

**Foundation of Computational Fluid Dynamics**  
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**Lecture – 01**

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Syllabus outline for the course

- Review of basic fluid mechanics including governing equations
- Taylor's series expansion procedure to obtain different finite difference formula
- Numerical errors, Stability criteria
- Finite difference formulation for different model equations
- Finite volume formulation in detail
- Time advancement methods for unsteady flows
- Pressure Velocity coupling
- Different Matrix inversion procedures
- A complete demo with Illustrative example including code display and explanation



Welcome to this MOOC course on Foundation of Computational Fluid Dynamics. I'll just do now course outline for this course. We start off with basic review on fluid mechanics which includes some important properties and governing equations. Then, important topic on Taylor's series expansion procedure to obtain different finite difference formula, numerical errors and stability criteria, finite difference formulation for different model equations... Then we go on to finite volume formulation in detail for solving full governing equations.

How to do unsteady equations? Which means time advancement methods for unsteady flows; then another important procedure what is known as a pressure velocity coupling, which is linking momentum equations and continuity equations. All these equations when discretized will result in what is known as linear algebraic equations. Then to solve we have to know different matrix inversion procedures. We will go over there procedures also. Then at the end, we will also see, a complete demo for two or three example problem discretization procedure, how a code is written, how a mesh is setup and what are the results and how to go about writing code etcetera.

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## Learning outcomes

At the end of course a student will be

- to understand discretization strategies
- to appreciate various numerical strategies
- to gain confidence either to write own code / to inherit code from open source and understand inner details with ease
- to understand theoretical background based on which commercial CFD softwares are built
- to gain confidence to apply CFD to a problem
- to be able to take up advanced course on any topic related to CFD



So, after going through this course, a student is expected to understand discretization strategies, and appreciate different numerical strategies like computational domain, boundary condition, what inversion procedure one has to follow and how to obtain results and interpretations. One also will get confidence on writing a code because we are going to see at the end, a complete working code, details of the code etcetera. And that will give you confidence to write own code or if a code is inherited from some other a person or source, then it also requires equivalent skills to understand that code.

There are many commercial CFD software and open source available, to use them one has to know details; otherwise, it will be a wrong selection of choices. So, one can understand at the end of this course, all the theoretical background based on which the commercial CFD software are built. You will also get confidence to apply any CFD code or own, commercial software or own code to any engineering applications problem. After this, this is a foundation course, so each of the sub topic is also available in the form of advanced course. For example, grid generation, finite volume method in detail etcetera. So, one can pursue those higher course, after this course.

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## Reference Text Books

- Anderson, D.C., J.C, Tannehil, and R.H.Fletcher, Computational Fluid Mechanics, Hemisphere Publishing Corporation, NewYork.
- Ferziger, J.H. and M.Peric, Computational Methods for Fluid Dynamics, Springer, 3<sup>rd</sup> Edition, 2002.
- Versteeg, H.K. and W.Malalasekera, An introduction to computational fluid dynamics – The Finite Volume method, Second Edition, 2007.
- Chung, T.J., Computational Fluid Dynamics, Cambridge University Press, 2002.



There are many text books available, and many online reference material available. So, I am listing here, particularly three or four text books, a student is expected to go through various other materials also. First book on Computational Fluid Mechanics written by Anderson, Tannehil and Fletcher; second book, Ferziger and Peric, book title – Computational Methods for Fluid Dynamics. Then there is a book exclusively on Finite Volume Method written by Versteeg and Malalasekera. There is a comprehensive text book on Computational Fluid Dynamics authored by T. J. Chung. As I mentioned before, there are many materials available, so please do not restrict yourself, only these four text books, you are also encouraged to ready many other online material available to gain confidence on this topic.

