. Now, I am going to call this by different name towards the end of the class. Let us now, right now call this as strain energy or strain energy density function.

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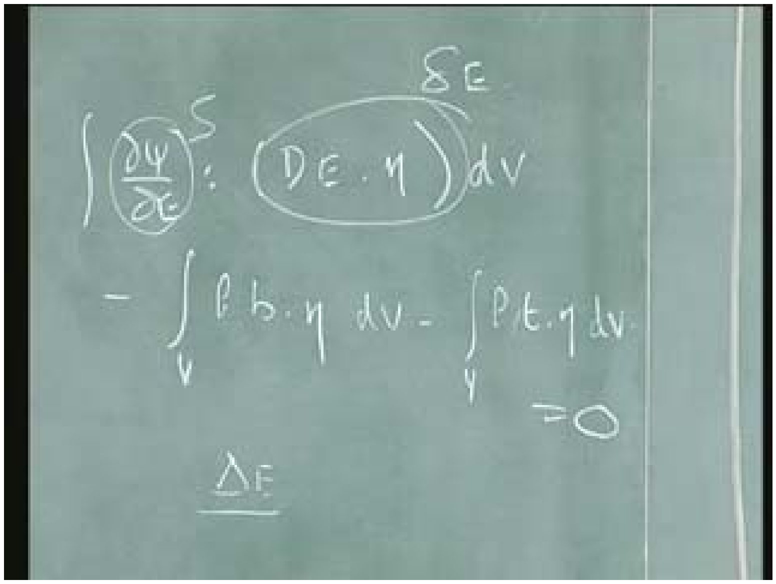

That first term can be written as dow psi by dow E into the directional derivative of E along eta, because that is what I am going to try this or that is what am going to do it here. So, the directional derivative of E along eta which can be written as DE dot eta dV that is the first term, first term there; just chain rule apply, you will see that that is what dow psi by dow E and directional derivative along eta. The second term obviously becomes minus integral rho b dot eta dV minus rho t dot eta dV. You can verify that by the simple Gateaux derivative.

If I write this as delta E, note that DE dot u is what we defined as delta E in the last class, so, this delta E is the E along any direction eta, then we get the virtual work principle and you see that this is the virtual strain and the first term gives rise to stress. We will see more about this in later classes. In fact, this would give rise to what is called as the second Piola-Kirchhoff stress and so, the first term is the internal virtual work and the second terms, of course, this is equal to zero; second term gives rise to, second and the third term together they give rise to the external virtual work.

In other words, this virtual work principle is the result of minimisation or in other words, the result of the application of Gateaux derivative or directional derivative to this functional phi. Is that clear? So, that is the, that is one of the major applications of this directional derivative, of course, we start our Newton-Raphson scheme at this place.

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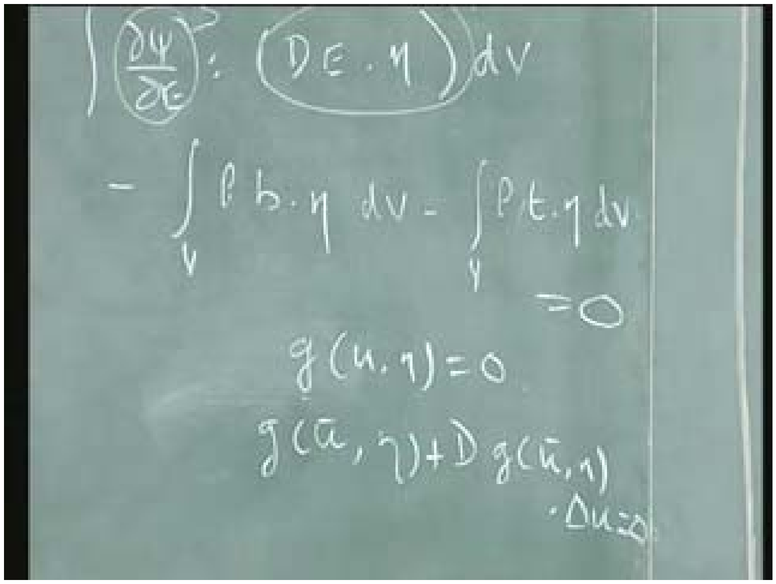

So, if I now write g of u comma eta is equal to zero that is the second or the virtual work principle to be written like that, then I develop a Newton-Raphson scheme from here and write that as g of say, u bar comma eta plus D g of u bar comma eta dot delta u is equal to zero. This is what it will be Newton-Raphson scheme. The directional derivative now, of g along delta u is what one requires in order to perform a Newton-Raphson scheme and this is one which would result in what is called as the tangent stiffness matrix. We will go into the details later, but I just wanted to point out how we can develop the Newton-Raphson scheme as well with the directional derivatives. We will come back to this after about four classes, four to five classes we will come back to this and develop the Newton-Raphson procedure for this kind of large deformation problems. That is in other words, without any frills attached to it, just the displacement based finite element analysis not mixed formulation or anything like that can be developed straight away from here. Of course, if you want to develop mixed formulation, then the functional that you take, of course you know, is going to be different.

We will just shift gears and now that we have studied stress and strain, we have to now look at a new thing. What is the relationship between stress and strain? That is the next thing, so, we have to shift gears and move away from directional derivatives. But before we do that, we have to see some very interesting things which probably you would not have realised in your earlier classes. These interesting things come from the fact that many of these phenomena that you see in solid mechanics are controlled by the laws of thermodynamics.

