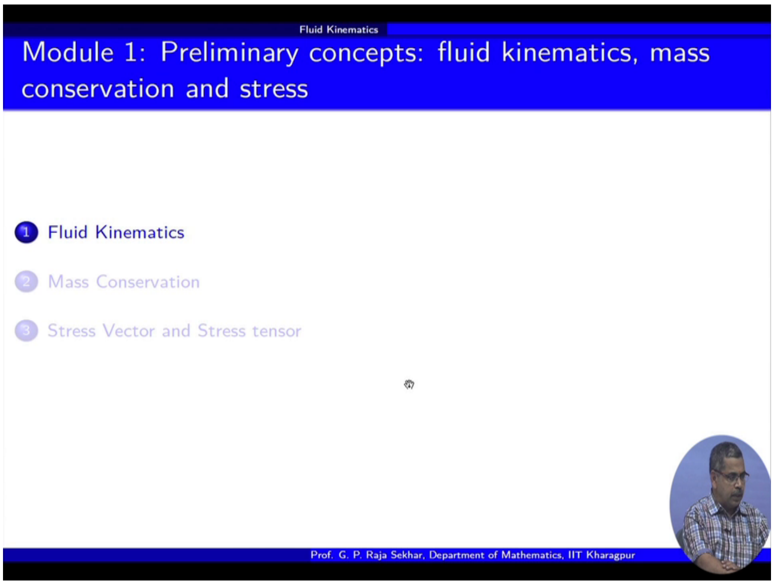
Modelling Transport Phenomena of Microparticles
Prof. G.P. Raja Sekhar
Department of Mathematics
Indian Institute of Technology - Kharagpur

Lecture - 1
Preliminary Concepts: Fluid Kinematics, Stress, Strain

Hello welcome to the course on modeling transport phenomena of microparticles. So this is done by two professors S.Bhattacharya and G.P.Raja Sekhar, both Department of Mathematics IIT Kharagpur, Okay. So as the title suggests modelling transport phenomena of microparticles, so what we would like to do in this course is we would like to run through basic tools to understand the transport of microparticles. So when we say micro particles are typically these are like viscous drops, soft colloids, microorganisms, or visit collides etc.

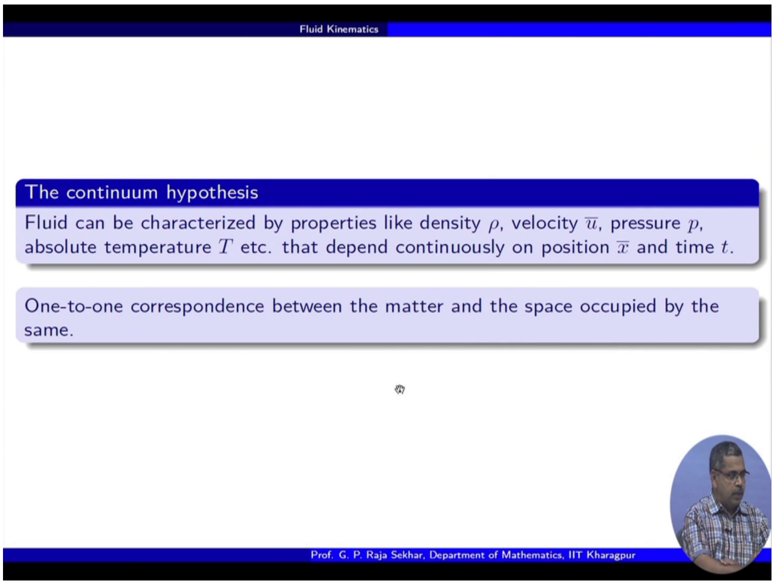
Most of these you can see in various applications in viscous environment and sometimes in addition to viscous environment you will see some external gradients like temperature or concentration or sometimes electric field etc. So the basic aim of the course is to give you some analytical tools and then now once that is done some computational tools okay. So let us see the module one.

(Refer Slide Time: 01:28)



Module one is preliminary concepts fluid kinematics, mass conservation, and stress, so these are the preliminary concepts, so when we say fluid kinematics, so typically when we start with the fluid kinematics, one would try to understand the basic Continuum Hypothesis.

(Refer Slide Time: 01:48)

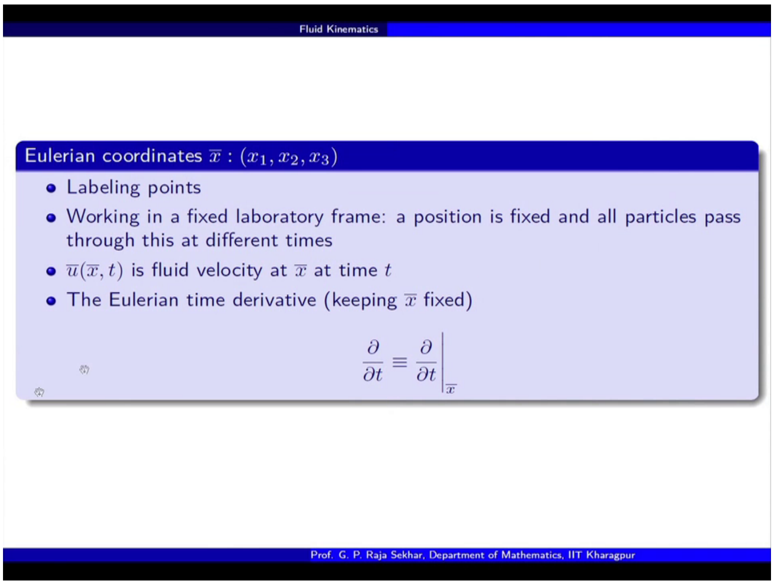


So what is continuum hypothesis typically a textbook definition is one-to-one correspondence between the matter and the space occupied by the same. So which means it is like this, so you have an object so now I kept here, so there is a one-to-one correspondence between the space occupied by the matter of this, suppose I move it so then again there is a one-to-one correspondence, so there is it is completely continuum okay.

