Computational Fluid Dynamics
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Lecture - 09
Scalar Transport, Mathematical Classification and Boundary Conditions

Welcome back to the last lecture in module 02 mathematical modeling, in this lecture you would finish of an unfinished business in governing equation that is you would obtain governing equation for transport of a generalized scalar quantity. Then you would focus on mathematical classification of governing equation in fluid flow. And look at what are the initial boundary conditions we require for numerical studies of the flow problems.

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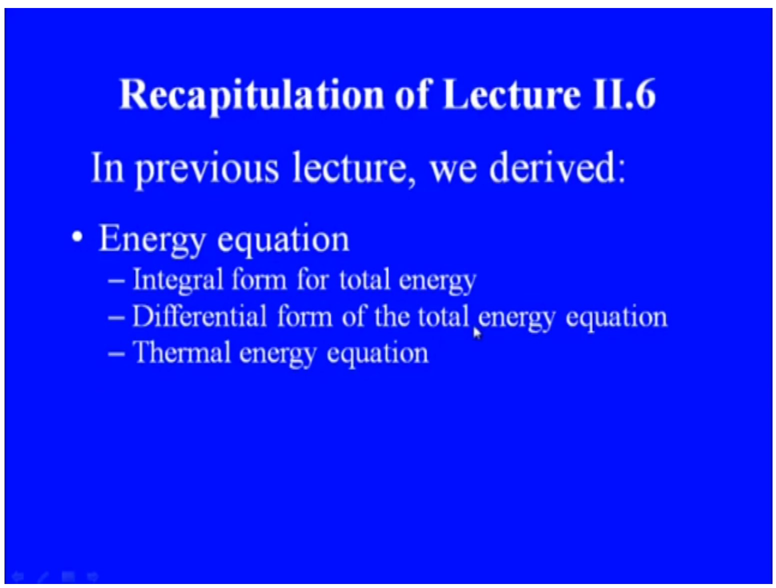

Let us see a brief recap of what we did in last lecture we derived energy equation starting from the first law of thermodynamics we obtained the integral form for total energy, and thereafter we invoked the Gauss divergence theorem to obtain the differential form of the total energy equation from that we subtracted mechanical energy equation and we obtained a thermal energy equation and in its different forms.

In this lecture we would focus on scalar transport, mathematical classification and boundary conditions which we require in flow problems, so this what our outline would be.

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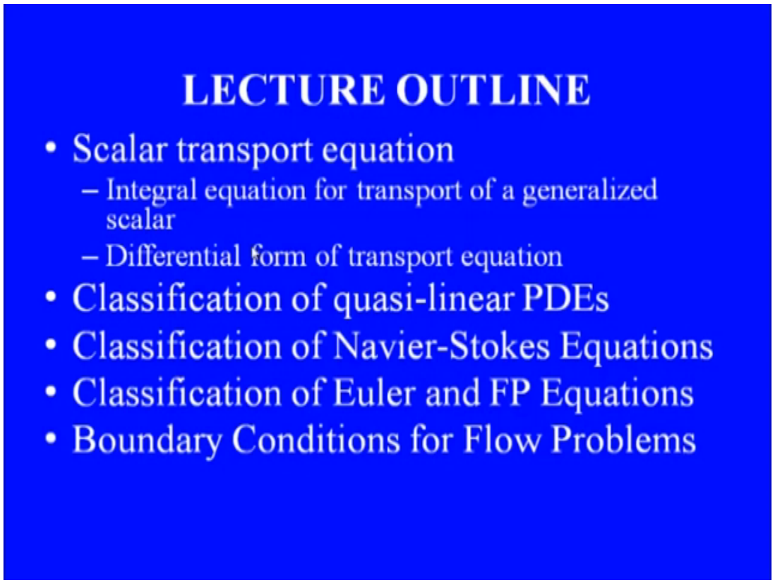

We would start off with scalar transport equation obtain an integral equation for transport of a generalized scalar quantity, and thereafter again we would obtain as usual a differential form of transport equation. Then we will have look at mathematical classification in particular the classification of quasilinear PDEs, and how we can extend this classification to the flow problems governing equation fluid flow.

And what we do the effect of choice of initial and boundary conditions, and we would also have a look at the classification of Euler and Full potential equations, and we will have a brief look at most commonly encountered boundary conditions for flow problems. So let us start off with conservation of a scalar quantity.

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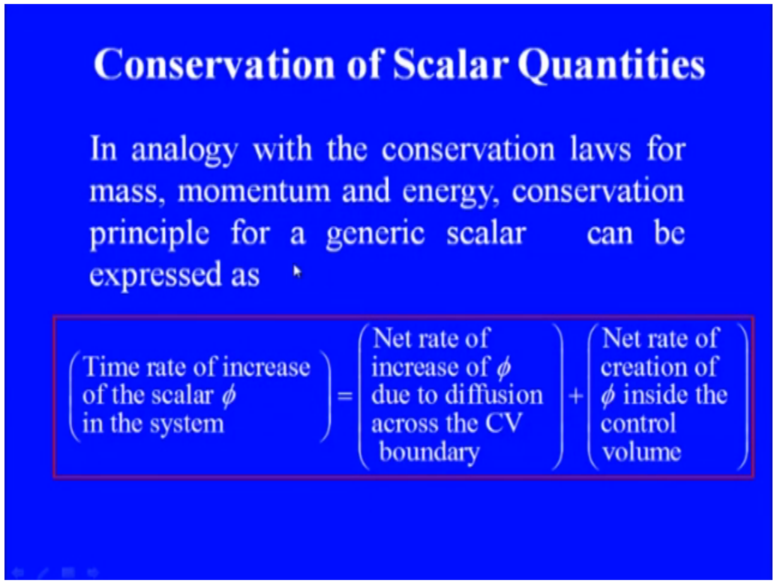

So we will invoke an analogy of what we said earlier in the case of energy equation or Momentum equation or mass okay, so we can extend the same conservation principle that is we want to find out the time rate of increase of the scalar quantity phi in the system. Now this increase could be due to two reasons, the first one is the sum amount of phi which is being transported across the control volume boundaries okay.

Net rate of increase of phi due to diffusion across the CV boundary + net rate of creation of phi inside the control volume, to understand this analogy further let us have a brief look at what we did earlier in the case of energy equation.