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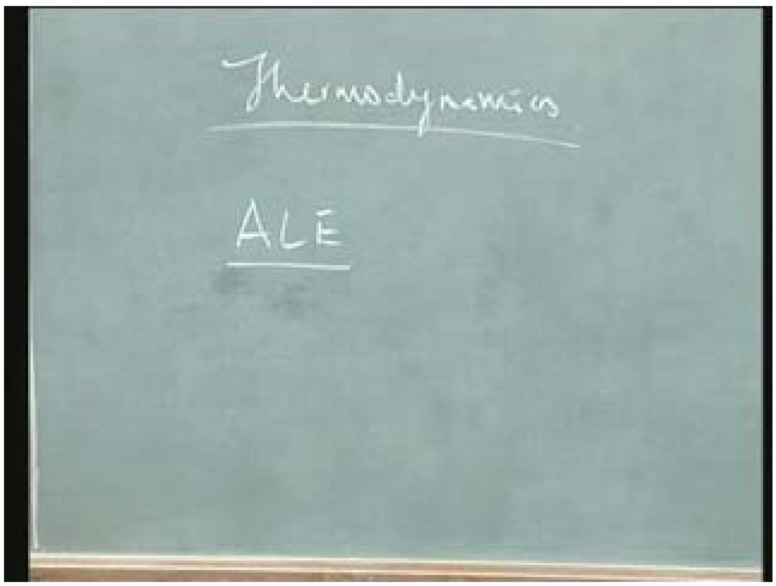

I have to develop certain very interesting or important principles from the laws of thermodynamics in order to explain certain physical behaviour of bodies of interest to us and I want to emphasise the fact that thermodynamics is a very general principle. The problem with most undergraduate courses is that thermodynamics you start separately and most of the things that are taught are associated with certain thermal cycles and hence thermodynamics is looked at as if it is a part of thermal engineering. I think that is not the correct approach. In fact, I want to clarify two things. I am going to do that may be in next two three classes, but right now I want to emphasise this fact, students would not have realised it, one is that the difference between a solid and a fluid now diminishes, when I look at it from a continuum mechanics perspective; so that is number one. In other words, continuum mechanics encompasses both solid mechanics and fluid mechanics. In fact, people who have studied courses in fluid mechanics would have realised that many of the things that we are developing now, for example, rate of deformation tensor, these things are useful in solid mechanics; maybe we have used that already as well, that is number one.

Number two is that all the major principles balance …… , as you call it many of them which we derived in the last course itself and some of the modifications I am going to make it now, today or may be in the next class are valid of obviously whether it is a fluid or it is a solid. Actually, what distinguishes the solid and the fluid is the type of constitutive relationship. All other things what we have developed now are valid, are valid for solids as well as for fluids. Many of the tensors we have talked about are valid for both solids and fluids. But, the only difference I want to point out is that, because of the fact that it is easier to analyse a fluid using an Eulerian co-ordinate system, the quantities of interest in fluid mechanics are ones which are restricted to spatial co-ordinates and the spatial derivatives; these are the things which we would be using.

On the other hand, it is just because it is easy to deal with things in a Lagrangian framework or material co-ordinate system that we deal for solid mechanics in terms of material coordinates derivatives and so on. Is that clear? These are for the ease of operations. It does mean not that in a solid mechanics you should not use Eulerian coordinates and for a fluid mechanics you should not use Lagrangian coordinates. But, it becomes very cumbersome, you cannot do it. But, in fact, today in solid mechanics, we use what is called as an arbitrary Lagrangian Eulerian procedure, A L E as it is called, where a part of the mesh is a Lagrangian mesh and a part of the mesh remains to be an Eulerian mesh. So it is very well within the frame work of solid mechanics to use Eulerian meshes as well.

What distinguishes actually the solid and the fluid is the principles of constitutive equations and before we go further into the constitutive equations, we should look at what these laws of thermodynamics are and why that is going to be useful to us. Is that clear?

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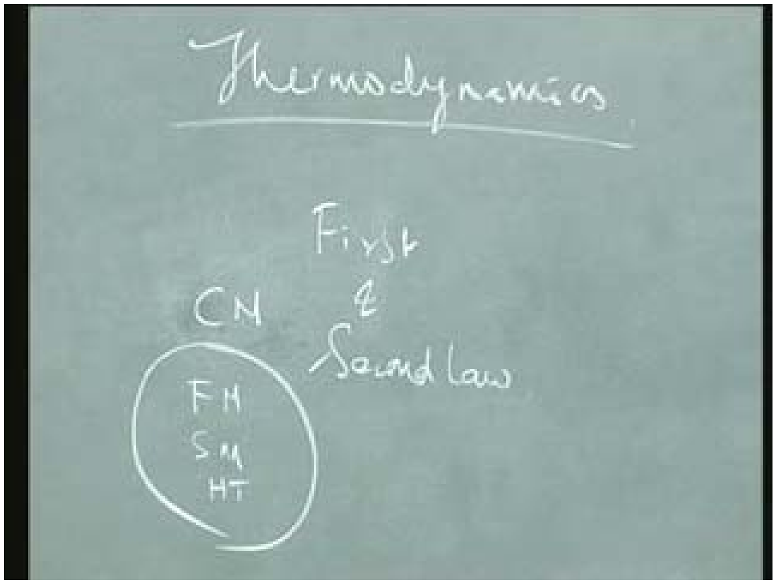

Now, what essentially we are going to use are the two laws of thermodynamics - the first and the second law of thermodynamics. These are the two things that we are going to use. People who already know, of course all of you know thermodynamics, would realise that the first law actually talks about, what? It is a balance law, it is actually the balance law and that the second law talks about the direction of these balances. First law does not tell you whether something is possible or not possible. That is given by the second law of thermodynamics and basically the first law is the one which talks about the balance of different types of energy.