So according to this, for example any fluid property like density, velocity, pressure, temperature, so they continuously depend on position and time. So it is once we have the continuum hypothesis typically fluid motion is described with the help of two approaches, one is Eulerian approach and other is a Lagrangian approach, so what is the big difference between these two.

The Eulerian approach is like we are sitting on a particular position and then let us say we are looking at it at that instant, whereas Lagrangian approach is like we are tracing the trajectory okay.

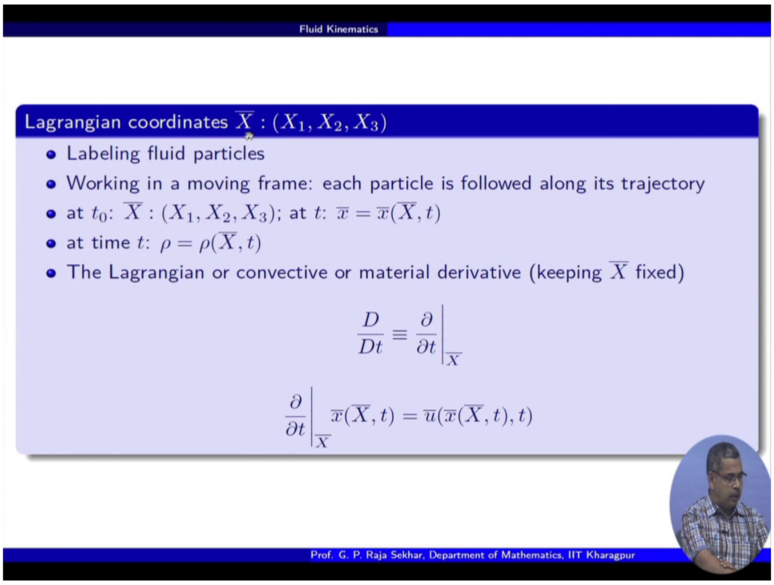
(Refer Slide Time: 03:10)



So let us see in detail Eulerian coordinates, so typically we are using a small x bar x1, x2, x3 Cartesian frame. So here it is nothing but labeling points which means we are working in a fixed laboratory frame, that means a position is fixed, so you are observing okay, who is passing by, who is passing by this at a particular time, who is passing at different time okay, so this is Eulerian approach okay, so a position is fixed and all particles pass through this at different times that what we are observing.

So accordingly, for example if you talk about velocity u bar x bar t this is nothing but fluid velocity at this position, at this time okay. So now corresponding to this Eulerian coordinate frame, what is the time derivative? So what we say is the position is fixed okay, so therefore the Eulerian time derivative is defined as the rate of change with respect to time while x bar is fixed okay.

(Refer Slide Time: 04:22)



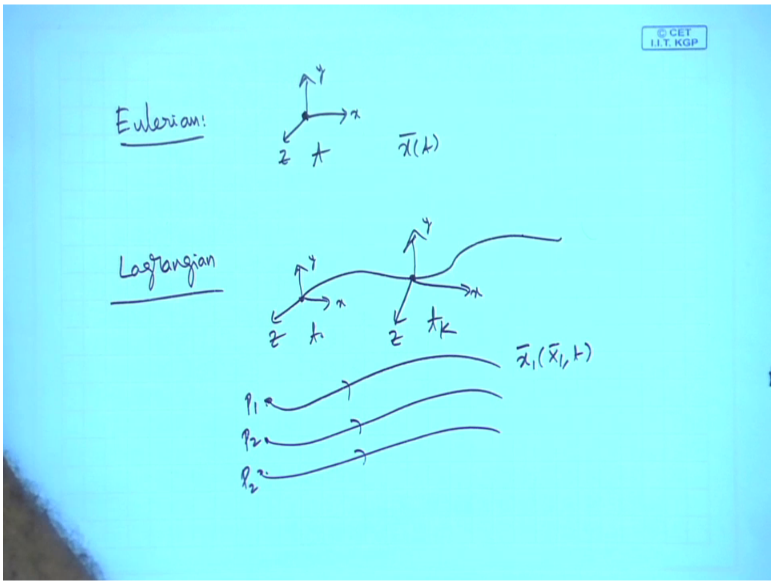
So now what is Lagrangian coordinate so this we are denoting by capital X bar again Cartesian frame and as I already indicated it is labeling fluid particles okay, so that means you are labelling your particle and then you are observing okay. It is like we are at a far off and then we are trying to see how a particle is moving okay.

Something like that okay, so accordingly at t0, so this is a reference position vector at time t, the position vector is expressed however you see in terms of the reference that means we are labelling the fluid particle with this reference position and then we are tracing okay. So for example if you take density, so this is explicitly in terms of the reference variable okay.

So now what these are corresponding derivatives in the Lagrangian frame, so this is called Lagrangian derivative or material derivative. So this is given this notation okay that means there is something more to be understood about this which we will, so you will see here it is a rate of change with respect to time with reference position fixed.

