**Introduction to Soft Matters**
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**Indian Institute of Science, Bengaluru**
**Lecture No 35**
**Constitutive modelling**

Welcome back everybody to one more lecture on Introduction to Soft Matter. So, what we have just finished discussing is a whole set of constitutive relationships that we derived, these were continuum mechanics level, constitutive relationship that were derived using a spring dash pot analogues. And we came up with certain relationships between stress and the strain, or the strain rate and we saw that there exist a general framework to describe them.

Now, since we are on the topic of constitutive relationships, this entire area has a lot of interesting insight. And so till now, which is simply used analogue, analogues of how energy can be stored or dissipated and we use that as our basis to derive them. But the whole area of continuum, constitutive modeling has very important principles that are embedded within it.

So, we want to discuss a little bit more detail, on the issue of this fundamental topic. So, we want to take a look at the important issues, that concern us when it comes to constitutive modeling. So, let us turn our attention to this slide here.

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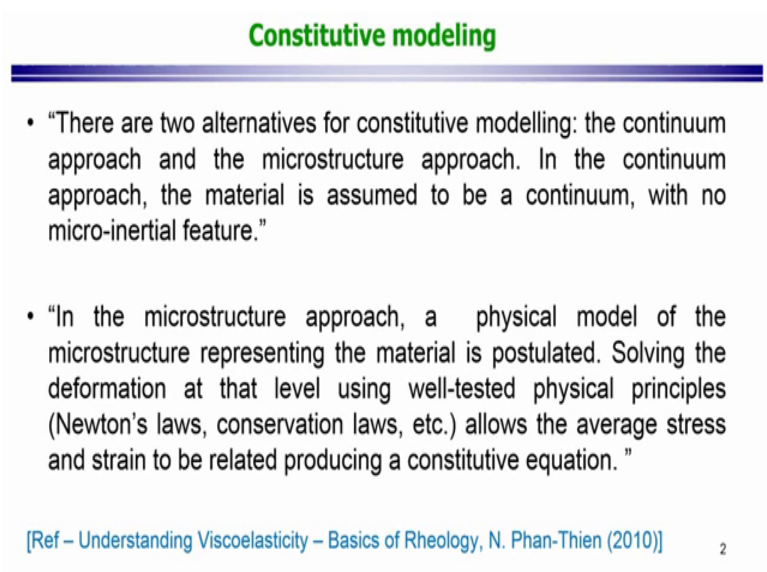

And so, this in the first line, so what I have done is, I have taken a few lines from the book called, “Understanding Viscoelasticity - Basics of Rheology”, and this is authored by N, Phan Thien. And he says that, there are two alternatives for constitutive modeling, the continuum approach, and the microstructure approach. In the continuum approach, the material is assumed to be a continuum, with no micro-inertial feature.

In contrast to the continuum mechanics approach, or the continuum approach, you have the microstructure approach, where he says that in the microstructure approach of physical model of the microstructure representing the material is postulated. Solving the deformation at that level using well tested physical principles like, Newton's laws, other conservation laws, extra, allows the average stress and the strain to be related producing a constitutive equation.

What he is trying to say here is that there are basically two different approaches to the whole topic of constitutive modeling. On one level, we can assume that the material is a continuum and that it is really, whether or not it is made up of molecules or not, or discrete particles is something that, we do not necessarily need to consider.

Rather we build or model based on certain phenomenological behavior, or and we model it just like we did in our particular case using the springs and dash pots, which was just analogues for how energy is stored and dissipated. But we did not necessarily say what the molecular scale process really is in that case.

So, the dash pot is represent a certain molecular phenomena, but we did not discuss the molecular phenomenon and how whether or not the dashpot is an adequate formalism for that process approach, also this was not discussed. But then there is the other side of it, where we take the microstructure, we assume that the molecular nature of the material is understood, maybe it is a polymer, where you have very large molecules, maybe it is a linear polymer and then you can try to use first principles.

So, you apply your first principles to that molecular structure, so maybe you have a model and then you say okay my Newton's, I will apply the Newton's laws and I will discuss, how the, how the particles interacts among each other. And from that, first principles approach, we calculate stress and strain and usually they turn out to be statistical theory is that, that can help you determine that. And once you do that, then you use the average quantities and you say that you have a molecular or a microstructure based physical model for this.