One of the misnomers that usually we have is that again heat transfer and solid mechanics are quite well separated. It is very unfortunate again. What I want to say actually is that in a large frame work of continuum mechanics, continuum mechanics, all these guys coexist; the fluid mechanics, solid mechanics or heat transfer, temperature, all these things, they coexist. In other words, it is because you cannot analyse certain things together that you make a very strict, I will say, demarcation and start operating them as separate regimes. In actuality it is not so and that is one of the reasons why we look at this whole system in totality using the most fundamental of all the laws, which is the laws of thermodynamics. Is that clear? So, they are all together, they cannot be studied separately.

Let me invoke some of the things that you already know in thermodynamics. I am sure certain terms ring a bell to you like state variables, thermodynamic process - these are things which I hope you remember. State variables are ones which depend upon the particular state of the body, now that state variables are going to be defined at every point and that the only difference is that you can look at, as I said deformation and temperature together and the state variables are more than what you had studied. In fact, you can take a, typically in a thermo mechanical process or thermo elasticity, you can say that there can be seven state variables which six of them can be related to strain and one is temperature.

You are going to see how we define temperature itself in thermodynamics, they are going to be different from what probably you would have studied before and before we go further, let us now first consolidate our first law of thermodynamics, move to what is called as an entropy inequality principle and explain how that is going to be useful for us in solid mechanics. Actually, in fact constitutive equations, though we call as relationship between stress and strain, strictly speaking you should say that constitutive equation is a relationship between thermodynamic variables. In fact, you can look at thermodynamic variables or in other words, you can look at even our heat conduction equations to be some sort of a constitutive equation. So, the relationships between these thermodynamics variables are the ones which are useful to us in defining or in modelling many of the processes.

In fact, though we may not have, we need not go into certain details, in fact, we would see that what goes into defining the variables, state variables, what can be there and what cannot be there again can be controlled by certain of these or many of these thermodynamic principles. Now before we go further, as I told you, we will look at the first law of thermodynamics carefully. In that process, we define certain, I would say definitions.

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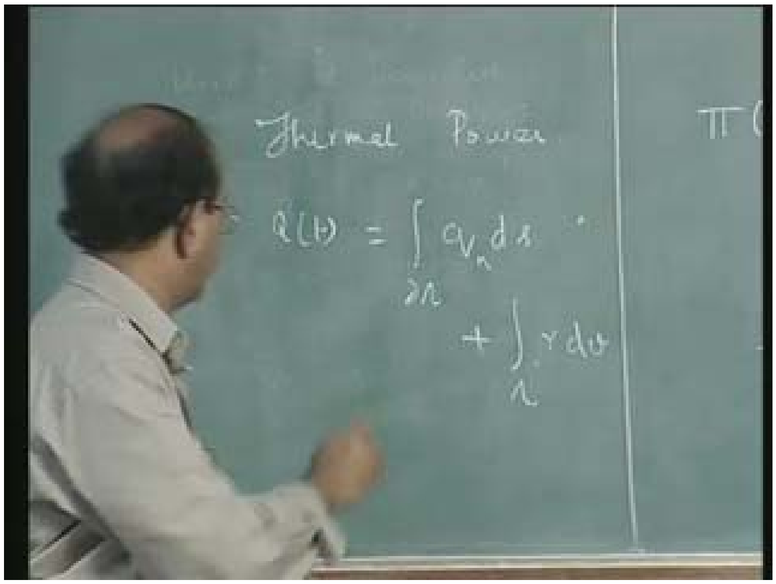

Let me define what is called as the thermal power and call this as say Q of t, Q of t. Note that it varies with time. So, we can call this as the rate of thermal work as well. The thermal power has two terms in it or the rate of thermal work has two terms in it - one is term which involves the flux which crosses the boundary, which can be, I have reasons for doing this; I will explain that in a minute, which for example can be given as qds dow s or dow omega plus an internal generation term, which can be defined as rdv. Actually we define this as q_n, to denote that $q_n$ds.

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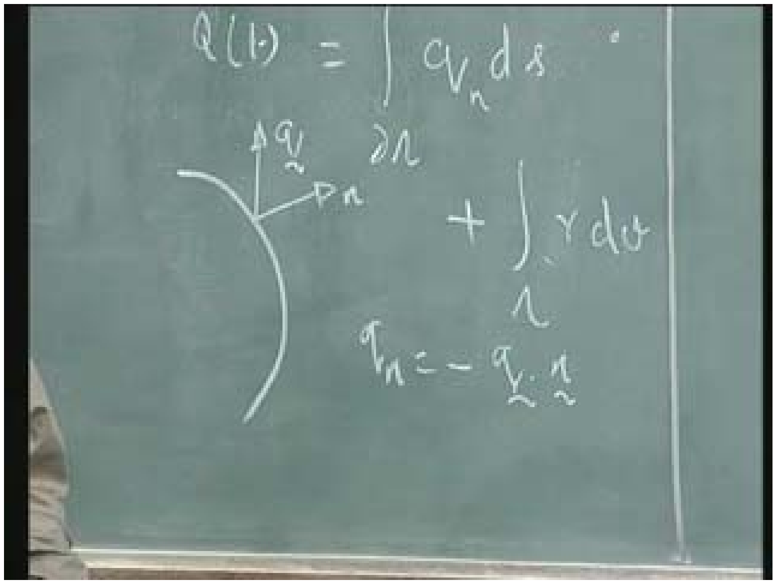

In other words, if I take a body, let us look at these terms carefully again; if I take a body and take a point here, let n be the normal and actually the q is the flux, then we define, this is the heat flux; then, we define q_n to be, q_n to be, minus of q dot n, obviously and many times we use this minus term to indicate that the heat is going out. So, that is the reason why we use this and note that this q can be function of small x and t.