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## Week 1 – Syllabus Content

- Review of basic fluid mechanics
- Review of basic governing equations and importance of terms
- Non-dimensionalization and its importance
- Vorticity-Streamfunction Transport Equation
- Classification of Equations, Examples and Solution nature
- Types of Boundary conditions
- Types of Problems
- Description about some test problems



Now, having discrete course content, expected outcome and reference text book. We now move on to actual course. So, in week one, I planned to do some important review on basic fluid mechanics, governing equations. We will do a derivation on one or some important terms of the derivation not in detail, they are expected in standard text book and some importance certain terms. There is some procedure called non-dimensionalization. So, we will go through that and find out why one has to do. There is a specific governing equation, what is known as a vorticity-stream function relation. We will do the derivation of the vorticity-stream function derivation. Then all these governing equations in fluid mechanics or heat transfer are mostly partial differential equations can classify them, and we will find out how to classify them based on the solution nature. And what is the procedure, how a procedure is different for different types of equation.

Then there are different types of boundary conditions available, so we will go through them also. Then there are different types of problem, we will see those types of problem with example. Then whenever somebody writes a code or setup a numerical strategy to solve any particular problem, there is a procedure called taking a standard test case and proving that code or proving your numerical strategy for the standard test case. So, we will go through few standard test case problems, explained the features in them; what kind of boundary conditions are imposed. And whenever you have to do a code

development or using a commercial software, you need to do this first step of proving your code for these test cases. So, this will be the course content for week one.

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### Different Co-ordinate Systems

- Relating Cartesian to cylindrical coordinates  $x = r \cos \theta$ ,  $y = r \sin \theta$

- Cylindrical to Cartesian

$$r = \sqrt{x^2 + y^2}, \quad \theta = \tan^{-1}\left(\frac{y}{x}\right) \text{ for } x > 0, \quad \theta = \pi - \tan^{-1}\left(\frac{y}{x}\right), \text{ for } x < 0$$

- Spherical to Cartesian  $(\rho, \theta, \phi) \equiv (x, y, z)$

$$\rho = \sqrt{r^2 + z^2} = \sqrt{x^2 + y^2 + z^2}$$

$$r = \rho \sin \phi; \quad \theta = \cos^{-1}\left(\frac{x}{r}\right) \quad (0 < \theta < 2\pi : \text{polar angle})$$



$$\phi = \cos^{-1}\left(\frac{z}{\rho}\right) \quad (-\pi/2 < \phi < \pi/2 : \text{zenith angle})$$

We now go on to review of basic fluid mechanics. We know we deal with lot of equations or mathematical terms, so we just do what is known as a different co-ordinate systems. So, we know there are basically three co-ordinate system, one is a Cartesian co-ordinate system – x y. Second one is the polar co-ordinate system – r theta, third one is a spherical co-ordinate system, which is r theta z. You can convert from any one co-ordinate system to any other co-ordinate system, there is a relationship. Now, why do you want to do this, because all the governing equations need not be only in one co-ordinate system, we should be able to convert from one co-ordinate system to other co-ordinate system and solve problem according to the co-ordinate system that you can described for the problem.

So, basic quantity for example, in two-dimensional co-ordinate, Cartesian co-ordinate system x and y is related to r theta co-ordinate system as x is equal to r cos theta and y is equal r sin theta. So, in cylindrical co-ordinate system, then we have r is equal to square root of x square plus y square, and theta is related to tan inverse of y over x, for x greater than zero, and different relationship for x less than zero. Similarly, spherical co-ordinate system to Cartesian co-ordinate system, in spherical co-ordinate system, you have three parameters to define. One is the rho, which is the radius; and theta is angle between two

sets of co-ordinate, and phi is angle between another two sets of co-ordinate. And they are related to Cartesian co-ordinate system x, y, z. In this formula, that is given here; rho is equal to square root of r square plus z square. So, this is available in any standard text book or anywhere else. So, we need to know how to convert from one co-ordinate system to another co-ordinate system.