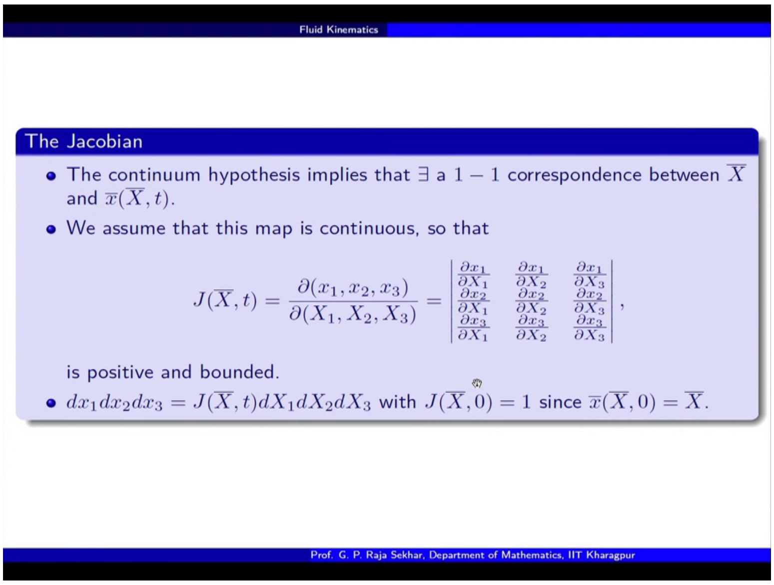
So for example if you take the position vector expressed in terms of this reference variable, so the Lagrangian derivative is the velocity but you can see the position vector is expressed in terms of the reference variable okay. So what is the basic difference?

(Refer Slide Time: 06:04)



So in one approach we have fixed the frame okay and in Lagrangian, we have taken a particle t0, so it is at some other time okay. So at some tk, so this is a trajectories each particle. So this is a particle one, particle two, particle three, so we are tracing the trajectories this is the Lagrange, so this approach you are observing sitting on that okay, then at that instant t. So this is nothing but, so here we have reference attached, so for example this is kind of okay. So this is the basic difference.

(Refer Slide Time: 07:19)



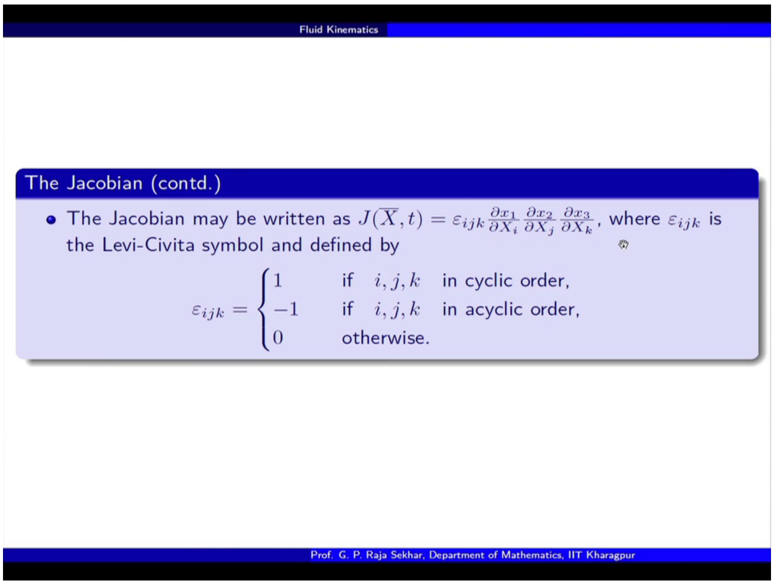
So once you have such a description then definitely we would like to use back and forth depending on the convenience. So the natural question to be asked is once you are given one description, how do you get back? Okay.

So naturally this is nothing but a coordinate transformation, so for any coordinate transformation what you require is the corresponding Jacobian right, so that is what we are defining. So as per the continuum hypothesis there exists a one-to-one correspondence between Lagrangian description and then earlier in description. So we assume that this map is continuous so that the Jacobian is positive and bounded and this determinant is non-zero by virtue of this.

So that the mapping is invertible and one can play with various descriptions okay. So correspondingly for any physical conditions you take it, and then model, and then let say you try to play with the corresponding coordinate systems, then you need a some volume element okay. So you see the volume element in Eulerian description is Jacobian times the volume element, the Lagrangian and you can see this Jacobian at time t equal to zero must agree with one because the position is agreeing with the reference okay.

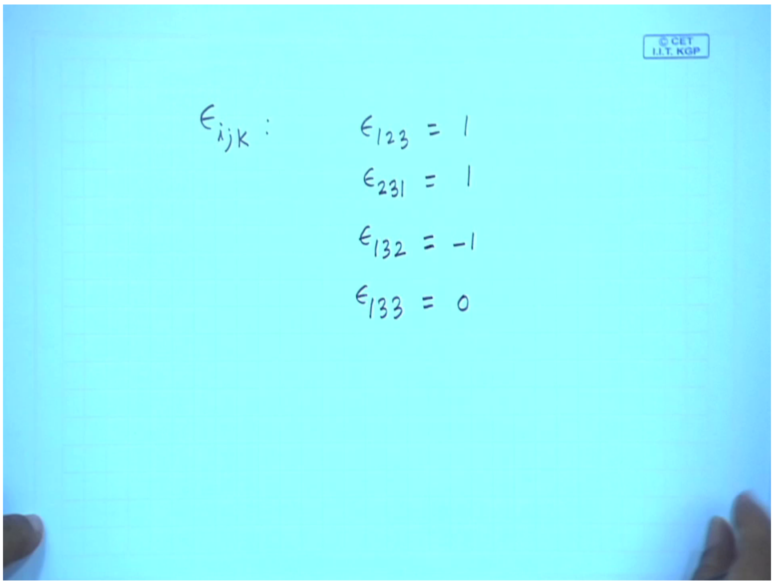
So that means there is no coordinate transformation right, so what is the use of this, use is like you one can now change the co-ordinate systems Lagrangian to Eulerian and Eulerian to Lagrangian using inverse transformation okay. So we will see the use of this very, very soon,

(Refer Slide Time: 07:19)