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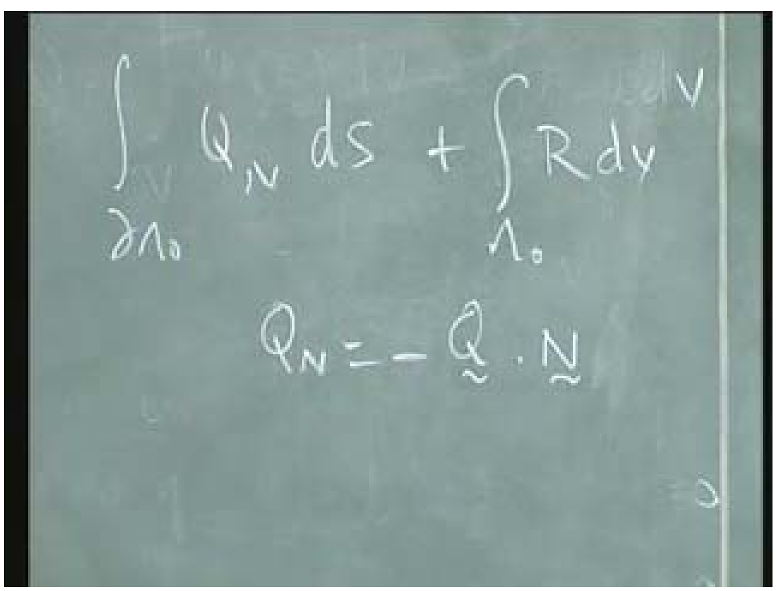

This same thing can also be written in terms of the reference co-ordinate system and in which case, you can write that down as with respect to omega$_0$. So, that can be written as dow omega$_0$, the flux written as capital Q and the normal written as N dS and the second term written as RdV with the original volume omega$_0$. Of course, Q_N is equal to minus Q flux dot N; sorry, Q dot N and that is what goes into the first term here. Now, the heat flux, of course, has to be the same. What crosses the boundary is going to be the same. Note the difference between what you have studied before and now. You would have studied a body which does not have any deformation and you would have said that this is equal to, the heat power is equal to what or the content, heat content or the rate of change if you want to call it, if there is a flux here and rate of generation of heat is just, you would not have bothered about the difference between this and this; you would have just said that it is the volume throughout. But, now this body, which was like this, is now deforming like that.

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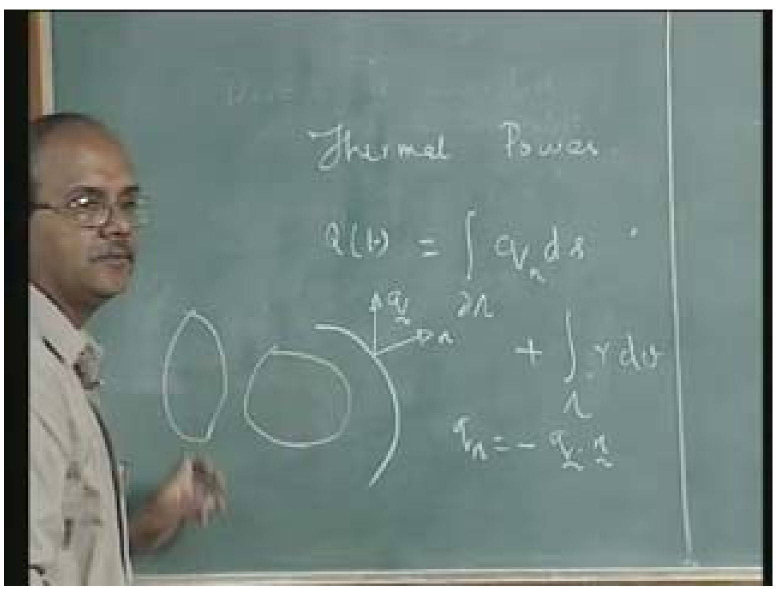

So, there is a deformation as well as there is a heat transfer and hence there is a difference between these quantities which are taken in the current configuration - spatial configuration and the material configuration and so, there is a difference between small q and capital Q. You cannot just like that write, though you would say that the flux, this is at a particular point of time, note that as well, though you can say that the flux can be calculated with respect to the original or the current configuration.

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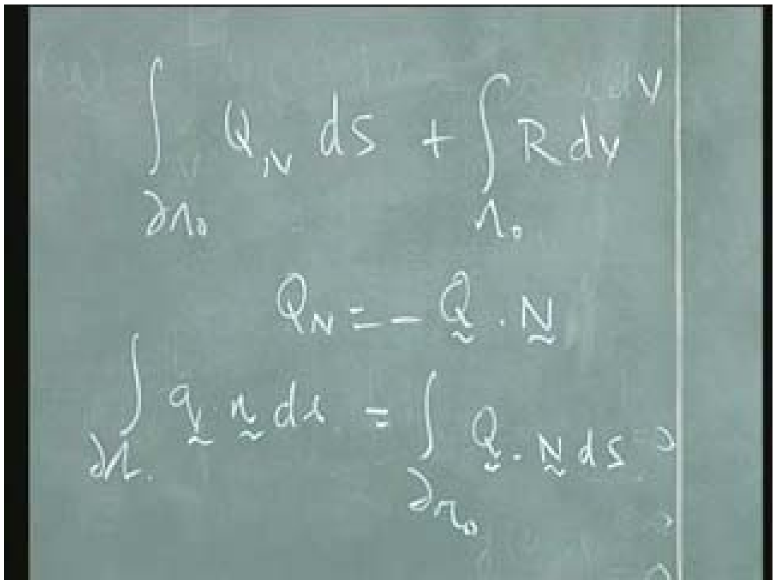