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## Vector Operators

- Gradient (scalar f)

$$\vec{\nabla} f = \frac{\partial f}{\partial x} \hat{i} + \frac{\partial f}{\partial y} \hat{j} + \frac{\partial f}{\partial z} \hat{k} \quad \vec{\nabla} f = \frac{\partial f}{\partial r} \hat{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{e}_\theta + \frac{\partial f}{\partial z} \hat{k} \quad \vec{\nabla} f = \frac{\partial f}{\partial r} \hat{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \hat{e}_\phi + \frac{1}{r \sin \phi} \frac{\partial f}{\partial \theta} \hat{e}_\theta$$

- Divergence  $\vec{V} = V_x \hat{i} + V_y \hat{j} + V_z \hat{k}$

$$\vec{\nabla} \cdot \vec{V} = \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z} \quad \vec{\nabla} \cdot \vec{V} = \frac{1}{r} \frac{\partial}{\partial r} (r V_r) + \frac{1}{r} \frac{\partial V_\theta}{\partial \theta} + \frac{\partial V_z}{\partial z}$$

$$\vec{\nabla} \cdot \vec{V} = \frac{1}{\rho^2} \frac{\partial}{\partial r} (r^2 V_r) + \frac{1}{\rho \sin \phi} \frac{\partial}{\partial \phi} (V_\phi \sin \phi) + \frac{1}{\rho \sin \phi} \frac{\partial V_\theta}{\partial \theta}$$

- Curl  $\vec{\nabla} \times \vec{V} = \left( \frac{\partial V_z}{\partial y} - \frac{\partial V_y}{\partial z} \right) \hat{i} + \left( \frac{\partial V_x}{\partial z} - \frac{\partial V_z}{\partial x} \right) \hat{j} + \left( \frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y} \right) \hat{k}$

$$\vec{\nabla} \times \vec{V} = \left( \frac{1}{r} \frac{\partial V_\theta}{\partial \theta} - \frac{\partial V_r}{\partial z} \right) \hat{e}_r + \left( \frac{\partial V_r}{\partial z} - \frac{\partial V_z}{\partial r} \right) \hat{e}_\theta + \frac{1}{r} \left[ \frac{\partial (r V_\theta)}{\partial r} - \frac{\partial V_r}{\partial \theta} \right] \hat{k}$$



There are different standard vector operations available. So, we first see what is known as a gradient. If there is a scalar function f, and if you do gradient of f then you get dou f by dou x i plus dou f by dou y j plus dou f by dou z k. You can also get a gradient expression in other co-ordinate system r and theta, which is defined as here, dou f by dou r and unit vector in r co-ordinate system as e r; similarly for second term and third term. The same way you can also define gradient operator in spherical co-ordinate system, which is given the last expression. Then another important operation is divergences. So, if you define elastic vector with the component and corresponding unit vector as V x into i plus V y into j plus V z into k, then divergence is defined as del dot v equal to dou V x by dou x plus dou V y by dou y plus dou V z by dou z.

Just like we did for gradient, we can also define divergence in other two co-ordinate system, r theta co-ordinate system and spherical co-ordinate system. Third important operator is a curl, which is defined as del cross V, so dou V z by dou y minus dou V y by dou z for i, similarly for second component dou V z by dou z dou V z by dou x into j,

then third component has  $\frac{dV_y}{dx}$  and  $\frac{dV_x}{dy}$  for  $k$ . So, you can extend this procedure for other two co-ordinate system, and we just defined here for  $r$  theta co-ordinate system as you can see here, the first component and second component and third component. Now, these are important, because it is easy or for any quantity later, you find them it is extremely useful.

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### Total Derivative of Multi-variable function

Scalar function:  $f(x, y, z, t)$

Total derivative at a point  $P(x, y, z, t)$  for the function is defined as

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial t}$$

$x, y, z$  are independent variables and function of 't' only

- The first term on RHS is called '*temporal derivative*' of the function
- The next three terms is called '*spatial derivative*' or '*convective derivative*'.



Then another important mathematical related quantity for fluid mechanics is what is known as total derivative. So, for a function, which is defined in  $x, y, z$  and  $t$ ; then one can define the total derivative of the function at a point  $P$ , and this is defined as capital  $D$  of the function by capital  $D t$  is  $\frac{df}{dt}$  plus  $\frac{df}{dx} \frac{dx}{dt}$  plus  $\frac{df}{dy} \frac{dy}{dt}$  plus  $\frac{df}{dz} \frac{dz}{dt}$ . Now, you can also recognize  $\frac{dx}{dt}$  is time rate of change of spatial co-ordinate, which is actually the velocity in  $x$  direction. Similarly,  $\frac{dy}{dt}$  is a velocity component in  $y$  direction, so all so for velocity component in  $z$  direction, because function  $f$  is dependent on three co-ordinate  $x, y, z$  and  $t$ , we have partial derivative define for that function in time as well as in other three spatial co-ordinate system.