So this can be expressed in this form in a compact form this is the summation notation maybe in some exercise I will include a few problems on summation notation, so that you can comfortably follow okay. So this Jacobian can be expressed in this form where epsilon i, j, k is a Levi-Civita symbol and the definition is hinted here, so this is one if i, j, k in cyclic order -1 a cyclic 0 otherwise. So what does it mean? It means,

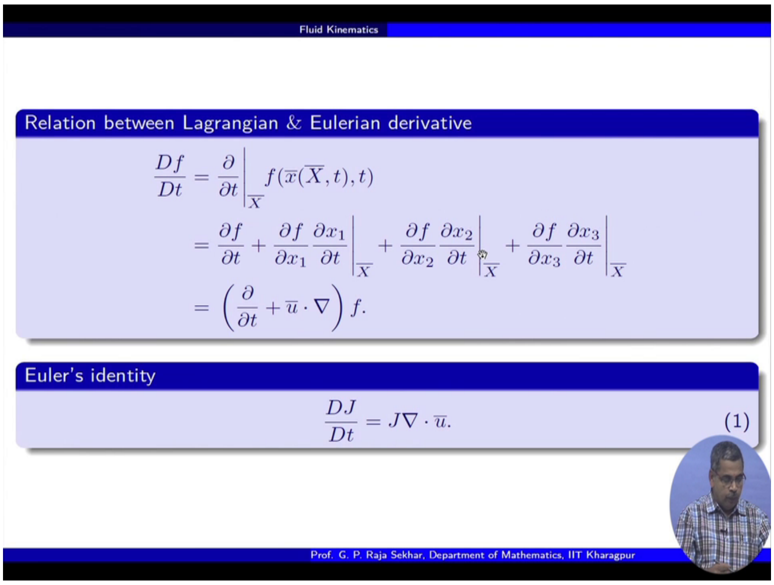
(Refer Slide Time: 09:48)



So you consider epsilon i, j, k, so suppose you take epsilon 1, 2, 3, since these are in cyclic order of the value is 1. Similarly suppose 2, 3, 1, so they are in cyclic order okay. Suppose 1, 3, 2, so the cyclic order is disturbed, they are in a cyclic order the value is -1, similarly suppose if you take 1, 3, 3, so there is index repeated so value is 0 okay, so one can easily and capture the Jacobian in terms of this okay.

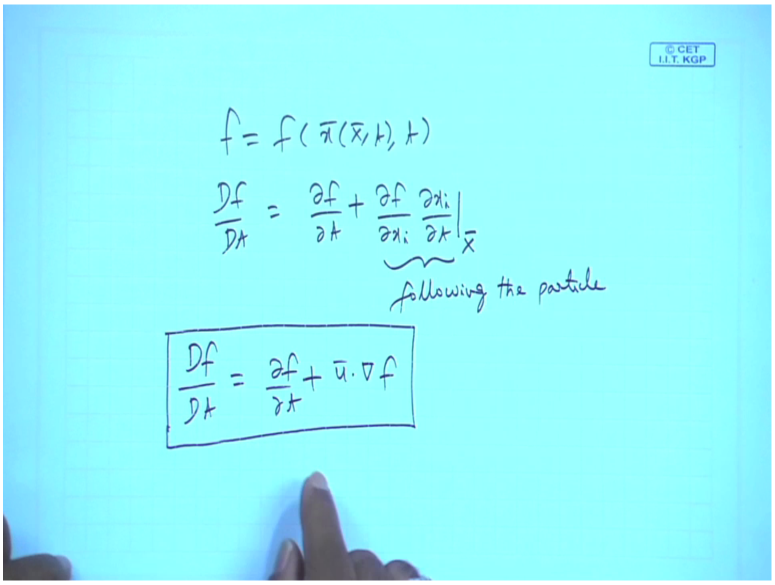
So this can be in exercise okay, this proof can be an exercise I will include.

(Refer Slide Time: 10:39)



So now once we have the corresponding Lagrangian and Eulerian derivatives what is the relation okay. So as you can see any fluid property f, it is expressed in terms of the position vector and time you can see this position vector is with the reference variable X bar expressed in terms of the Lagrangian. So now therefore the Lagrangian derivative or the material derivative of this fluid property is nothing but the local rate together with following the trajectory. So we would like to get the corresponding derivatives.

(Refer Slide Time: 11:28)

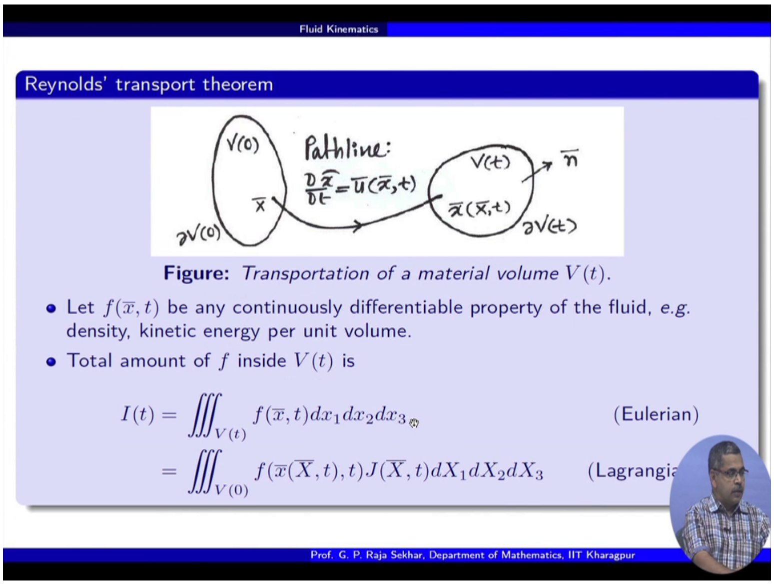


So you have an f, which is X bar of this so Df by Dt is the local rate + the following the particle so this is nothing but, following the particle okay. This is a local rate, so now this is nothing but velocity, so which we will see. So you can, so in Cartesian frame, so the summation I have expanded here so del f by del xi, del xi by del xt is expanded and you can see this is a u bar so the entire thing can be expressed as this.