Now, this is just my personal to this, and that is when the continuum mechanics approach, the continuum approach can be related to a certain type of microstructure approach. So, you can construct a corresponding microstructure approach, which accounts for the molecular basis of the springs and the dashpot, for example. But on another hand you can even think of them at some scale as being purely phenomenological.

So, it is driven by just understanding or an observation of how the phenomena occurs, and then you construct an equation that has some certain unknowns, that can we perhaps be even, be resolved with experiments. And there is a certain advantage in trying to understand or think of constitutive equations in this form, is because there might be cases where this constitutive equations are relevant, which cannot be model or cannot be easily thought of from a molecular perspective. So, what I have done here, let us just go to the next slide.

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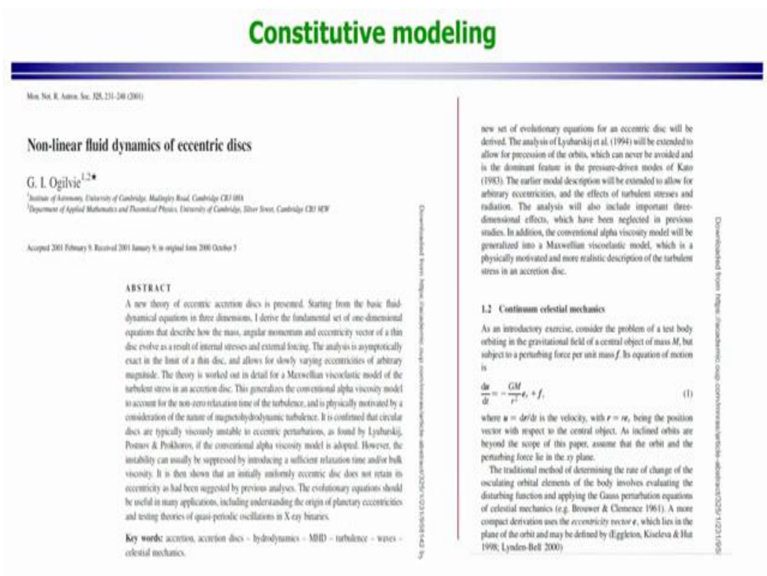


So, for example, I just taken, these are the pages from a paper called Non-linear fluid dynamics of eccentric discs and it is authored by Ogilvie, and here he is looking actually at a theory of eccentric accretion discs, which in a astrophysical phenomenon and the important part is.

So, this is on your left hand side, you can read the abstract for that and this on the right hand side, this is separate page of the manuscript, and the important thing just before the section 1.2, if you see he says, that he is actually going to use the Maxwellian viscoelastic model. And you can take a look at the whole paper, but this is the outside of the scope of our discussion, but I just wanted to point out that you can use these models in areas that are really far off from your initial areas of guess.

So, we discussed polymers extra as soft materials, but our point in enumerating them was just familiarize ourselves with difference of materials. But the ideas that we are being discussed can be extended to a very different scale altogether and here you might have a lot of difficulty trying to understand it, from first principles. What is there at the molecular scale? That might be really, really complicated, but you can still phenomenologically apply some of the models discussed.

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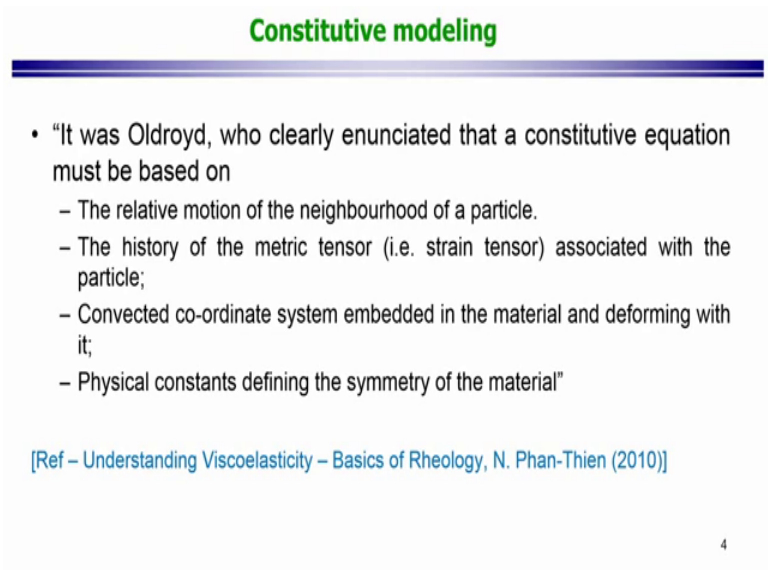