Now, such as derivative is defined here as capital  $D$  by  $D t$ , which is known as material derivative or substantial derivative or total derivative. The first term on the right hand side, which is  $\frac{df}{dt}$  is called temporal derivative, because it is derivative taken

with respect to time. The other three terms are called spatial derivative or convective derivative. So, this gives local acceleration and this give convective acceleration.

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### **Fluid as a Continuum**

- Properties are considered to be continuous functions of space and time
- Modeling fluid as a continuum assumes that it is continuously distributed and fills the entire region of space it occupies.
- This assumption does not allow properties to become infinite or to be undefined at a single isolated point.
- In view of the particulate nature of matter, it may seem appropriate to question the validity of the continuum assumption.
- However, the governing equations derived based on this assumption have withstood the test of time and the assumption of fluid medium as a continuum has got firmly established.



Now, we restrict ourselves to fluid as a continuum, which mean properties are considered to be continuous functions of space as well as time. We have just seen a function of  $f$ , function of  $x$ ,  $y$ ,  $z$  and  $t$  and that is considered to be continuous, there is no gap in between. So, modeling a fluid as a continuum assumes that properties are continuously distributed and fills the entire region of space it occupies. Now, this assumption does not allow properties to become infinite or to be undefined at a single isolated point, but there are some branches what is known as molecular dynamics where there is a question whether this continuum assumption is valid. But in this course, we are going to restrict ourselves only took situation where fluid is treated as continuum. Hence all the governing equation and whatever procedure we are going to do to deal with those governing equations or restricted only for fluid as continuum and it has been tested by several people and different situation and this assumption holds good. So, we are restricting ourselves only to situation where fluid is treated as a continuum mechanism. There is another subject called rarified gas dynamics where it is treated not as continuum.



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### Viscosity

- Viscosity is the property of fluids which describes the internal resistance of the fluid to flow and may be thought as a measure of fluid friction. All fluids possess some resistance to stress.
- The fluid which has no resistance to shear stress is said to be an *ideal fluid* or *inviscid fluid*.
- Two definitions of viscosities  
Absolute or dynamic viscosity  $\nu = \frac{\mu}{\rho}$   
Kinematic viscosity (momentum diffusivity)

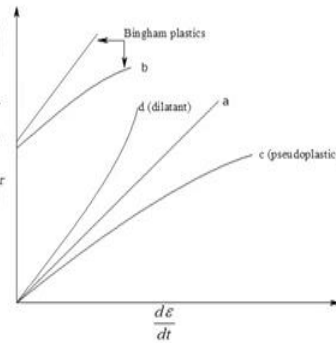


There are many properties, first is the viscosity. So, it is the property by which internal resistance to a fluid flow is defined and it is just a measure of fluid friction. So, all fluids supposed to have some resistance to the flow and because of the resistance it develops some stress. Fluid where resistance is assumed to be zero or no effect is there, such a fluid is called ideal fluid or inviscid fluid. So, in some situation, you can assume ideal fluid situation or inviscid calculations can be done to obtain first level of results or approximation then that inviscid solution can be taken as a initial condition for subsequent viscous calculation. So, this stage-by-stage, numerical simulation is helpful to overcome any numerical difficulties. There are two definitions available; one is absolute or dynamic viscosity, second one – kinematic viscosity, it is also called momentum diffusivity. And these two are interrelated.