So that means so we have the corresponding, sometimes called substantial derivative is given by okay, so this is the very useful because this will indicate how a particular fluid property is varying following the particle, so not only local time also the spatial trajectories okay. So that is the advantage.

So once you have the convective derivative we have discussed Jacobian and then we have convective derivative, so you have applied convective derivative on the Jacobian we get this, and this one can do using simple algebra, so I would like to include this in exercise, I am sure you will be able to do it okay right.

(Refer Slide Time: 13:15)



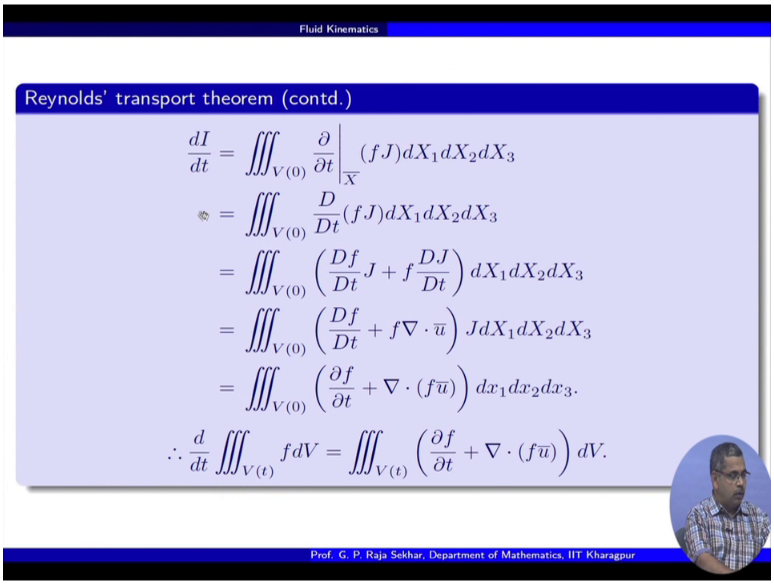
So we have now discussed how fluid motion can be described using Euler in Lagrangian approach and then how any fluid property let it be velocity, density, or temperature how it gets converted okay, so these variations we have discussed. So now we would like to derive the mass conservation but before that we would require some tools okay. So let us see the first tool namely Reynolds transportation theorem.

So basically this indicates the variations of any fluid property or a fluid element and how it is changing with time okay. So this is a Reynolds transport theorem you can see we have considered a fluid element at time t equal to zero bounded by volume V and the corresponding boundary is this, and this is the reference position vector and it is along a trajectory it has moved and then this is the corresponding volume element at time t.

So we have indicated to the normal as well here, so now we would like to understand if there is any fluid property f which is continuously differentiable how it gets converted and what is the rate of change of that particular fluid property over this volume element okay. So you can see once you have f the total amount is the integral of f over the volume element okay. This one so you can see this is the Eulerian description.

So now you come back to Lagrangian description so this position vector is expressed with reference to X bar and the corresponding Jacobian and the corresponding volume element and the Lagrangian is given.

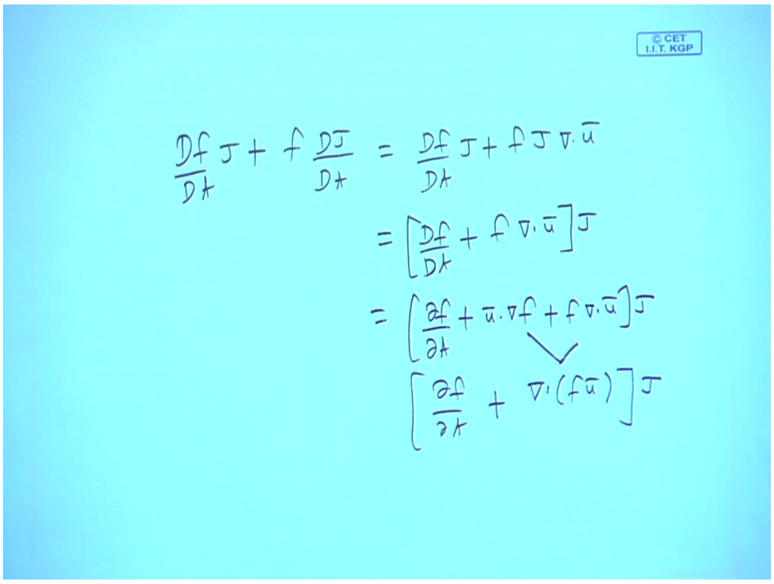
(Refer Slide Time: 15.25)



So now we would like to discuss the rate of change of this total amount accordingly we compute the derivative, so this is nothing but we are in Lagrangian frame, so this is the corresponding Lagrangian derivative okay. So you see this is nothing but the Lagrangian derivative, convective derivative okay. So you expand this is a simple calculus so once you do this we use Euler's identity here okay.

So one step is missing, so I would like to do this step here, so consider this okay and then we use Euler's identity.