In fact, the relationship between them is very straight forward and what we mean to say is that q dot n d small s which is taken at the current configuration is equal to what is taken at the reference configuration and that is given as the Q dot N dS, both of them indicating that the flux comes out from the surface of the body and at a particular point of time, they are the same. I understand, I mean there are always confusions; I understand these confusions. Please note that the flux, which we are talking about by these two equations, are at a time. They are not a flux which happens when the body was in the reference configuration and when the body has moved after deformation to current configuration; we are not equating those two. At a particular point of time, what is the reference is what we are concerned about. At a particular point of time the reference if it happens to be the current configuration, then this is what we are dealing with, sorry, this is what we are dealing with and at a particular point of time, when I want to refer all my quantities to the reference configuration then this is the quantity. So, do not, please do not get confused between the two; how can the flux be the same. At a time, it is the same. Hence, I can equate these two.

Now, what I am going to do is very straight forward. I want to develop a relationship between small q and capital Q. Can you do that? What do you do, what is that you apply? Fantastic; Nanson's formula, so, apply Nanson's formula here.

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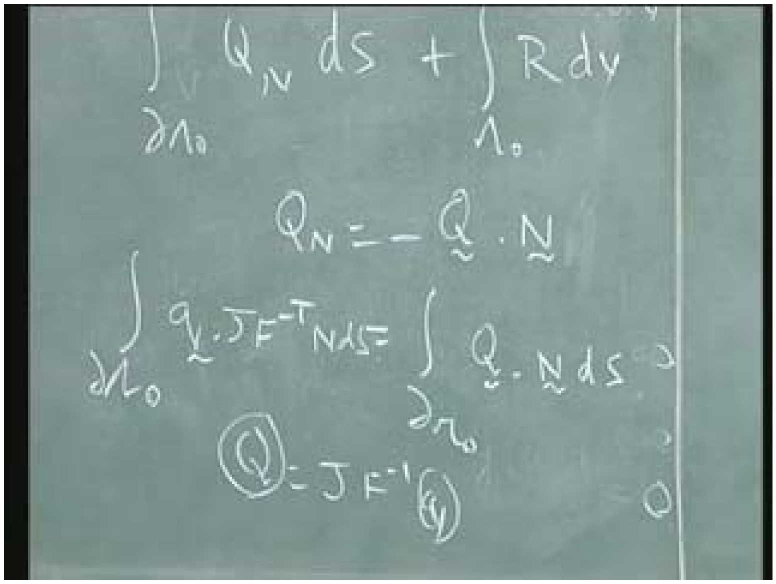

J F inverse NdS, so, this can be replaced by q dot J F inverse NdS or F inverse transpose NdS. I have to now use the definition of transpose, so that ultimately I can define Q to be J F inverse q. This is the definition of u dot a v is equal to v dot a transpose u. That is what I use it, so, this transpose of this, it becomes just minus 1.

No, no, that does not matter, because ultimately when I substitute this, this will become q dot NdS, so, both of them are the same. By Nanson's formula, what I am essentially doing is to convert this also. It is like converting the reference configuration to the, sorry, current configuration to the reference configuration. So, I am, I am converting d small s to d capital S by Nanson's formula and the ensuing relationship is what you get. Do you remember what the corresponding quantities in, remember what you had before? You did a very similar thing, for example, when you looked at the force terms; the force that is acting at the current configuration and the force, the same force acting in the reference configuration and the result was a, what was the result? What did you get? From

Cauchy's stress, you had Cauchy's stress sigma dot N d small s, you got P dot N; P dot capital N dS. What was that? It is the first Piola-Kirchhoff stress. People call this also as, this q to be Cauchy's heat flux and this to be Piola heat flux.

Student: Still F is a deformation gradient.

Yes, F is of course the deformation gradient and what I have essentially used is to relate d small s and d capital S and please note that the d small s and d capital S are related by the deformation and hence obviously deformation gradient comes into picture. So, the first Piola-Kirchhoff stress has an equivalent in heat transfer, which we call as the Piola flux. Sometimes people call this also as Piola transformation from one to the other. Of course, when you, when you do not have deformation, when you are treating a pure heat transfer problem, you do not have any of these issues, because $omega_0$ or omega or omega naught or omega does not exist; they are all only one. So, obviously, we have a deformation gradient which comes into picture. Is that clear, no other questions?

Yeah, Piola transformation, this is called as Piola heat flux and that is called as the Cauchy heat flux, just to pick up an analogy between what you do in the heat transfer and in solid mechanics. Now that we have both these things together - the deformation as well as the heat transfer or heat or thermal power together - we have to look at certain other things also more carefully; for example, the internal energy term. Now, if you look at the internal energy term, the internal energy term has two things in it.