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## Newtonian and non-Newtonian Fluids

- In a Newtonian fluid, there is a linear relation between the magnitude of applied stress and the resulting rate of deformation (marked 'a')
  - In a non-Newtonian fluid, there is a non-linear relationship between the value of applied stress and the rate of deformation.
  - For time-independent fluids, a power-law model of the following form is commonly proposed.
- $$\tau = k \left( \frac{d\delta}{dt} \right)^n = k \left( \frac{d\delta}{dt} \right)^{n-1} \left( \frac{d\delta}{dt} \right)$$
- $$= \eta \frac{d\delta}{dt} = \eta \frac{du}{dy}$$
- Fluids for which apparent viscosity decreases with increasing deformation rate ( $n < 1$ ), are called 'pseudoplastic' (marked 'c') or *shear thinning fluids*.
  - If apparent viscosity increases with increasing deformation rate ( $n > 1$ ), the fluid is termed 'dilatant' *shear thickening fluid* (marked 'd')



So, having defined viscosity, stress and strain one can classify fluid based on how they behave. So, major classification Newtonian fluid or non-Newtonian fluid. In Newtonian fluid, there is a linear relationship between applied stress and resulting rate of deformation. In non-Newtonian fluid, there is a non-linear relationship between the value of the applied stress and the rate of deformation. So, there is a graph available; so on y-axis, we have the stress – tau; on x-axis, we have the rate of strain – d by dt of epsilon, which is strain. So, a is a linear straight line, so linear relationship between applied stress and the resultant strain that behavior, which is marked here as a is known as Newtonian fluid. Any other behavior, which is marked in this figure either b, citation d or citation c, where the linear relationship is not followed, we are called non-Newtonian fluid. So, we have example tooth-paste is the example for non-Newtonian fluid; blood is example for non-Newtonian fluid, grease is example for non-Newtonian fluid.

So, whenever we have a non-Newtonian fluid, there are different models available to describe them. A popularly used a power law model, where the stress is related to rate of deformation by power law, so it is d by dt of strain to the power of n, n is the index of the power. And you can separate as d by dt of delta to the power of n minus one and the remaining one part is written separately. This product k into d delta by dt to the power of n minus one, this term alone is referred as apparent viscosity which is written by the symbol eta, so d by dt of remaining term delta and which is related to strain d u by dy, this is velocity strain. So, this is because in general in for Newtonian fluid, we write tau

equal to  $\mu \frac{du}{dy}$  or  $\mu \frac{du}{dy}$ ; so for non-Newtonian fluid also we would like to have a similar expression and that is written here as  $\eta \frac{du}{dy}$ . The difference here is  $\eta$  is apparent viscosity,  $\mu$  is another viscosity.

So, we can go one more small sub classification; fluids where apparent viscosity which is  $\eta$  decreases with increasing deformation rate which means  $n$  is less than one is called pseudo plastic which is marked here as  $c$  in this curve. So, the relationship between stress and rate of strain is decreasing with an increasing, so on x-axis as you go, it increases; whereas, the rate here is smaller in the other axis. The second situation, if the apparent viscosity increases with increasing deformation rate, which happens for dilatant fluid which is marked here as  $d$ . So, there are situations where there is a stress required then the fluid will start moving so that is the meaning of situation where  $b$ . So, they will not start flowing up to some definite pressure is set for plastic.

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### Scalar and Vector Fields

- A field is a quantity which can be defined as a function of position at every point in space.
- The quantity may be a scalar, which has magnitude alone, or a vector, which is characterized by magnitude as well as direction.
- When a scalar quantity is defined as a function of position, it is said to be a scalar field.
- Similarly, when a vector quantity is specified at every point as a function of position, it is said to be a *vector field*.

Scalar field:  $T(x, y, z)$ ;      Vector field:  $\vec{V}(x, y, z)$

- The components of the vector field are scalar field functions
- The direction at each point along which the resulting rate of change is oriented is associated with gradient of scalar field and makes it a vector.



Flow field:  $\vec{V}(x, y, z, t) = u(x, y, z, t)\hat{i} + v(x, y, z, t)\hat{j} + w(x, y, z, t)\hat{k}$

We also now go to the next topic what is known as scalar or vector fields, because in fluid mechanics we talk about velocity, temperature or concentration, so we should know what is the scalar field and what is the vector field. A field is a quantity which can be defined as a function of position at every point in space. This may be a scalar, which has only the magnitude or vector which has both magnitude as well as direction. When a scalar quantity is defined as a function of position then it is said to be a scalar field.