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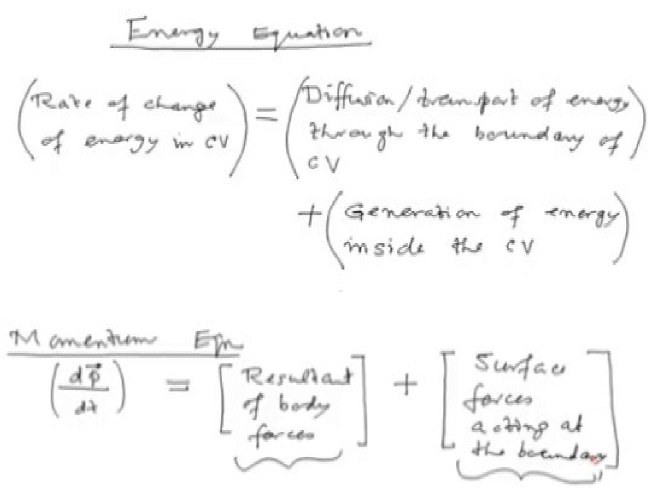

Let us explore the analogy further and let us go back to the statement of energy equation, so what we had in the case energy equation we had rate of change of energy in our control volume, this was contributed by two terms the diffusion or in general we can say the transport of energy through the boundary of a problem domain + the second one we had was the generation of energy of energy which could be due to a chemical reaction inside the control volume.

In fact we will find similar sort of things happening in the case of momentum equation, so let us also have a look at the momentum equation, what we had the rate of change of momentum dP/dt. Now this can be caused because of two things, first is we have got a body force which is similar to a source term inside the body, so resultant of body forces, so this body forces are sort of represent what we call sources of as a force present inside the body + surface forces acting at the boundary.

Now the second part, if you look at the surface forces this could be thought of as diffusion of momentum or this happens because of the transport momentum across the control surface. So this explains the analogy which we had invoked in this case for a a generic scalar, you can say the time rate of increase of the scalar phi is because of two things, net rate of increase of phi due to diffusion across CV boundary + net rate of creation of phi inside the control volume.

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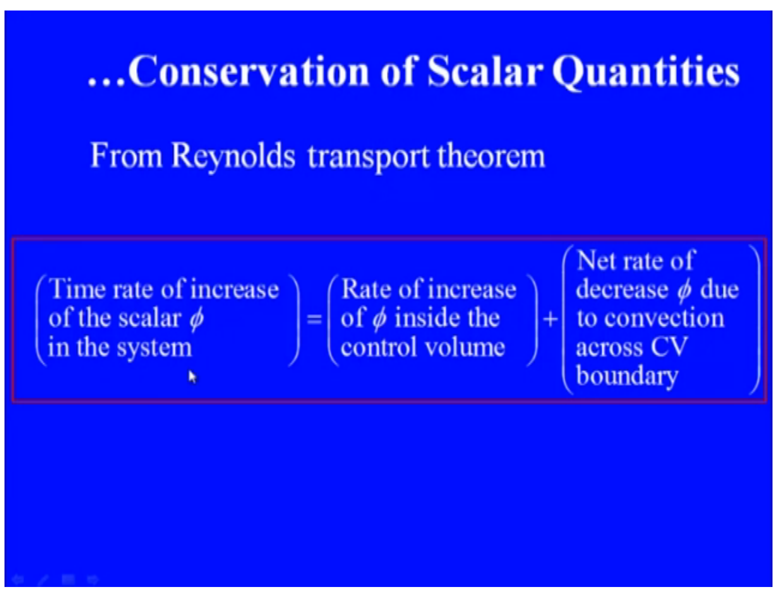

Now we can invoke the Reynolds transport theorem to convert the rates for a system to that our control volume, the time rate of increase of scalar in the system this = rate of increase of phi inside the control volume + net rate of decrease of phi due to convection across the CV boundary.

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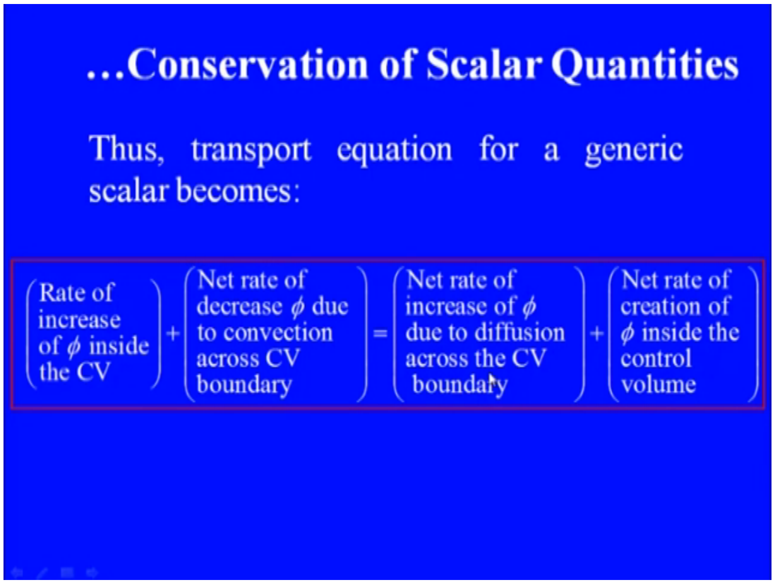

So we combined these two equations together and the left hand side we will get rate of increase of phi inside the CV + net rate of decrease of phi due to convection across a CV boundary = net rate of increase of phi due to diffusion across the CV boundary + net rate of creation of phi inside the control volume. So let us have a relook this rate of increase of phi inside the CV this would be essentially a time derivative of volume integral.

And this convection term that could be because of a surface integral the convection of phi because of fluid flow, and the RHS again you got increase of phi due to diffusion across the CV boundary, so this again be represented by surface integral and the last term would be due to a volume integral which is a net system of different sources inside the volume. Now to obtain the formal equation let us have a detailed look at each one of these terms.

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Scalar Transport

$$\left\{ \begin{array}{l} \text{Time rate of} \\ \text{increase of } \phi \\ \text{inside the CV} \end{array} \right\} = \frac{\partial}{\partial t}\int_{\Omega} \rho \phi \, d\Omega$$

$$\left\{ \begin{array}{l} \text{Convection of } \phi \\ \text{through CS} \end{array} \right\} = \int_{S} \rho \phi \, \vec{V} \cdot d\vec{A}$$

Rate of generation ϕ inside CV

$$= \int_{\Omega} \dot{q}_{\phi} \, d\Omega$$

$\dot{q}_{\phi}$: source term (volumetric generation rate)

Diffusion ϕ through control surface

$$= \int_{S'} \underset{\sim}{q} \cdot d\vec{A}$$

So on the left hand side we had the term that is rate of increase of phi sorry, scalar transport time rate of increase of phi inside the CV, now this a simply the temporal derivative of rho small phi here we have assumed this phi is an intrinsic quantity, so it is essentially this phi represents our physical quantity per unit mass d omega. And convection of phi through control surfaces this would be given by a surface integral across our control surface rho phi v dot dA.