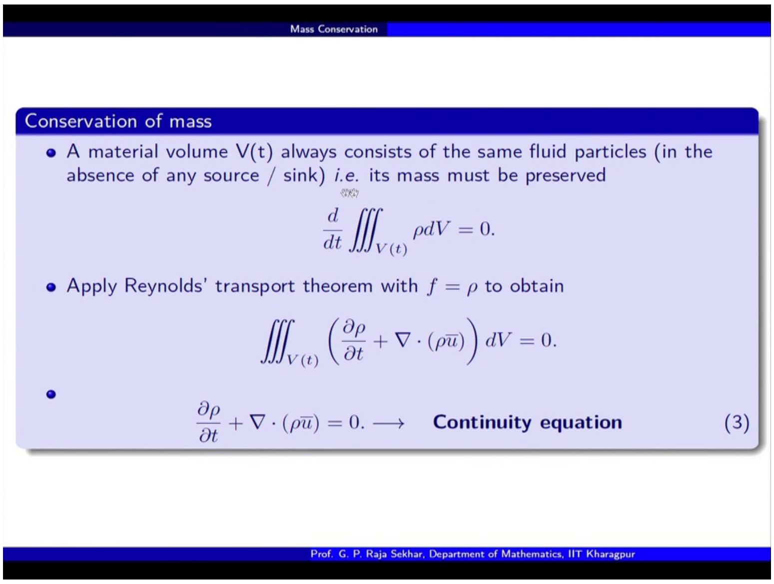
(Refer Slide Time: 16:11)



So once you will Euler's identity we get see you have two terms Df by Dt J + f DJ by Dt. So we are using Euler's identity so fJ so this is nothing but Df by Dt + so we have taken the Jacobian out further use the convective derivative. So this will be u dot grad f + f divergence u J. And these two are combined so therefore we get okay; this is what we have written here okay, so that what we have got okay.

So the total rate of the total amount is equals to this, so that means if you take any fluid property f let it be density or temperature or energy, so over a fluid element how it is changing is indicated by this okay. So this is very useful tool to derive conservation of mass okay. So as I indicated, so we are very much interested in the next conservation of a mass which is a first fundamental principle okay.

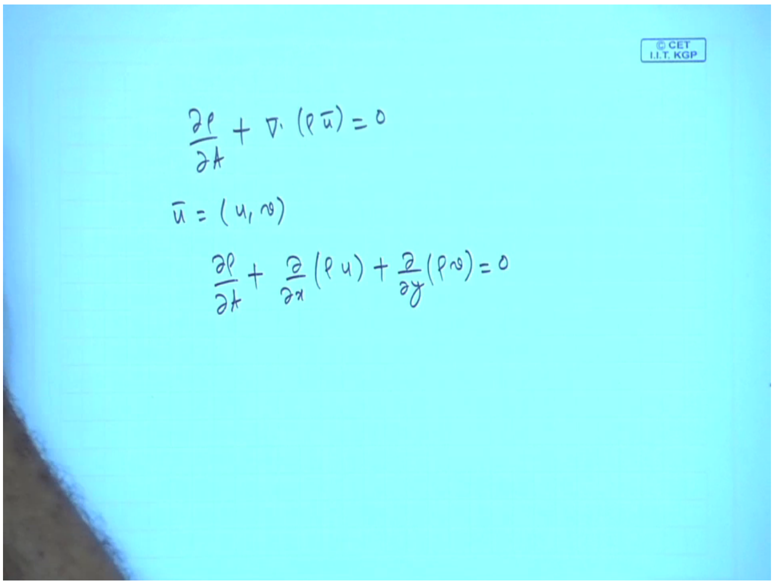
(Refer Slide Time: 17:59)



So according to this a material volume we always consists for example, if you do not have source and sink so then accordingly what will happen, once you have a mass that stays so no addition and the no deletion is taking place then total mass is conserved, so always consists of same fluid particles okay. Therefore mass must be preserved so accordingly the rate is in this is the mass and then rate is zero okay because the constants the derivative of that will be zero.

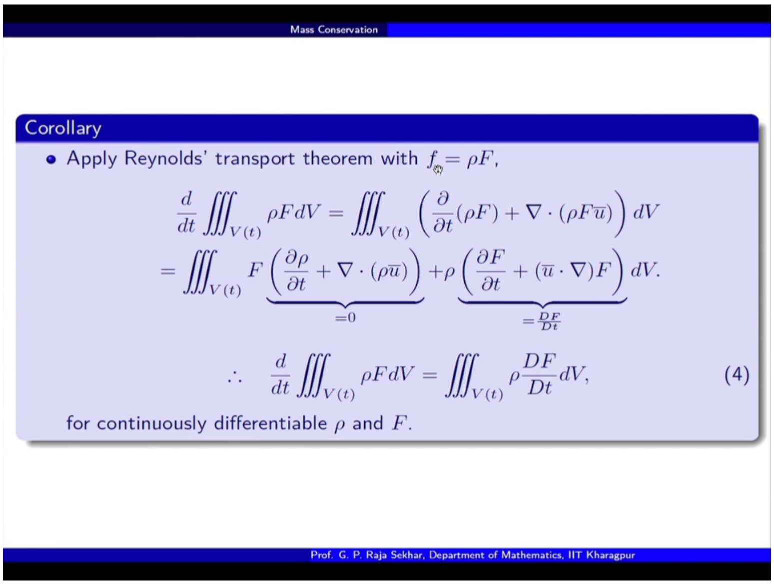
Now apply Reynolds transport theorem with f equals to the density okay. So you see this we have the Reynolds transport theorem if you take f equals to Rho right density, so then this will be the mass and if the total mass is comes out d by dt of this is 0. And then correspondingly f will be Rho we get the following okay, and you can see this holds for any arbitrary volume element so therefore the integrand is 0, which is a called a equation of continuity, so which is a fundamental equation.

(Refer Slide Time: 19.15)



So this is a general where you have density is varying for example let us say you have a 2D so then the above equation will be Rho u, Rho v = 0, so correspondingly if you have three dimensions or polar coordinates one can write a similar form okay. Right so now there is a corollary to Reynolds transport theorem.