Similarly, when a vector quantity is specified at every point as a function of position then it is said to be vector field. So, for example, temperature is a function of x, y, z and if you prescribed temperature then it becomes scalar field. Similarly, vector velocity is defined then it becomes velocity field, because it is direction dependent.

You can also take a component, so component of vector field or called a scalar field function, so just like velocity vector  $V$ , if we take a component in x, y, z then we get corresponding component of velocity in that direction. Though it is defined as a scalar field, it keeps on changing, so even if you take only the velocity component as it keeps on changing in x direction. For example, then the direction along which the change happens results a vector. So, for a flow field, velocity vector  $v$ , which is a function of spatial co-ordinate x, y, z also as a function of time; we have a three component u, v, w and all three also varies as a function of x, y, z as well as time. And to get to get back velocity field – vector field, you multiply magnitude with a corresponding unit vector i, j, k. So, one can obtain from the scalar field, vector field this way.

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**Vorticity Vector**


$$\vec{\omega} = \omega_x \hat{i} + \omega_y \hat{j} + \omega_z \hat{k} = \frac{1}{2} (\vec{\nabla} \times \vec{V}) = \frac{1}{2} \vec{\Omega}$$

Cartesian:  $\vec{\Omega} = \left( \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \right) \hat{i} + \left( \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \right) \hat{j} + \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \hat{k}$

In cylindrical polar,  $\vec{V} = V_r \hat{e}_r + V_\theta \hat{e}_\theta + V_z \hat{k}$ ;  $\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \frac{\hat{e}_\theta}{r} \frac{\partial}{\partial \theta} + \hat{k} \frac{\partial}{\partial z}$

$$\vec{\nabla} \times \vec{V} = \left( \frac{1}{r} \frac{\partial V_z}{\partial \theta} - \frac{\partial V_\theta}{\partial z} \right) \hat{e}_r + \left( \frac{\partial V_r}{\partial z} - \frac{\partial V_z}{\partial r} \right) \hat{e}_\theta + \left( \frac{1}{r} \frac{\partial}{\partial r} (r V_\theta) - \frac{1}{r} \frac{\partial V_r}{\partial \theta} \right) \hat{k}$$

- A fluid particle moving without rotation in a flow field cannot develop a rotation under the action of a body force or normal surface forces.
- Development of rotation in a fluid particle, initially without rotation, requires action of a shear stress on the surface of the particle.
- Since the shear stress is proportional to the rate of angular deformation, then a particle initially without rotation will not develop a rotation without a simultaneous angular deformation.



Next quantity of interest is vorticity vector, and  $\omega$  is the symbol used to define this vorticity; expression for  $\omega$  is shown here with its component. So,  $\omega = \omega_x \hat{i} + \omega_y \hat{j} + \omega_z \hat{k}$  and that is also equal to half times  $\nabla \times V$ , where  $V$  is the velocity vector and that is equal to half rotation vector which is capital  $\omega$ . And in terms of detail Cartesian component, rotation is given here as

$\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}$  into  $i$  – this is the x component; similarly expression for y component  $\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}$  into  $j$  plus expression for third component  $\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$  into  $k$ . Expression for cylindrical co-ordinate system is also given here.

Now, we know in a fluid, a fluid particle is subjected to body force or normal force as well as shear force. A fluid particle moving without rotation in a flow field cannot develop rotation under the action of body force or normal force. Development of rotation in a fluid particle, initially without rotation, requires action of a shear stress on the surface of the particle. If the rotation or vorticity is zero, that is  $\text{del cross } V$  is zero, such a flow is called irrotational flow. Since the shear stress is proportional to the rate of angular deformation, then a particle without initial rotation will not develop rotation without any simultaneous angular deformation. So, for a fluid to have rotational viscous force, which actually results in the form of shear stress is responsible for rotation.

In this first module, a outline syllabus for the entire course, outcome of this course, what is expected from this course, reference text book, important fluid properties, basic review on mathematical operations, viscosity, and something about rotation. So, next class, we are going to continue this and slowly move onto governing equations.

Thank you.