Anyway, but the basic point that we want to discuss, is the issue of constitutive modeling. And that these constitutive equations should be based on some general principles, and there are around the 1950s fantastic work occurred in this area, where important principles that should govern constitutive equations were laid down and one of the pioneers of this was professor Oldroyd, who, his full name was James Oldroyd and he was a professor in Applied Mathematics at the Universities of Wales and Liverpool.

And his work was one of the first where he laid down clear basis for different, clear basis for principles that should govern constitutive equations. And again I am taking this set of sentences from the book by Phan Thien and he says that, it was Oldroyd who clearly enunciated the constitutive equation must be based on, the first point is the relative motion of the neighborhood of a particle.

The history of the metric tensor or the stress tensor, sorry, the strain tensor here, associated with the particle converted coordinate system embedded in the material and deforming with it. Physical constants defining the symmetry of the material and there are models which are named as Oldroyd AB and A and B fluid in honor of the work that he has done in this particular area.

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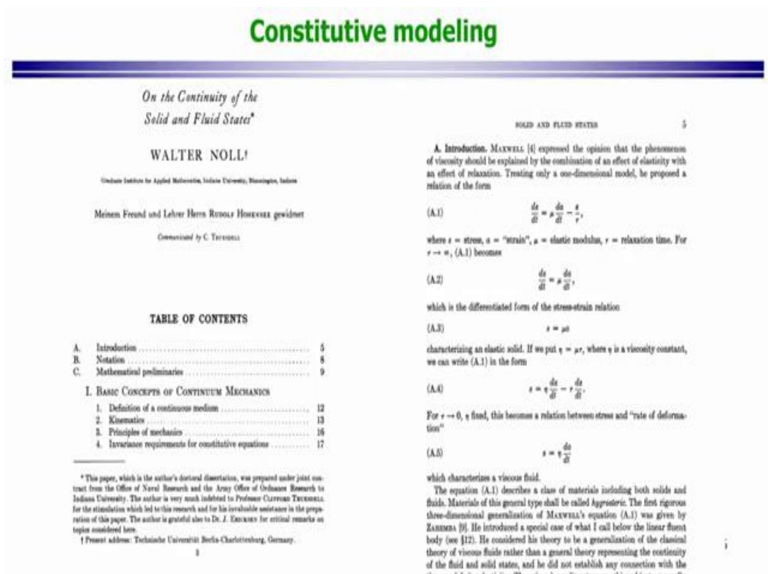


*On the Continuity of the Solid and Fluid States**

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Meinem Freund und Lehrer Herrn Rudolf Hoheisel gewidmet

*Communicated by* C. Truesdell

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SOLID AND FLUID STATES 5

**A. Introduction.** Maxwell [4] expressed the opinion that the phenomenon of viscosity should be explained by the combination of an effect of elasticity with an effect of relaxation. Treating only a one-dimensional model, he proposed a relation of the form

(A.1) $$\frac{ds}{dt} = \mu \frac{de}{dt} - \frac{s}{\tau},$$

where $s$ = stress, $e$ = "strain", $\mu$ = elastic modulus, $\tau$ = relaxation time. For $\tau \to \infty$, (A.1) becomes

(A.2) $$\frac{ds}{dt} = \mu \frac{de}{dt},$$

which is the differentiated form of the stress-strain relation

(A.3) $$s = \mu e$$

characterizing an elastic solid. If we put $\eta = \mu\tau$, where $\eta$ is a viscosity constant, we can write (A.1) in the form

(A.4) $$s = \eta \frac{de}{dt} - \tau \frac{ds}{dt}.$$

For $\tau \to 0$, $\eta$ fixed, this becomes a relation between stress and "rate of deformation"

(A.5) $$s = \eta \frac{de}{dt}$$

which characterizes a viscous fluid.

