Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 15
Numerical Solution of PDE-Finite volume method

In this lecture, we are going to talk about the finite volume method of analysis and solving the partial differential equation systems.

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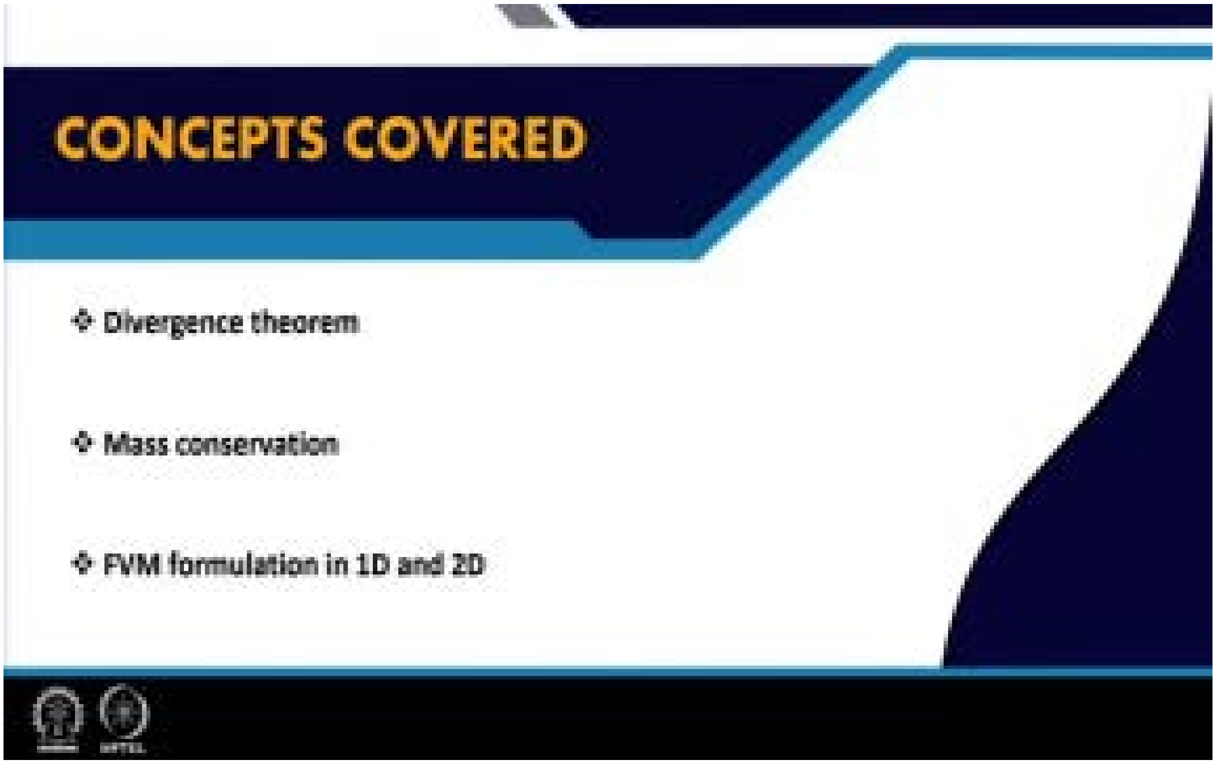

Now, what is the finite volume technique? The finite volume is essentially based on the divergence principle as well as the mass conservation.