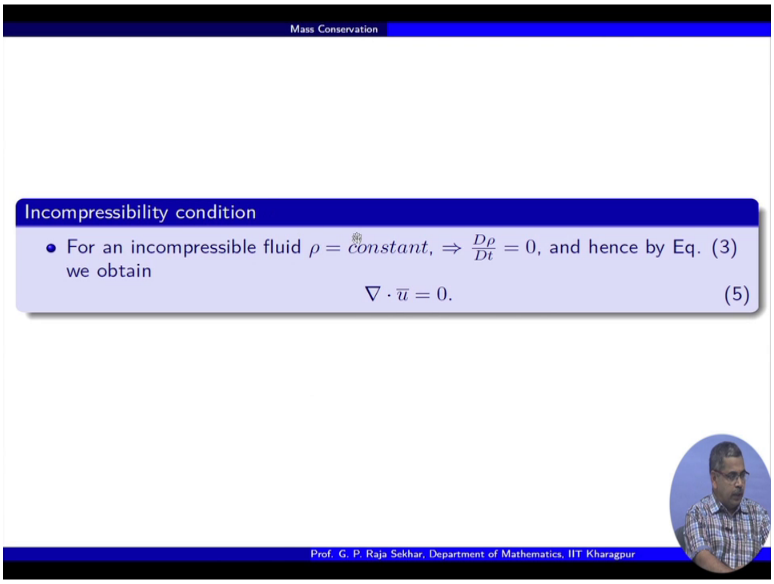
(Refer Slide Time: 19:56)



So let us say instead of f equals to Rho you take f equals to Rho f so then d by dt over a volume element row f dV is we apply the Reynolds transport theorem and we expand one term is coming here, one term from this coming here okay, similarly one term is here and one term is here and this is nothing but the df by dt and this is nothing but equation of continuity, which we have seen just now therefore this is zero and this is the convective derivative.

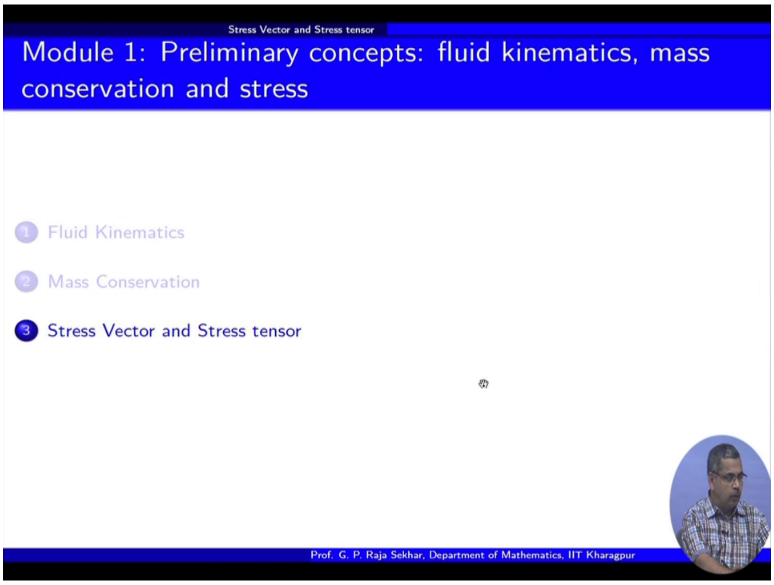
So therefore one useful identity we get is d by dt of Rho times any fluid property is Rho times we convective derivative okay. So this is very useful identity which will use it while deriving various other balance principles okay.

(Refer Slide Time: 20:58)



Okay so now incompressibility condition for an incompressible fluid so that means, we are talking about density variations are not there either with respect to space or time so correspondingly you have Rho is constant and then you get d Rho by dt = 0 and hence from equation of continuity we get divergence of u is 0, so this is a typically equation of continuity for incompressible.

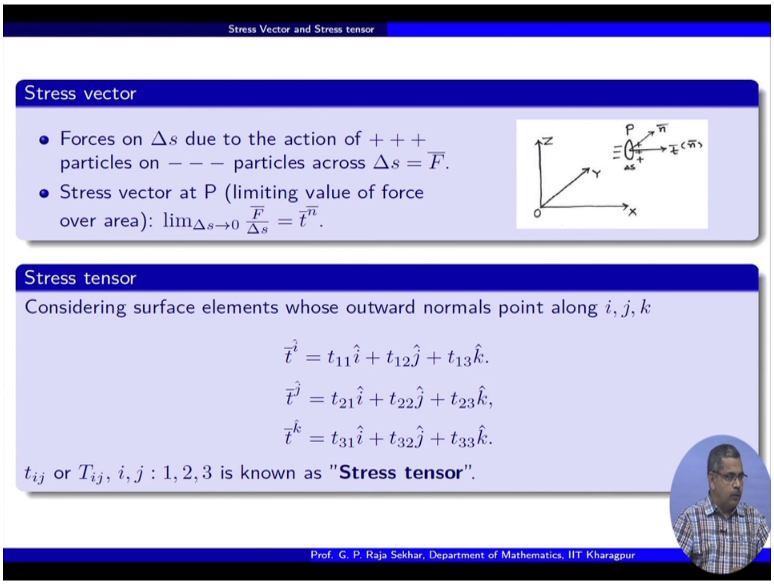
(Refer Slide Time: 21:30)



So it is okay so now we, so far we have discussed the corresponding fluid description and then Reynolds or transportation theorem, which is, which gives you how a fluid property gets convicted along, so once we do this we should move on to the corresponding momentum balance because that is the next natural principle okay. But before we go to this we need to understand about forces so when you say forces on a fluid element so these are expressed captured in terms of stresses okay.

Typically either in solid mechanics or fluid mechanics forces are captured in terms of stresses, okay or vice versa stress is captured in terms of course so we would like to understand the concept of stress so that we are in a position to move forward and get the conservation of momentum okay.