Next, let us talk about the terms which contributes to it are the interactions from sources and the transport of phi across the boundary. The first one is rate of generation of phi inside CV, this can be expressed as the volume integral of q subscript phi dot d omega, now here similar to what we saw in the case of energy equation, this q dot phi this represents the source term we can call it as a volumetric generation rate.

And the last term which we had that is diffusion of phi through control surface, now this we can represent by a surface integral of a flux like quantity, let us say that q is the flux of phi which is being transported across the control surface q dot dA integrate over our surface, that will give us the efflux or net rate of efflux of q across the control volume surfaces. So now you can substitute these 4 integrals which we obtained in our verbal equations which we derived earlier, and that leads to the integral form of the scalar transport equation.

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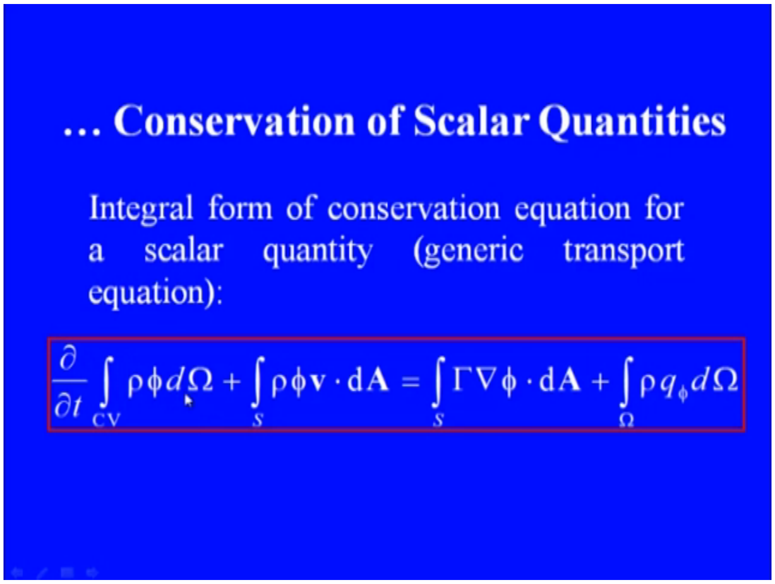

So this is the form conservation equation for a generic scalar quantity, so we can also call it generic transport equation del/del t of rho phi d omega +phi times rho v dot dA=surface integral of gamma times gradient of phi dot dA, now this gamma times gradient of phi we have put here assuming that this is the this q can be represented in terms of a diffusion coefficient gamma and gradient of scalar quantity phi, so gamma gradient of phi dot dA+rho times q phi d omega.

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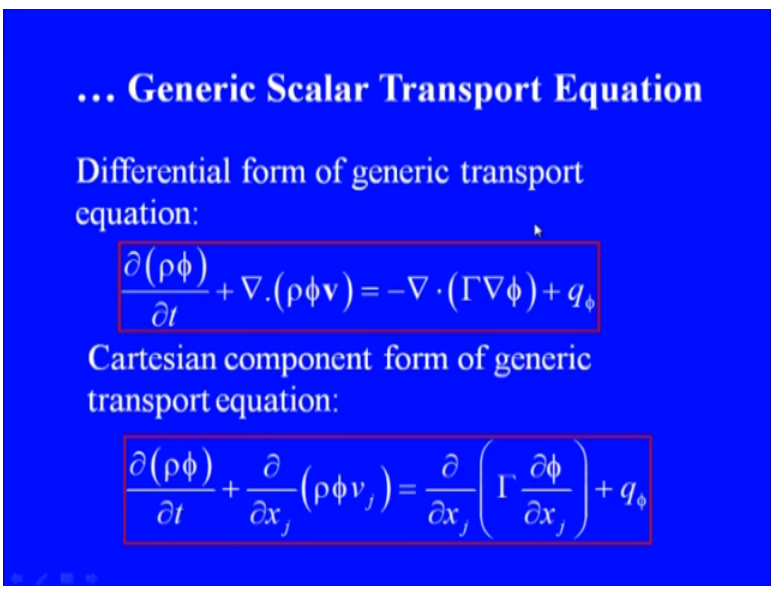

Now let us obtain the differential form of generic transport equation, now this we can again doing by following the same method which we had adopted earlier for derivation of the differential forms starting from the integral forms.

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Differential form of generic transport equation

$$\frac{\partial}{\partial t}\int_{\Omega} \rho\phi \, d\Omega \equiv \int_{\Omega} \frac{\partial(\rho\phi)}{\partial t}\, d\Omega$$

Gauss divergence theorem

$$\int_{S} \rho\phi\vec{v}\cdot\vec{dA} \equiv \int_{\Omega} \nabla\cdot(\rho\phi\vec{v})\, d\Omega$$

$$\int_{S} \vec{q}\cdot\vec{dA} \equiv \int_{\Omega} \nabla\cdot\vec{q}\, d\Omega$$

$$\boxed{\int_{\Omega}\left[\frac{\partial(\rho\phi)}{\partial t} + \nabla\cdot(\rho\phi\vec{v}) - \nabla\cdot\vec{q} - \dot{q}_{\phi}\right] d\Omega = 0}$$

It holds if and only if the integrand vanishes everywhere in Ω.

$$\Rightarrow \frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\phi\vec{v}) - \nabla\cdot\vec{q} - \dot{q}_{\phi} = 0$$

$$\Rightarrow \boxed{\frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\phi\vec{v}) = \nabla\cdot\vec{q} + \dot{q}_{\phi}}$$

$\Uparrow$ Differential form of generic transport eqn.

So differential form of generic transport equation, so let us first write down our integral form we had first one was time derivative del/del t of rho phi d omega, now for a fixed control mass or fixed mass we can represent it as an integral of the time derivative that is del rho phi/del t d omega, the second term which we had on the left hand side of our integral form that was surface integral that was rho phi v dot dA which represents the convection of phi across the control surface.

Now this can be changed using Gauss divergence theorem into a volume integral, so this is divergence of rho phi v d omega. Similarly, we had a surface integral on the right hand side which was because of the flux term, so S q dot dA this can be transformed into a volume integral divergence of q d omega. So let us now combine all these terms together and transfer everything on the left hand side.