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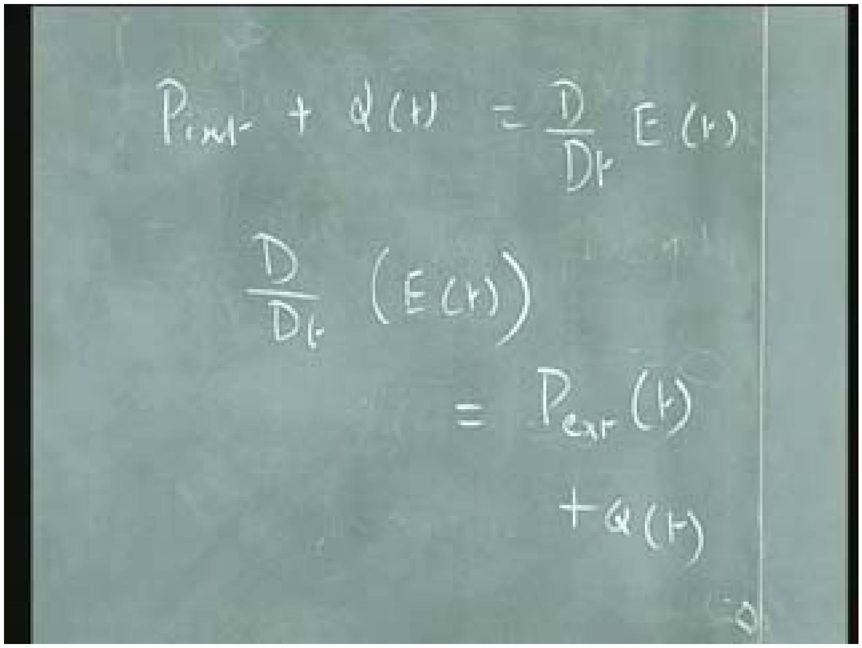

Let me call that as P internal; P internal plus Q, if I can call it as the thermal work or thermal part of it. This is, the first part is due to the mechanical work, the second part is due to the thermal work. Both of them go to raise the internal energy of the system and so, we can write that as equal to D by Dt of E(t). Note that both these quantities are rate quantities and both these quantities, if written in the reference configuration, can result in the rate of change of internal energy D by Dt of e. So, both of them raise internal energy. Both the work, mechanical work that is done as well as the thermal work or the thermal power, so, both of them, they raise the internal energy.

Now, let us write down the familiar first law of thermodynamics. How do you write down the first law of thermodynamics? You can, how do you, what you say, if you do not want say, kinetic energy, so, you can say that D by Dt of E(t) is equal to, this is what you called it as, I do not know what symbol you used; delta E, right? Delta E is equal to delta P plus Q. This is what probably you would have written in your first or second year classes or today, even in high schools. So, the first term is the external, P external, the work done by the external forces. If it is rate, then obviously, it is rate quantity plus the Q term that goes in, Q(t).

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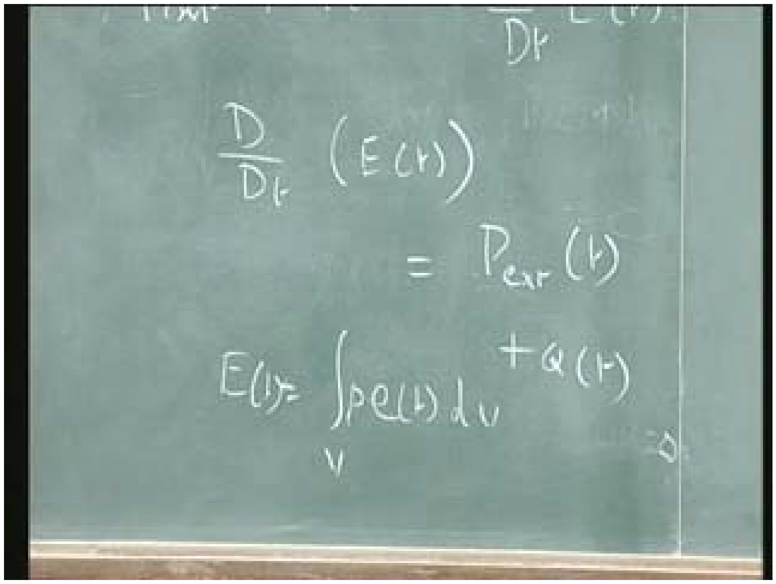

Of course, E, you can, you can define it through what is called as from thermodynamic principle, thermodynamic concept can be defined as or through what is called as specific internal energy e, small e, if you want E(t), then e(t) dV, depending upon whether you can define it with respect to per unit volume or per unit mass, there may be a rho or there may not be a rho in it. Is that clear? Now, what is P external?

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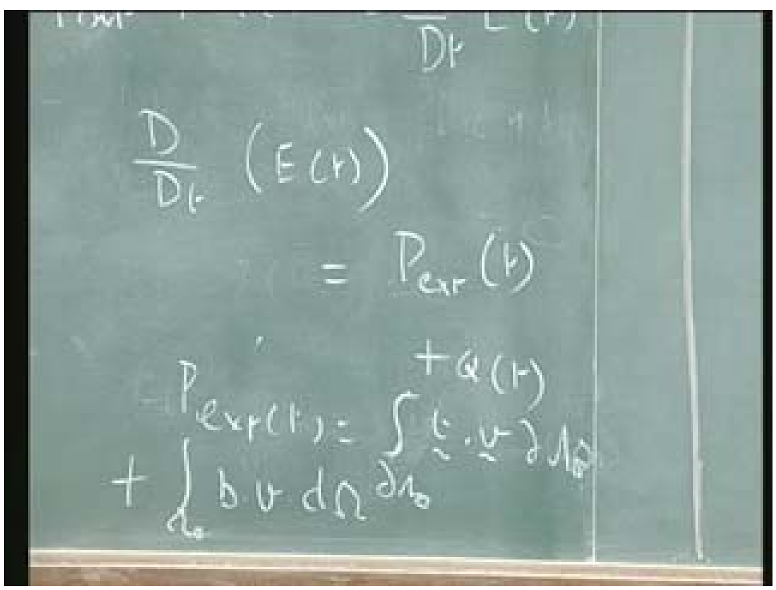

P external is nothing but what has been done, external work and so, the P external term can be written as d omega$_0$, now, how do you write that? Previously it was t dot u; now, since the rate quantities are involved here, so, it becomes t dot v, velocity, so, t dot v d omega$_0$. The whole thing can also be written in terms of the spatial co-ordinates, does not matter, plus b dot v; plus integral omega$_0$ b dot v d omega or dV. Omega$_0$ I said, can also be replaced by v$_0$. I am using it deliberately between these two, because it is a style to write omega$_0$; it is the writing style is omega$_0$ or v$_0$. I just want to tell you that in many books one or the other is used. So, this is the external work done. This probably you would have written in your earlier classes as P dV and so on. That is external work and of course, Q is the thermal power or the thermal work which we had already put up.