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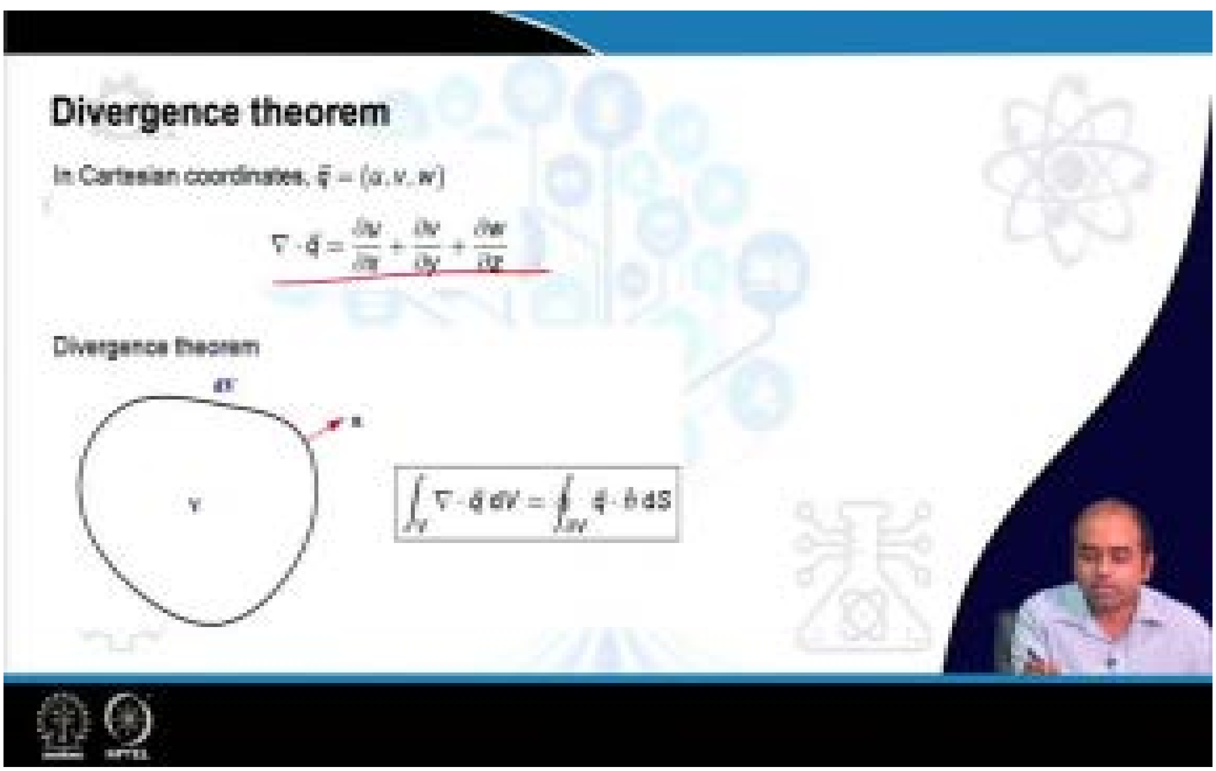

So, what is the divergence theorem? So, the divergence theorem tells us that the surface integral of a vector field over a closed surface which is clogged the flux through the surface is equal to the volume integral of the divergence over the region inside the surface, it is equivalent to the volume integral of the divergence over the region inside the surface and this is what is represented in front of you in the mathematical form.

Let us say this q is a flux variable and on the left hand side you see the volume integral of the divergence of this flux and the right hand side it is the surface integral of this vector field that is q over this that is closing this volume or the boundary of this volume and and this is on the top you see for the Cartesian coordinate this is how we write the divergence (of) for vector field and essentially, this divergence represent if you try to get a physical picture, this divergence represents the volume density of the outward flux of a vector field from an infinitesimally small volume around a given point.

So, this is the background this is almost the heart of the finite volume technique and this is an integral approach based on this divergence theory.
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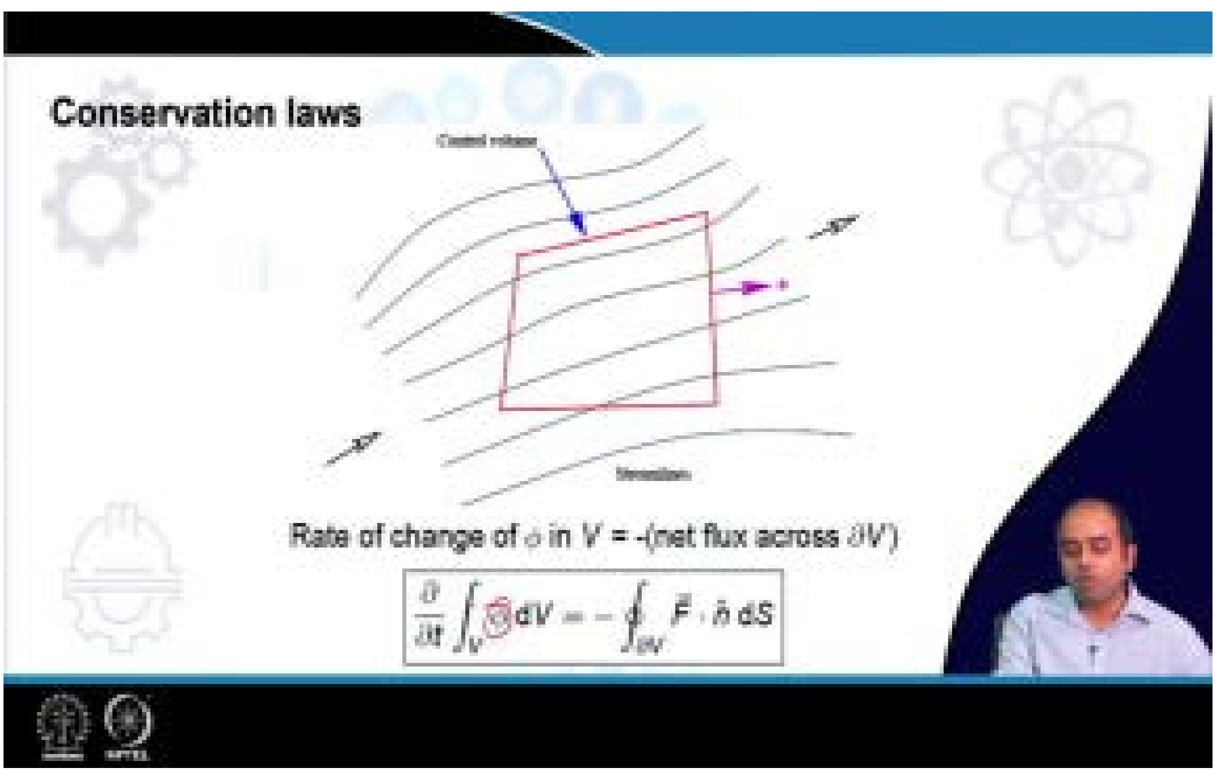