So we have big volume integral [del rho phi/del t+ divergence of rho phi v - divergence of q-q phi dot] d omega= 0, so once again we get an integral which is 0 and this integral will be 0 irrespective of our chosen control volume omega okay. So this usual argument again applies it holds if and only if the integrand vanishes everywhere in omega, that is our time derivative of rho phi + divergence of rho phi*v - divergence of q-q dot phi= 0.

So now let us keep an unknown term on the left hand side transfer rest on the right hand side a slight re-arrangement, so del/del t rho phi+ divergence of rho phi v= divergence of q+q dot phi, so this is our differential form this is differential form of generic transport equation, it is not too difficult to realize that look this equation can represent any of the equations which you have derived earlier, for instance if you replace phi by 1 what do we get?

So let us do for a shake of exercise that this generic form which we have derived that is it or it can be made to represent few transport equations which we have derived earlier.

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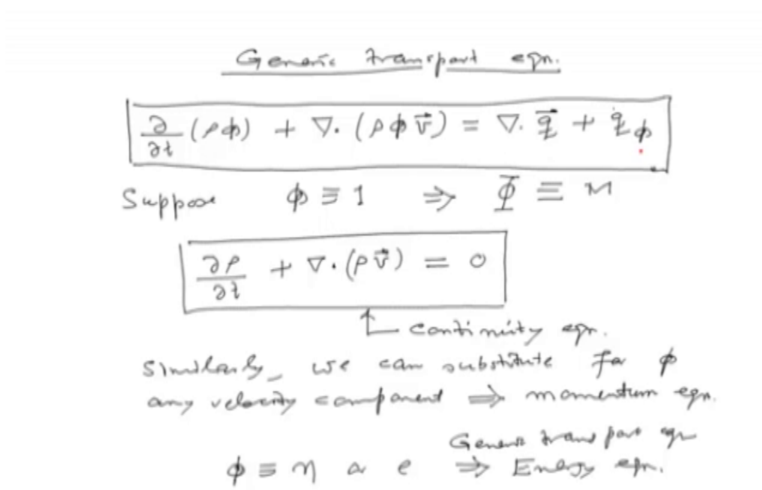

Generic transport equation let us rewrite it again, so del/del t rho phi + divergence of rho phi v = divergence of q+q dot phi, we can call it a generic transport equation only if it can be used for a different conserved quantities, so suppose we take phi= 1 what does that mean? That is the transported quantity capital PHI that must be mass, so if you substitute phi= 1 in the previous equation what do we get? We get del rho/del t+ divergence of rho v.

And in this case if you are dealing with a mass of system there is no diffusion of mass through the control surface not any mass source inside, so the right hand side must be 0, so what do we have got? This is precisely the continuity equation which have derived earlier. Similarly, we can substitute for small phi any velocity component and this will lead us to an appropriate form a momentum equation of course we will have we have to interpret flux in that case our q would be given in terms of a stress components or divergence of stress.

And that is q phi that would be given in terms of body forces, so and if I we take phi= small e, eta or small e, now our generic transport equation would lead us to energy equation, so that is what we say that so called this generalized transport equation which we have derived that can be made to represent the transport of any conserved quantity. So in the reminder of the course in fact the first half of the course of CFD we would primarily focus on our attention on finding out or deriving the numerical schemes which can solve this generic transport equation.

And only thereafter, we would apply those techniques or we will extend those techniques for a solution of full Navier-Stokes equations. Now before we can proceed with the numerical solutions we have to grab with few issues that what should our choice of the governing equations be that is one thing that will depend on the physical phenomena.

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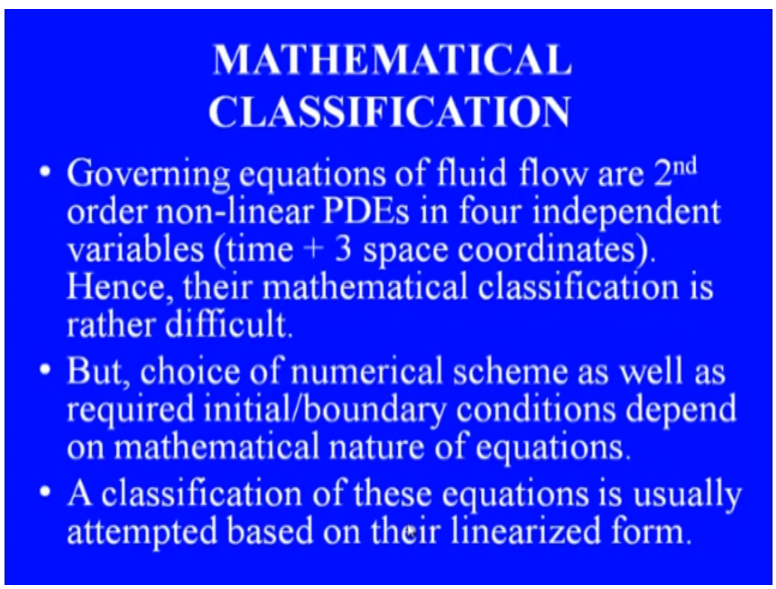

And based on the physical phenomena physical situations we can derive the way we have learned our governing equations, that is the basic conservation laws which will give us the questions for continuity Momentum and energy, but you should know what is the nature of these equations because that will dictate the choices of the numerical schemes which we can use. So if you look at any of the equations of governing equations of fluid flow the second order nonlinear partial differential equations in 4 independent variables.

A time dependent problems time is 1 and 3 space coordinates, so mathematical classification of this nonlinear PDEs is a rather difficult task, but we have to get some picture at least some qualitative picture because choice of numerical scheme as well as the number of initial and boundary conditions which will be required that depends on the mathematical nature of our governing equations.

So if you have got no options but to explore or at least get some estimate before we can proceed with the choice of numerical schemes, so what we normally do is that we try we attempt to do a classification of our governing equation that as Navier-Stokes equation and energy equations usually based on their linearized form. So our first task would be to have a look at the classification of this linear or quasi-linear of second order partial differential equations.