(Refer Slide Time: 22:39)



So what is the stress vector, so you apply a force on an element okay, so that means let us say you have any surface and then you apply force okay? So what will happen the force is applied on a particular surface so then what is the stress we would like to capture, right so the stress is defined as the force limiting of the force on a particular area, that means the area is approaching to 0 and then the force acting on a particular surface element while the surface element is approaching 0, so that is the stress okay.

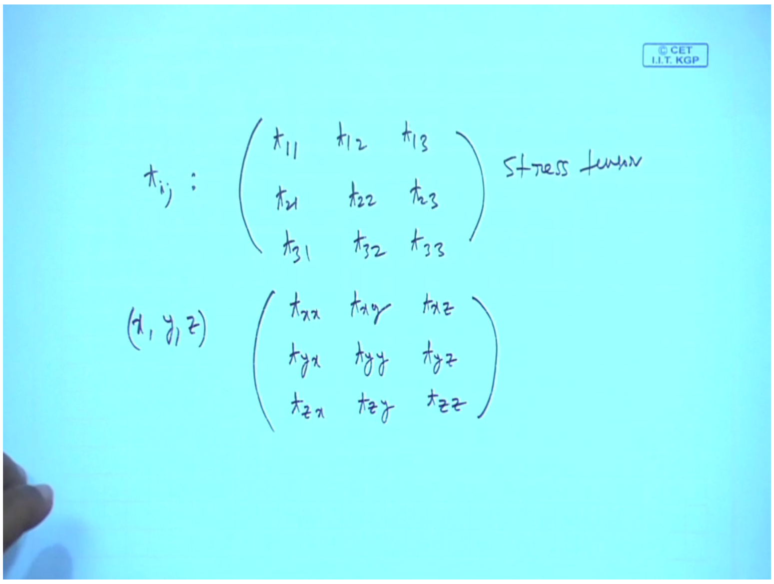
So accordingly you see we have taken a small element okay, which has a normal and then let us say this is the stress which we are going to define, how we are going to define is force on a particular surface element these are indicated with plus these are indicated with negative, so action of these particles on these particles, across small surface element, so this is the force.

Now how a stress is defined as I mentioned just now limiting value of the force our area okay. Which means F bar by delta s is the stress vector okay, s as delta s approaching 0, okay, so now once we say stress vector then that means this has components so those components are defined in terms of something called stress tensor okay.

So let us understand this stress tensor, suppose you consider surface elements whose awkward normal's pointing along i, j, k, okay. So then the stress factor ti indicates that we are considering a surface element whose outward normal is pointing along i then it can be resolved along the three components so one is t11, t12, t13, so here you see we are talking about i. So let us say i is 1 so normal is along i where we are talking about stress on a surface having normal along i.

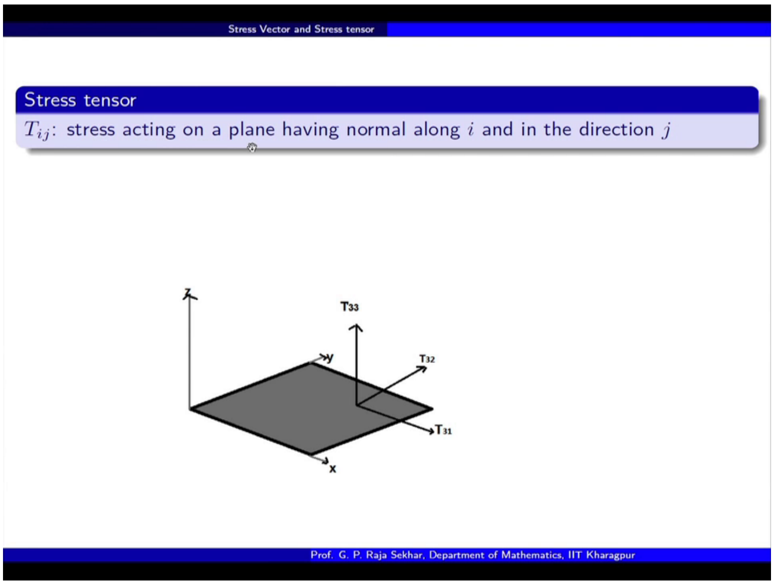
So then this is the i component, j component, k component, similarly you consider a surface element whose outward normal pointing along j, so then here j is fixed, you can see then this is the i component, j component, k component, similarly this is on a surface which is having normal along k. So therefore three, we have three so then now this is X along I component, J component and K component.

(Refer Slide Time: 26:10)



So that means once you have a stress vector we have 11, 12, 13, 21, 22, 23, 31, 32, so this is called stress tensor, so we have nine components, three dimensions so this is called stress tensor okay.

(Refer Slide Time: 26:40)



So to be more precise this is what I indicated Tijs stress acting on a plane having normal along i and in the direction j, so let us take an example, so this is the plane you can see normal is along k okay, z axis along k, so therefore this is stress acting on a surface having normal along z and x component normal along z, y component, normal along z, z component okay.

So these are the corresponding stress components, so in Cartesian suppose if somebody is using x, y, z. So this can be written as xx, xy, xz, yx, yy, yz, zx, zy, zz okay. So this is in Cartesian similarly if you are using polar correspondingly one can write down the corresponding components okay, so now the most interesting is what will be the stress xy and yx that means we are considering this means what, stress acting on a surface whose normal is along x axis and the component is along y.

And this one is stress acting on a surface whose normal is along y and the component is x, so we will see in later modules there will be interesting the relation between these two, so which will be useful okay, so understanding stress is a very much important because this will give you the contact forces okay, so as I indicated once you have conservation of mass what will be the next one is balancing momentum right.

So momentum means we are balancing the forces, so contact force are very much play a role so in order to compute the contact forces we have to capture the stress and then integrate the stresses okay, so we will discuss the next module the how the stress will be integrated to get the momentum balance, okay thank you.