The equation (A.1) describes a class of materials including both solids and fluids. Materials of this general type shall be called *hygrosteric*. The first rigorous three-dimensional generalization of Maxwell's equation (A.1) was given by Zaremba [9]. He introduced a special case of what I call below the linear fluent body (see §12). He considered his theory to be a generalization of the classical theory of viscous fluids rather than a general theory representing the continuity of the fluid and solid states, and he did not establish any connection with the

His work was also followed by very outstanding work by Walter Noll, and here Walter Noll laid down some of the, in an axiomatic form. He laid down some of the basis on which constitutive equations must be developed. And this is again pages from one of his, this is of paper published, I believe in 1955 and this is considered a very seminal work in this area and the interesting reason I just wanted to point it out is, he begins with the maximum model again.

So, he starts off with the idea that the Maxwell expressed the opinion that the phenomena of viscosity should be explained by combination of an effect of elasticity within the effect of relaxation. And treating only a 1-dimensional model, he proposed relationship of the form and we have seen this equation. So, this is something that is familiar to us. So, what we are going to do is? We are going to discuss this basis.

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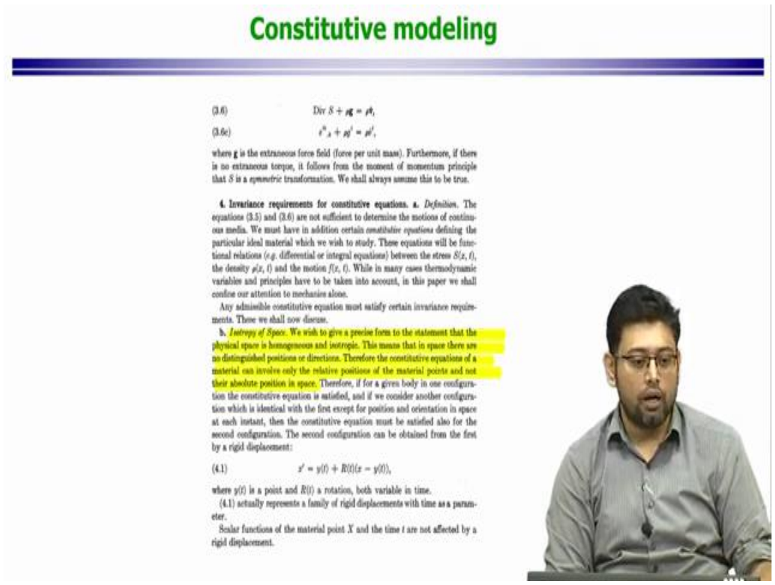


So, Noll in a seminal work, he points out an important issue that we will discuss in a bit of detail today and that concerns the isotropy of space. And just to read out from his manuscript, he says, that we wish to give a precise form to the statement that physical space is homogeneous and isotropic, this means that in space there are no distinguished positions or directions.

Therefore, the constitutive equations of a material can involve only the relative positions of material points and not their absolute position in space. And this becomes, this idea has evolved into a very important governing principle. So, we will stop discussing the work of Noll, et cetera. and we will start to.

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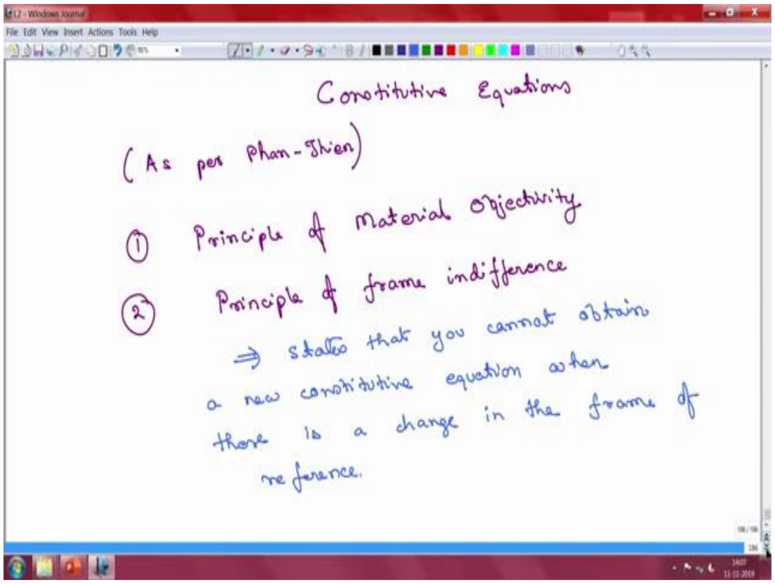


So, what we will do now is we will discuss and here what I am trying to do is you can read some of these seminal manuscripts and go through them, but the particular format in which I am going to discuss this is the format as laid down by Phan Thien in his manuscript. So, we are discussing the issue of constitutive equations and as said so there are different people who put this in different ways, so that is why I am pointing it out that I am discussing it as per Phan Thien as he has laid out this in his book.