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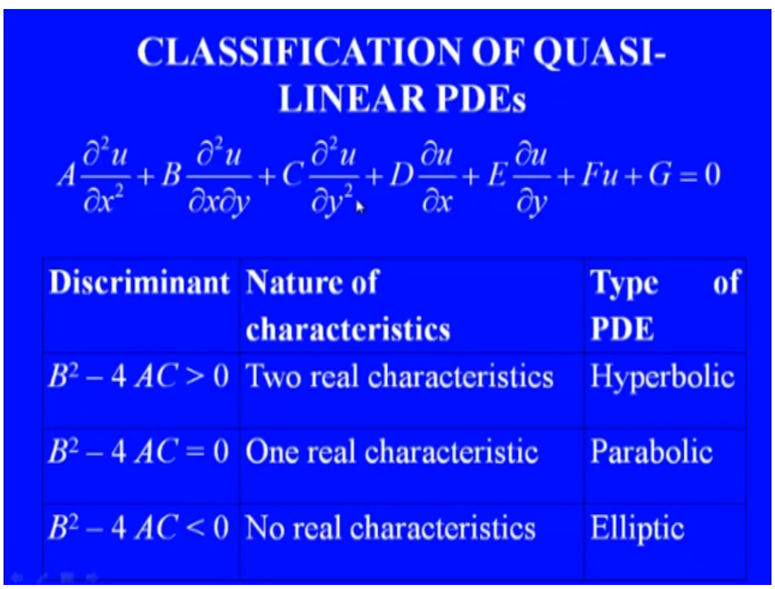

So now let us have a look at a generic or generalized quasi-linear partial differential equations which we can represent this forms suppose for time being we will dealing with an unknown function unknown variable u which is dependent on 2 variables x and y. So first this situation we can write our generic second order PDE as A times del 2 u/del x square+B times del 2 u/del x del y+C times del 2 u/del y square+D times del 2 u/del x+E times del 2 u/del y+F times u+G=0.

Now here A, B, C, D, E, F and G these would in general be functions of x and y, what would be the nature of this particular equation? We can derive the so-called equation for characteristics for this case and those characteristics are basically given by so-called discriminant B square-4 AC okay. Now this particular term B square-4 AC in fact it comes if we compare this equation will be the second order algebraic equation.

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Second order algebraic eqn

$$\boxed{Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0}$$

↳ represents a conic section

Discriminant $B^2 - 4AC$

$$\text{If } B^2 - 4AC > 0 \Rightarrow \text{hyperbola}$$
$$B^2 - 4AC = 0 \Rightarrow \text{parabola}$$
$$B^2 - 4AC < 0 \Rightarrow \text{ellipse}$$

So let us have a detailed and let us have a look at what second order algebraic equation in 2 variables, so we can write as A x square+B times xy+C times y square+D x+E y+F=0, if you recall from geometry this second order equation represents an equation of a conic section. So it represents a conic section, by conic section we mean it could be circle it could be a parabola or ellipse or a hyperbola, so what are the conditions for each type of conic section?

So what would we see that, that would depend on the discriminant B square-4 AC. So we say that if B square-4 AC>0 this equation represents a hyperbola, hyperbola essentially a curved in fact it contains 2 different curves combination of two curves. B square-4 AC=0, so in this case we have got a single characteristics and we called this curve as parabola. And B square-4 AC<0, we do not get any characteristics and we call this equation as or rather this equation represents geometric shape called ellipse a circular forces specialized case of an eclipse.

So our classification for PDEs is basically are the nomenclature which we use that follows what nomenclature used in geometry for classification of hyperbola, parabola and ellipse. Let us have a look at B square-4 AC now if it is >0 we have got 2 real characteristics, the characteristics of the ones basically the space curves along which an information would propagate, B square-4 AC>0 that says that will have 2 real characteristics.

And in this case of equation or PDE would have what we call hyperbolic nature, because that is what we have got in the case of hyperbola we have got 2 different or 2 distinct branches of an hyperbola, so that is the same analogy which has been used in this classification. B square-4 AC=0, so we have got one real characteristics that is we have got only a single branch in the case of parabola and the same terminology been used here B square-4 AC=0 this equation would be called parabolic.

And a B square-4 AC<0, we have got no real characteristics and in that case we will term of a quasi-linear PDE as elliptic. Now let us have a look at one example of each of these types of equations and what do these mean?

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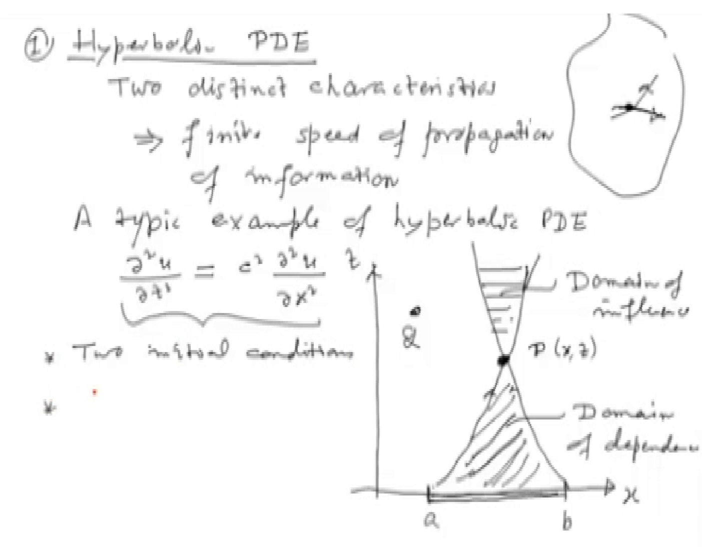

So let us have a look at hyperbolic equation, now this in the case of hyperbolic PDE we have got 2 distinct characteristics okay and the information that is to say we have got problem domain, we introduce at some point some disturbances, that disturbances propagates along these characteristic lines they have characteristic lines along which the information propagates and information propagates at a finite speed.

So we have got finite speed of propagation of information regarding where the particular disturbances would introduced and what is its effect on the field, so a typical example of this equation would be a wave equation, a typical example of a hyperbolic PDEs that is del 2 u/del t square=c square del 2 u/del x square, let us see what is this geometrically means? We have got 2 independent variables here x and t.

And suppose we say that extent of our physical domain in x is along A and B, so our information would propagate or if you look at any particular point P we want to see what would happen at a given instant of time, the things that P would be influenced by the information contained when this region the characteristics which are propagating through P originating from either side, so what would we say in this particular slant has domain which would be called is domain of dependence.

So solution at point P that depends only on this slant hatched portion and whatever happens at point P that affects only this narrow region contained between these characteristics let us put these as horizontally hatched region, so this region we would call as domain of influence or simply means if we introduced a disturbances at point P that will affect the solution only on this small region of this space and time this at any point let us say if you got a point Q located here anything happening at P will not affect what happens at Q.

So it is a basic nature of the hyperbolic PDEs that domain of dependence and domain of influences both fairly confined and well-defined regions in space, and in this case we will typically need a second order PDE in times we will need 2 initial conditions and 2 boundary conditions given at points a and b.