Now, where is that q? I think, yeah, yes, it is here. q dot n minus q dot n ds. Now, I can apply of course, let me look at this more carefully. I hope, if you have understood this, I will just remove it and of course, I can apply the divergence theorem to this first term and I can write this in a slightly different fashion as well and how do I write that?

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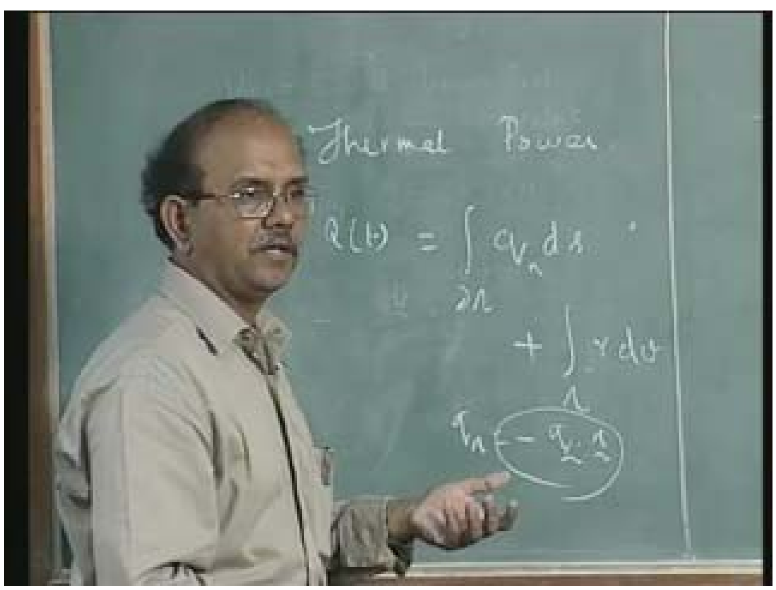

First term, if I use the divergence theorem, q_n replace it by this quantity. So, why do I use that? I want to remove this surface term and put a volume term there, so that I will get dv r.

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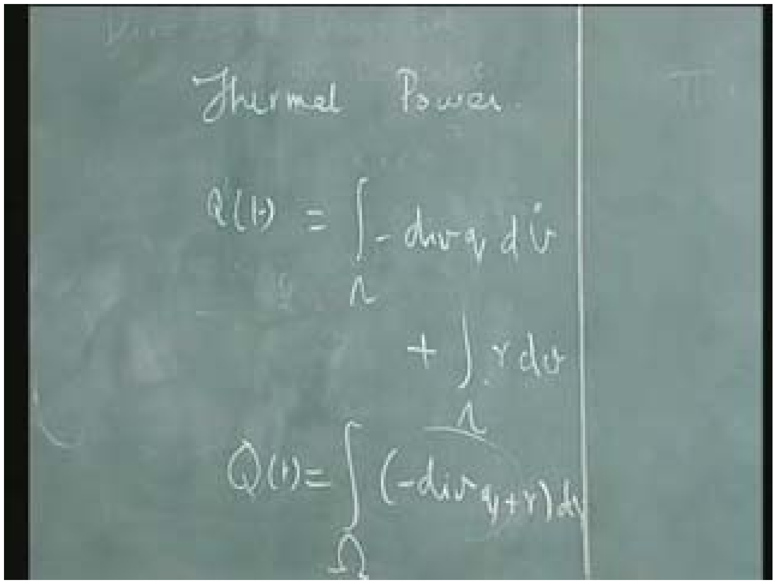

That is correct, that is the divergence of q, minus divergence of q dv, so that it can be written as well. So, q term can also be written as minus Q plus R. So, together they can also be written as minus divergent q plus r dv is equal to Q. What is this internal term, P internal term? We are looking at every term. So, this comes also from here. I have this q term here. What is this internal term? This we had seen just couple of classes back.

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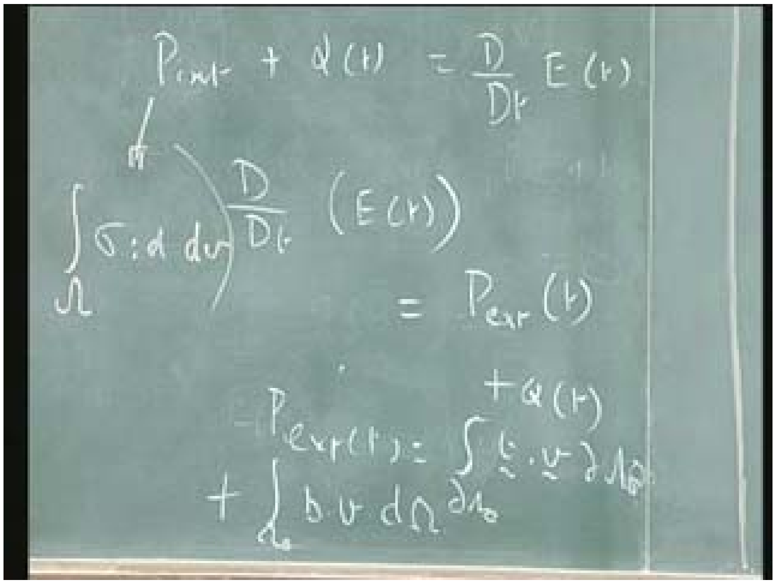

So, this can be written as, if it is in the spatial co-ordinates, then this can be written as integral, correct, sigma d double dot d. Yeah, this is the rate of deformation; rate terms have to become, have to come in, so, that is the rate term is there dv, where it is the current co-ordinate that is this term. Put them together, put them together and you can write a beautiful expression in the current co-ordinates and you can also write down a similar expression in terms of the reference coordinates as well. Put them all together and please write down, let us see; write down one equation. Since then, substitute this, substitute for this and then put that in the other one. So, the equation now, the first equation now becomes, in fact, you can substitute from here and then write that term.