So, there are four important principles, and the first of this principle is called the Principle of Material Objectivity. This principle we are going to discuss in more details. So, I am going to leave it out for the time being. I will come back to this again. Then there is a Principle of frame indifference and Noll, sorry, Phan Thien points out that to obtain a new constitutive equation, when you cannot obtain a new constitutive equation when there is a change of frame.

So, the operator or the basic constitutive operator should be independent of the frame that you are using. So, this principle, its states that you cannot obtain a new constitutive equation when there is a change in the frame of reference.

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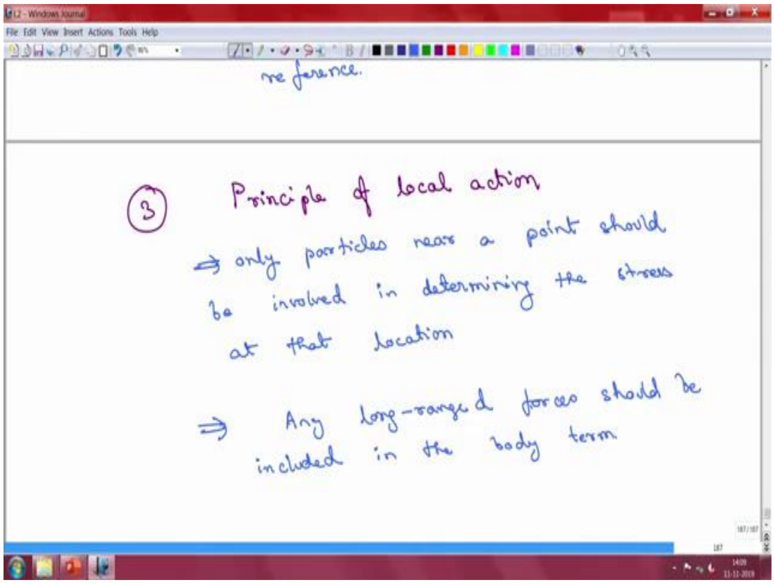


Another important principle is what we call the principle of local action, this principle states that only particles near a point should be involved in determining the stress at that point. So, only the neighborhood of a particle is involved in the deciding the current state of stress at that particle, some particle far away, some for example, the state of stress in a fluidic body on earth cannot be decided by other fluidic body, maybe outside of our solar system.

So, that is a very simple idea that the local bodies or the local location is what is, what plays the determining role in the state of stress. So, stress is the only particles near a point, near a point implies the immediate neighborhood should be involved determining the stress at that location, special location. So, any long range force, any long ranged forces should be included in the body term.

So, this is where we separate the action of the faraway system versus the local body or the local neighborhood, because we know that for example gravity does have a role and gravity from far away bodies can have a role in determining a stress, but that is considered as a body first term.

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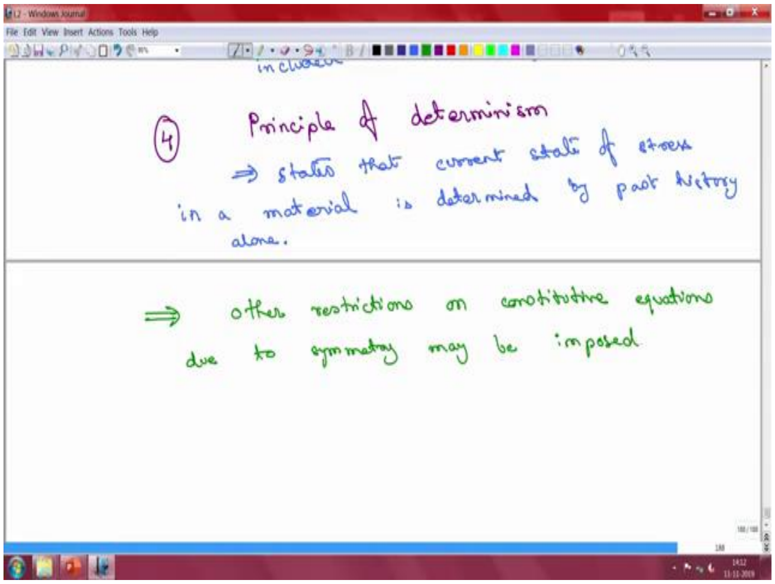