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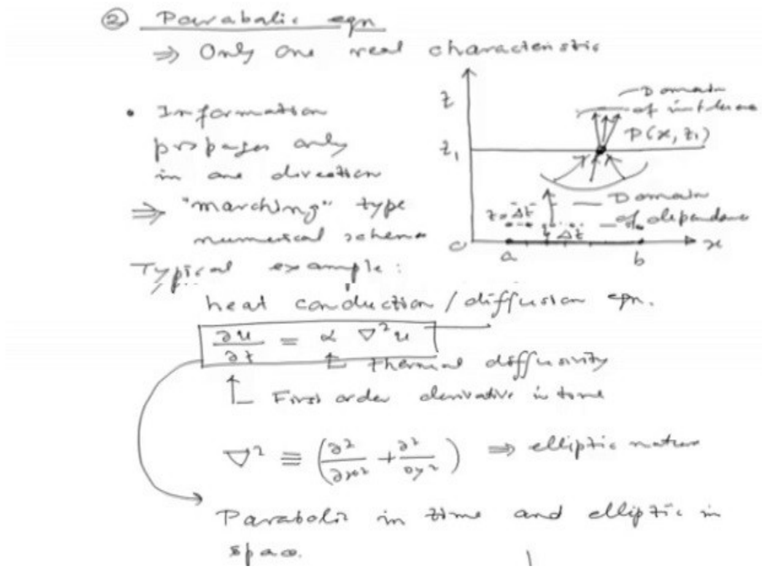

Next, let us have a look at the next type that is parabolic equation, now in this case of parabolic equations we have got only one real characteristic, and let us say it will propagate along only one directions for instance if you have a time dependent problem, suppose one dimension in space and one dimension in time. So now in this case whatever has happened in our domain or physical problem domain at time prior to a time t1 that will affect our solution at point Px, t1.

So whatever happens before P in terms of time that will affect the solution of P similarly, the happenings at point P they will affect only the solution behaviour only at future times not at the prior times, so now in this case this becomes what we call our domain of dependence and on the later times are what we can say is domain of influence. So beautiful thing about this parabolic PDE is that at information propagation, the information propagates only in one direction.

And this simplifies your task a quiet a bit that we can do what we can say marching or we can apply marching type numerical schemes, that is if we have got the time= 0 we know what solutions of different points are using this solutions we obtain or we can obtain the solution of times slightly afterwards let us say time t= delta t, now we can use this solutions at these values and obtain the solution at t=2 delta t and so on, and thereof thereby we can just keep marching along the time direction.

So this solution procedure is fairly simple in the case of parabolic. And the typical example of such equations as our heat conduction equation or we can also call it heat diffusion equation, so we can write it as del u/del t=alpha times del square u this alpha represents of a thermal diffusivity. Let us have a look at carefully here now this first order derivative which involved in time derivative in time.

And the right hand side what we have got if you will look at the expanded form of our del square operator this is del 2/del x square+ del 2/del y square, and this operator we would see it is got so called elliptic nature, so in fact some people called this heat diffusion equation as parabolic in time and elliptic in space.

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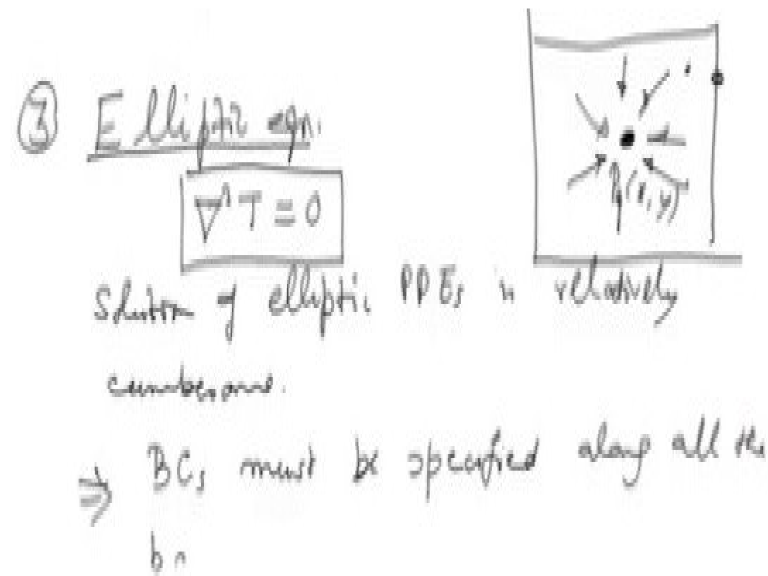

Now the last type which we discussed is elliptic equations, a typical example which is our steady state equation del square T=0, now in such cases suppose you have got a problem domain if you look at a specific point P x, y the solution at this point depends on whatever happens anywhere in the domain, so if you introduce a small disturbances at any point at the boundary or inside the domain anywhere that influence the solution at our specified point P x, y.

Similarly, if you introduce the disturbance at P its effect is failed everywhere in fact we would theoretically call here that this speed of propagation of disturbances that speed is infinite, now that introduces some complications since the solution at or disturbances at one point affects the solution everywhere, the solution of elliptic PDE is relatively compression, and in this case we must specify BCs must be specified along all the boundaries okay.

Now this is general description about nature of the PDEs or what we call quasi-linear PDE, we had looking at some of the examples. Now can we extend this classification to our flow problems, so we would be primarily solving Navier-stokes equations and energy equations, so what is the nature of Navier-Stokes equations or energy equation?

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Classification of N-S and Energy Eqn

(1) Incompressible flow

- Unsteady $\Rightarrow$ parabolic in time and elliptic in space

$\Rightarrow$ We require one set of initial condition at $t=0$ and boundary condition specified everywhere on CV boundary for $t > 0$.

- Steady case $\Rightarrow$ elliptic

$\Rightarrow$ BC on the domain boundary.

(2) Compressible Flows

Nature of equations $\Rightarrow$ mixed

$\Downarrow$

Depends on local Mach no. (Ma)

(i) If Ma < 1 everywhere (subsonic)

$\Rightarrow$ nature is similar that of eqn. for incompressible

(ii) If Ma > 1 everywhere

$\Rightarrow$ Hyperbolic nature

otherwise $\Rightarrow$ mixed nature

So classification of Navier-Stokes and energy equation, there are broadly 2 cases which we would like to deal with, let us first take the case of incompressible flows where the situation is rather simple. So incompressible flows if the problem is time dependent on a steady case so the nature of equation is what we called parabolic in time because we have got a first order derivative in time and elliptic in space.