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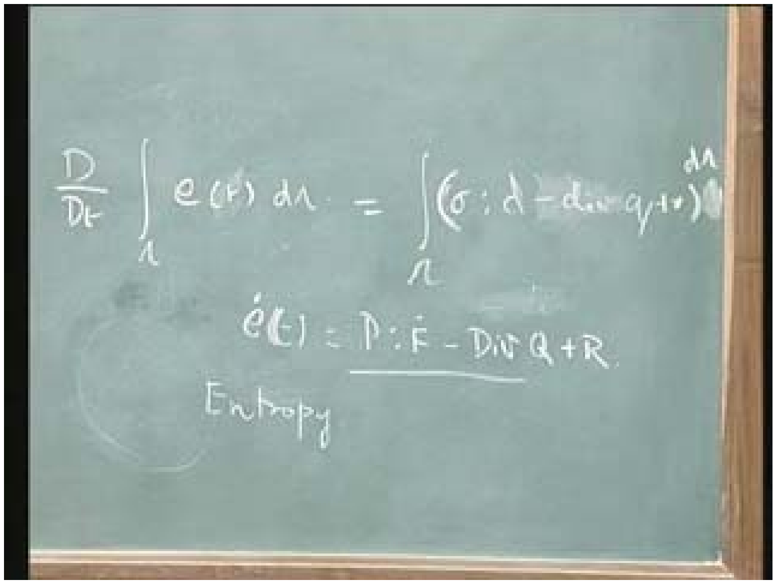

First let us write this down, e in terms of, so, D by Dt whatever, e, is specific, if you want, you can write that as t, d omega d omega; that is the first term D by Dt is equal to integral sigma d omega d omega term minus the second term divergent, minus divergent, sorry, I can do that later may be, minus divergent q plus r whole thing dv, or sorry, d omega; I will use the same symbol, d omega. So, the material time derivative of e is equal to all these things. Corresponding quantities in terms of, if I want to write it in terms of, the reference configuration it is much simpler. Then I say, see, material time derivative of e is equal to instead of sigma and d, it will be, if you remember we had done that P dot colon or double dot F dot minus divergence of Q plus R.

If you had noticed, do not get confused with capital E dot, because I do no want to use that term, because then you will get confused with the, our strain term. That is why when I put this dot that means that it is the material derivative, material time derivative of e automatically. That is why I have used this term e dot. This means that the material derivative is equal to P colon F dot and so on. Note that the first law basically what it talks about is nothing but the energy principle. So, the only thing is that now the energy, so, P internal plus Q(t), the energy also comes from two terms - one from the external or the work done as well as from the heat transfer that takes place inside the system and if you remove this Q, in fact, Q term it is nothing but the P internal is equal to what comes out of the P external terms.

That is the first part of the story and what is important here is this definition. We will come back to this definition later and whether such an energy change, what really it talks about is the conversion of one form of energy to another form of energy. Whether such an energy change takes place is given by the second law and one of the most important quantities which the second law goes or throws up is what is called as the entropy. Entropy means that, en is a Greek word; en means in, tropy - direction. So, the word itself says how the direction of this kind of transformation can take place.

Let us look at the second law, which gives rise to what is called as the entropy inequality principle and Clausius-Duhem inequality as it is called, in the next class and see how this can be used for defining the material behaviour. Is there any question? The only thing which I did not do here is to leave out the kinetic energy part of it.

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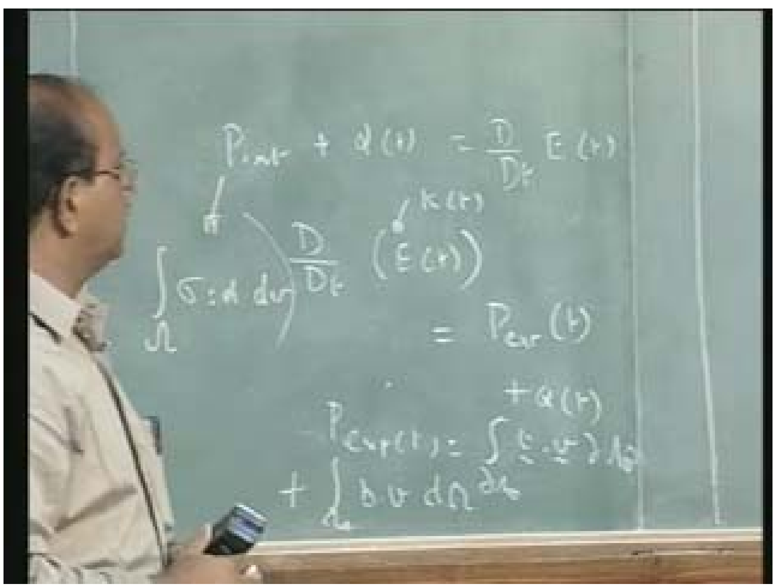

In fact, you can add kinetic energy part of it as well and you can write that down as well, which I had not done. Anyway, you can add that also. We will stop here and we will continue with the second law of thermodynamics in the next class.