And then finally, there is the principle of determinism, the principle of determinism is the belief that the current state of stress is influenced by history but not by future. So, when you are taking the effect, when we say there is a memory that means that in the integral it is okay to integrate it from minus infinity to T, but not beyond any point given the current time. So, this again states that, the current state of stress in a material is determined by past history alone and not the future.

So, these four principles, there is a reason why they are being stated, so why we are using the word principle. And this is because they are basically axioms, which means that we stayed them, this is our belief that these are true and hence these are to be expressed letter on in mathematical form. But we do not necessarily need to have to prove any of these.

So, the correct way of looking at these principles are that they are axioms on which we will base the rest of the theory. Apart from all this other restrictions can also apply, for example, based on the symmetry of the material. So, other restrictions on constitutive equation due to symmetry may be imposed.

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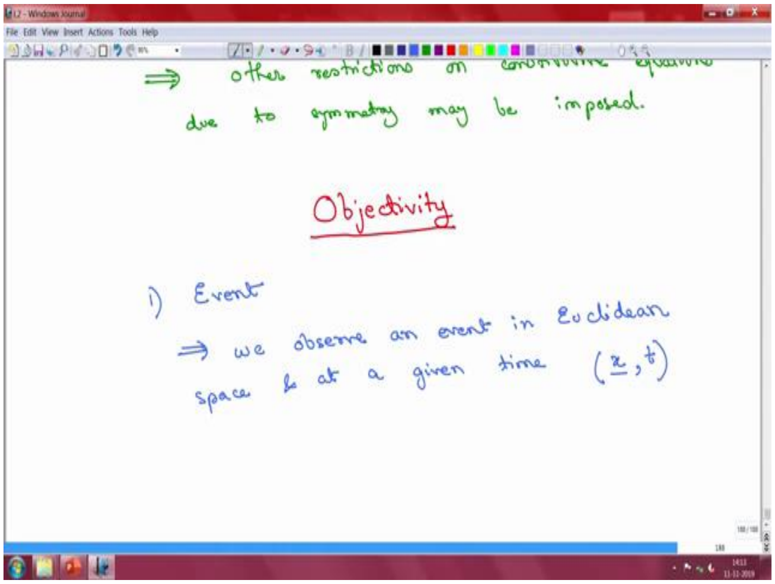


But we are not going to look at all these different issues the one issue that will consider in a bit of a detailed is the principle of objectivity. So, before we discuss objectivity, we want to discuss a some of the more general principles underlying this. So, let us before we discuss objectivity, we need to, we need to agree upon a few other things. So, we have to agree upon that, there is something called as an event. An event is something that we observe; we observe an event in Euclidean space and at a given time. So, you have some special location and time with which you can associate the event.

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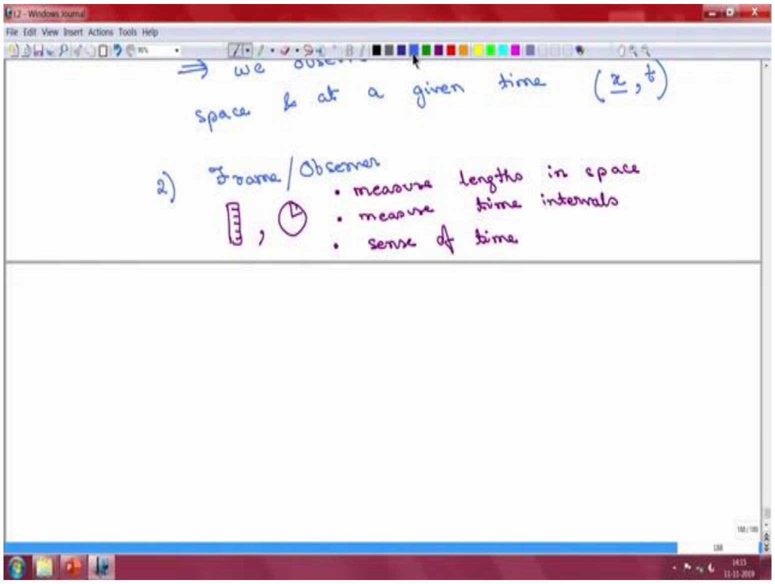