Or this elliptic in space this nature comes because of the presence of second derivative with respect to x on the right hand side of both Navier-Stokes and energy equations, and the consequence is that we require 1 set of initial conditions at t=0 and boundary conditions specified everywhere on CV boundary for t>0. For steady case the nature of both of these equations Navier-stokes as well as energy equation that is elliptic.

So we only require here BCs on the domain boundaries. Next, let us moves to compressible flows, now in the case of compressible flows the life is bit difficult, the nature of equations is what we will call mixed and in fact it would depend on of non-dimensional number called Mach number, so depends on local Mach number and because local Mach number we can make certain observations.

That is first if Mach number Ma if Ma<1 everywhere, so typical of what we called subsonic flow okay, now in this case nature is similar to that of equations for incompressible flow okay. Now if Mach number>1 everywhere that means our flow equations both Momentum as well as energy equations they would have what we called hyperbolic nature. Otherwise, we will have mixed nature.

Similar type of classification we can extend in the case of Euler's equation and for details we will have a look at few references to which you can have a look at that how do we classify energy, so Euler equation and Full-potential equations. And next, we will have a brief look at boundary conditions before we close this module.

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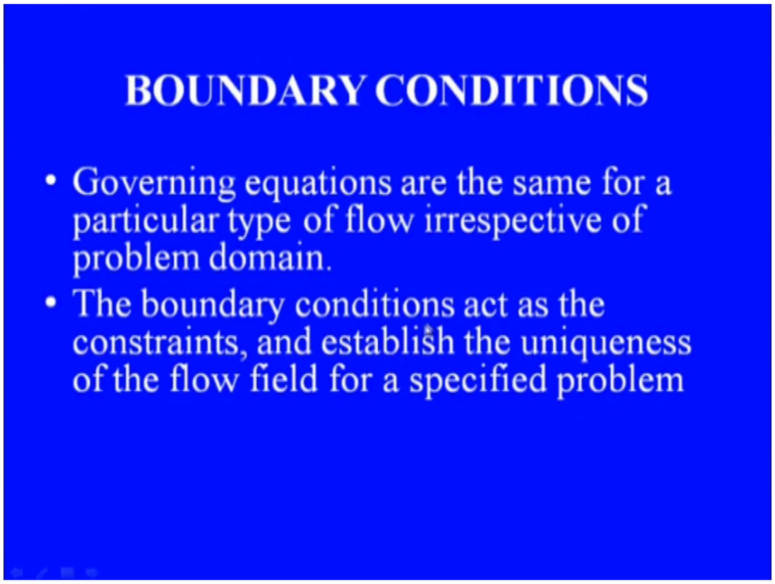

So let us see governing equations which we had continuity, momentum or energy equation, they would be the same irrespective of the problem domain. Then what makes each problem unique that uniqueness is imposed by what we called boundary conditions which act as the constraints and establish the uniqueness of the flow field for a specified problem. Now in normal flow simulations we will encounter 2 types of boundary conditions.

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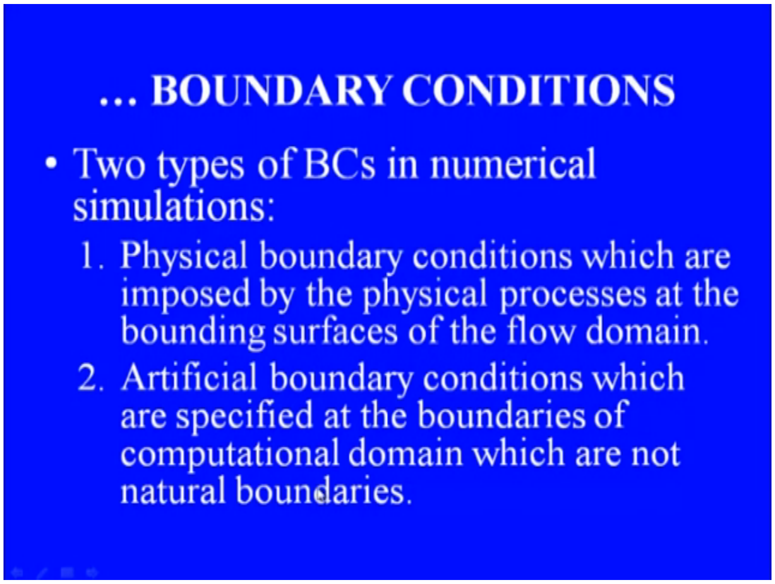

The first situation we would be looked we have got some physical boundary conditions, if you got the physical boundaries which are actually present there, and we can say the constraints which are imposed by this physical processes happening at the bounding surfaces, so we will call these things as physical boundary conditions. The second case would be artificial boundary conditions which are specified at the boundaries of computational domain which are not natural boundaries.

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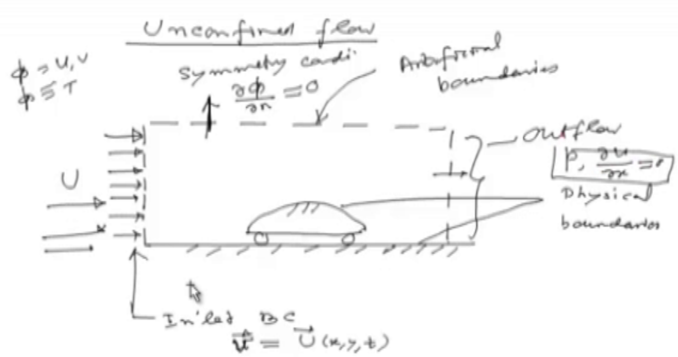

To understand the second aspect let us have a look at an unconfined flow around a black body, so unconfined flow or it could be a car we want to simulate the flow around the car, now in this case how do we specify our problem domain, the car is moving in an unconfined here, so we cannot take this unconfined domain in numerical solutions, so we have to somewhere break or put what we called artificial boundaries.

And by putting these artificial boundaries we introduce what we called artificial surfaces, and we have to specify what type what would be the reasonable boundary conditions at these artificial boundaries, so these are artificial boundaries, and of course in this case we can also have a set of physical boundaries that is car surface and our route surfaces, so these are our physical boundaries.