The second thing we have to agree upon is to what we understand by frame or an observer. So, frame or an observer is, if we think of it is, if you are wanting to think of observe as a person, let us think of that person as a guy who is holding let say a scale and has a stopwatch. So, that guy has a scale, scale bar with which he is going to measure distances, because he wants, the observer wants to observe events.

So, he needs to figure out what access, and to do that he must be able to measure lengths. And then he should be able to measure time. So, he also has us a watch with him, so the observer should be able to measure lengths in space, a length basically is special intervals. And similarly, he should be able to measure time intervals and finally he should also have a sense of time. So, time is not something which flows like or time has a special property that flows in one direction.

So, the observer must also understand which direction time is flowing because you cannot step into history like you can go and plus minus X, you cannot do the same thing with time. So, once we have an observer, we need not have only one type of observer, we can have many observers. So, are there, is there something called an equivalent observer?

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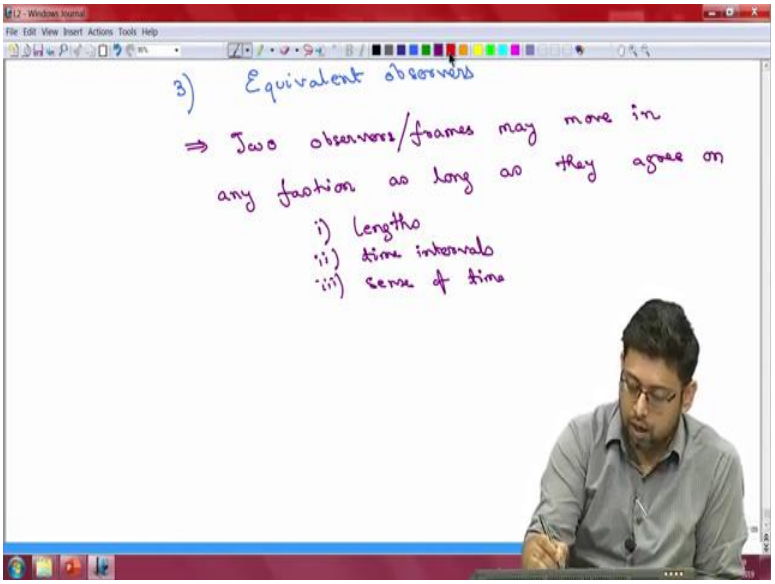


So, we say that two observers are equivalent, so we say that two observers or frames are equivalent, if they are moving. So, these two equivalent observers may move in any fashion with respect to each other of course, may move in any fashion as long as they agree on, one is lengths, two is time intervals, and three is sense of time.

So, two observers move in any fashion as long as they agree on lengths, time intervals and sense of time. We see that this, the third point is also very important, they need to agree upon a time flows. So, not only should they be able to measure distances in space, they should be able to have a common time interval. And they should have the same sense of time.

So, we are not going to consider for example, relativistic conditions. So, here the speeds are supposed to be much lower than the speed of light. So, we are just looking at the non-relativistic issues here. So, for example I am observing this room, I am one of the observers. So, let say I can see the distance between the two of you, I can measure it. And I will associate a certain distance between the two of you. And I know that this is true at this current time only.

And then some other person comes in, that other person observe us the way his going to look at the perspective is going to be very different. He is observing you guys and the chairs everything that is there in this room, to be placed at different special location with respect to him. But both of us can agree upon the distance between the two of you, both of us can agree upon that this event is only to at this given time.

So, that we can say that what I am going to measure later on, or what you are going to measure later on should be similar. They cannot be very different from each other. So, that simple idea is the basis of this discussion. And, so what you can show that these two observers.