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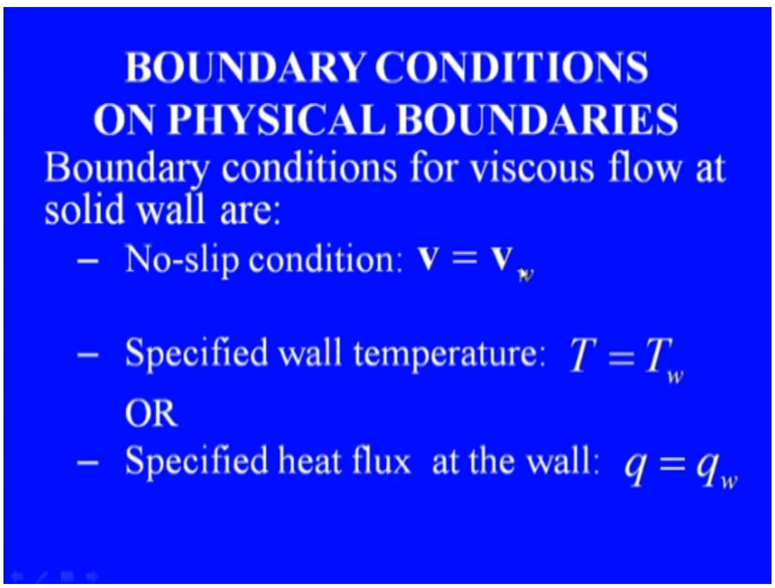

Now for a typical boundary which conditions we confined for viscous fluids at physical boundaries that is say if you are dealing with a flow surface or solid surface, so since the flow is viscous the velocity of the flow would be same as that of the solid wall, so we have got the impose what we call no-slip country conditions which is given by V=Vw where Vw tell us the velocity of this solid surface, in majority of applications Vw would simply be 0.

For energy equation you have to specified the wall temperature that depends on the physical process which are happening maybe in some cases the solid surface has got a constant wall temperature, so in that case we will put T = Tw or you would have a specified heat flux that is q=qw, so this would be typical conditions for viscous flows. If you are dealing with inviscid flows then by inviscid means there is no viscosity present.

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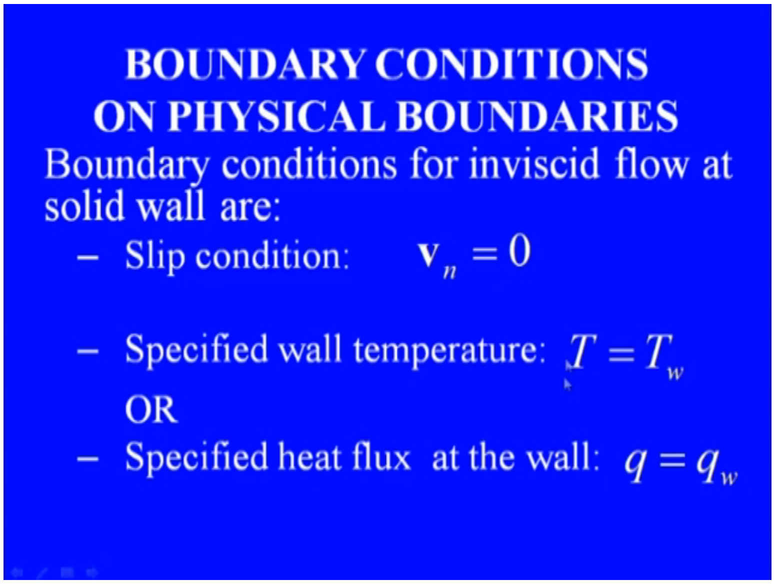

So there could be a slip between the solid surface and the fluid but one thing is very sure that the fluid cannot penetrate the solid surface, so we will impose what we call as slip condition Vn, n is stands for the normal velocity, velocity component normal to the surface so Vn=0, rest these 2 conditions one of these 2 conditions have to be specified for energy equations that is specified wall temperature or specified heat flux.

The only difference in the case of inviscid flow would be that in the case of velocity that is we have to impose what we call slip condition by setting the normal component of velocity has 0.

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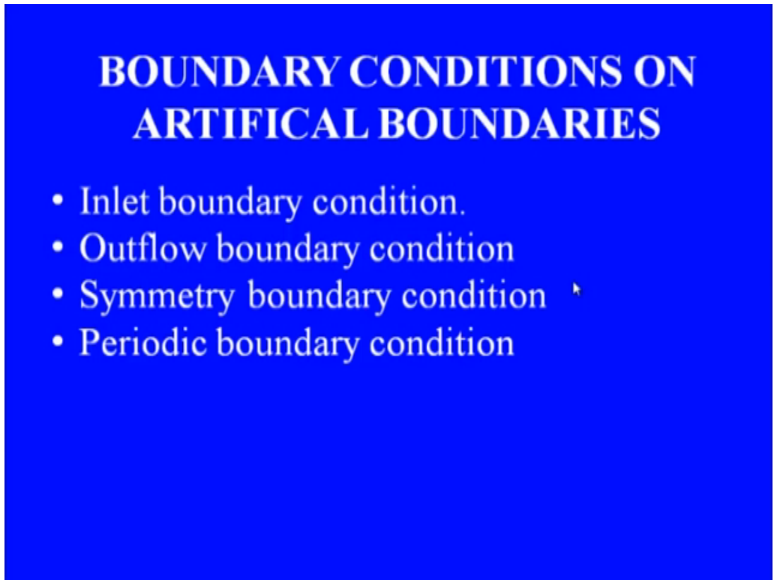

What other boundary conditions we encountered? We have what we called inlet boundary, now that inlet boundary conditions could be at both physical as well as artificial boundary conditions. We have got outflow boundary conditions, symmetry boundary conditions, and periodic boundary conditions and so on. The variety of these types now solving these we can have a brief look here.

For instances let us get back to our example of simulation of flow around the car at upstream end we have got to specify the velocity everywhere, so this would become what we call as our inlet boundary or inlet boundary condition, so you have to specified as a function of or the velocity has to be specified as a function of spatial coordinates and time. What happens at this stop artificial surface we would say that the flow or temperature does not vary across the surface.

So we can impose what we call a symmetry conditions here at the top that is for any flow variable del phi/del n= 0, there is no variation of a given quantity of phi could be any velocity component or it could be temperature it does not vary along the normal direction. Similarly, on the downward side we can specify what we call outflow boundary conditions, so you have to specify pressure and we can say that look this no variation in the velocity components along the outflow directions so that completes our outflow boundary conditions.

So further details about these boundary conditions and mathematical classification you encourage to read these few very nice books is Computational Fluid Dynamics by Anderson, and Computational Methods for Fluid Dynamics by Ferziger and The Introduction to Computational Fluid Dynamics by Versteeg and Malalasekera each of these 3 books they gives some description about the derivation of governing equations.

They contained a very nice detail about classification procedure and they also have they are generally useful as a text book for numerical schemes you are going to learn later on. So that is we are going to now put a full stop to this module, and in the next module will start off with Finite Difference Methods.