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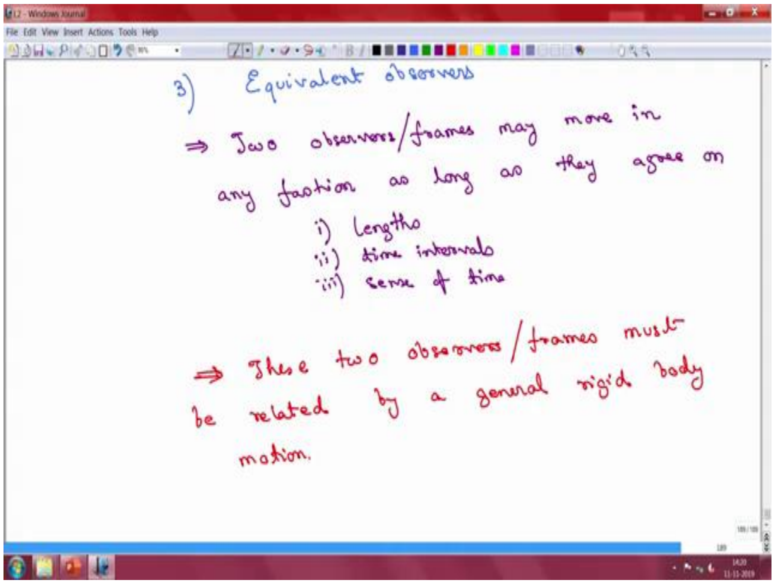


So, I will just make a note of it here, that these two observers or frames must be related by a general rigid body motion, a rigid body motion involves rotation and displacement. So, where are we trying to go from, go here?

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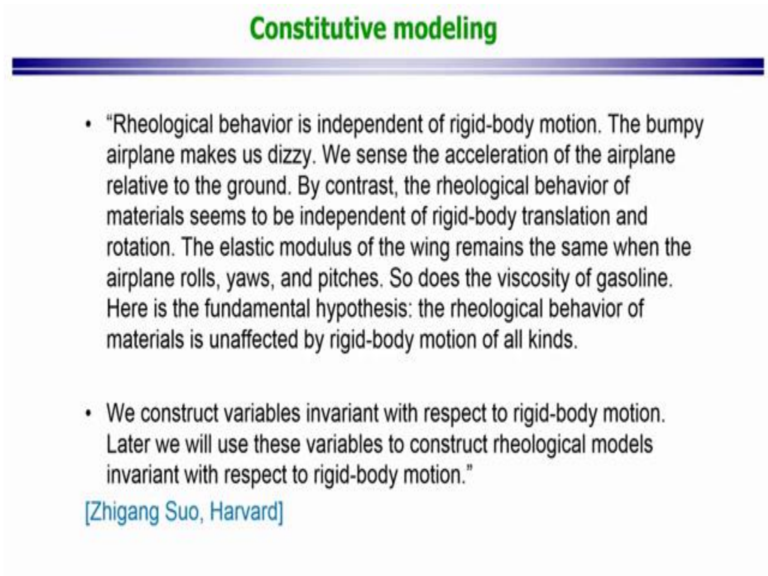


So, what we want to discuss or where we are getting to is this point and I am going to quote processor Suo here, I have taken this from set of his notes and he says that, "Rheological behavior is independent of rigid body motion. The bumpy airplane makes us dizzy. We sense the acceleration of the airplane relative to the ground. By contrast, the rheological behavior of materials seems to be independent of rigid body translation and rotation.

The elastic modulus of the wing remains the same when the airplane rolls, yaws, and pitches. So, does viscosity of gasoline, here is the fundamental hypothesis: the rheological behavior of materials is unaffected by rigid body motion of all kinds. And then he goes on to say later, that we construct variables in variant with respect to rigid body motion, later we will use this variables to construct rheological models invariant with respect to rigid body motion.

So, we just discussed the two observers, equivalent observers are basically related to each other by a general rigid body motion. So, basically this hypothesis is trying to say that the rheological behavior of materials should be the same for two equivalent observers. So, if I make some measurement or let us say, what is the? So, as I have a spring and you place it on a rotating disc, when you had done the experiment previously you must have determined a spring constant for that spring.

But when you put it on a rotating disc, the spring constant of the spring should not change, should be the same value just because now it is in a rotating frame compared to what lab frame we had use earlier cannot imply that the material behaviors have now changed totally. So, we are going to look into more details so this is the fundamental idea governing objectivity and we will discuss this more in the next class. So, we will stop here today.