Now, what is the conservation law and the mass conservation tells us that the rate of change of the variable phi (it could be a scalar variable) let us say in this volume V is equal to is equal to the negative of the net flux across this control volume of del V. So, this is what the mass conservation tells us the rate of change of the scalar quantity phi in this control volume V is equal and opposite to the net flux through the boundary of this control volume.

And this is what has been mathematically represented here, you see that the temporal derivative of this variable phi over this region of the control volume is equal to the negative of the and it is the sum of these two is equal to 0 it has to conserve always then the total flux coming out from the surface of (the) this control volume in the normal direction or outward normal flux is equal and opposite.

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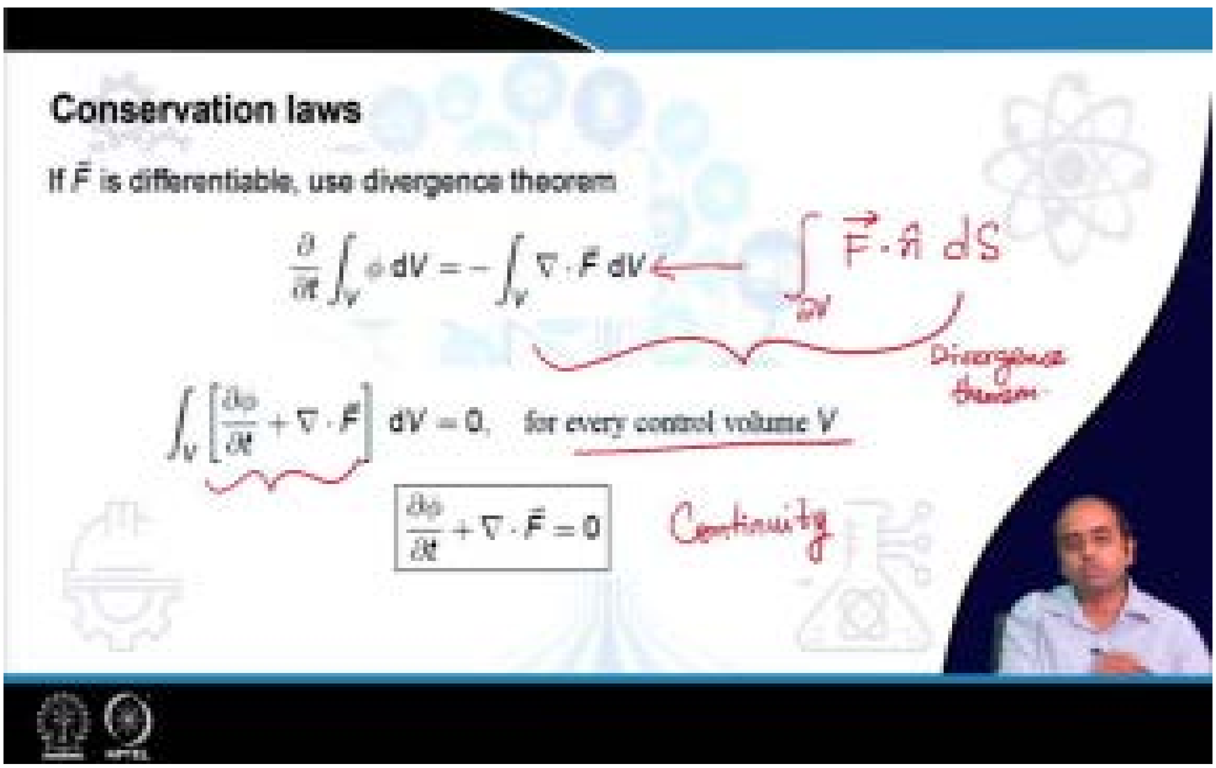

Now, if you apply this divergence theorem and it is possible only when F is differentiable or the flux is differentiable this quantity this this is equal to the from the mass conservation whatever we got. So, this equivalence of the flux is from the divergence theorem that is why we use it. And what is the immediate consequence I bring in on the both side and I can easily say that this quantity is equal to 0 then only then this integration will be equal to 0 this has to be satisfied for every control volume V.

So, this continuity equation that we are used to or familiar with or the mass conservation equation for any fluid element is based on the divergence theorem and the integral formulation tells us that this quantity on the left hand side over this integral volume or this over this control volume has to be equal to 0.

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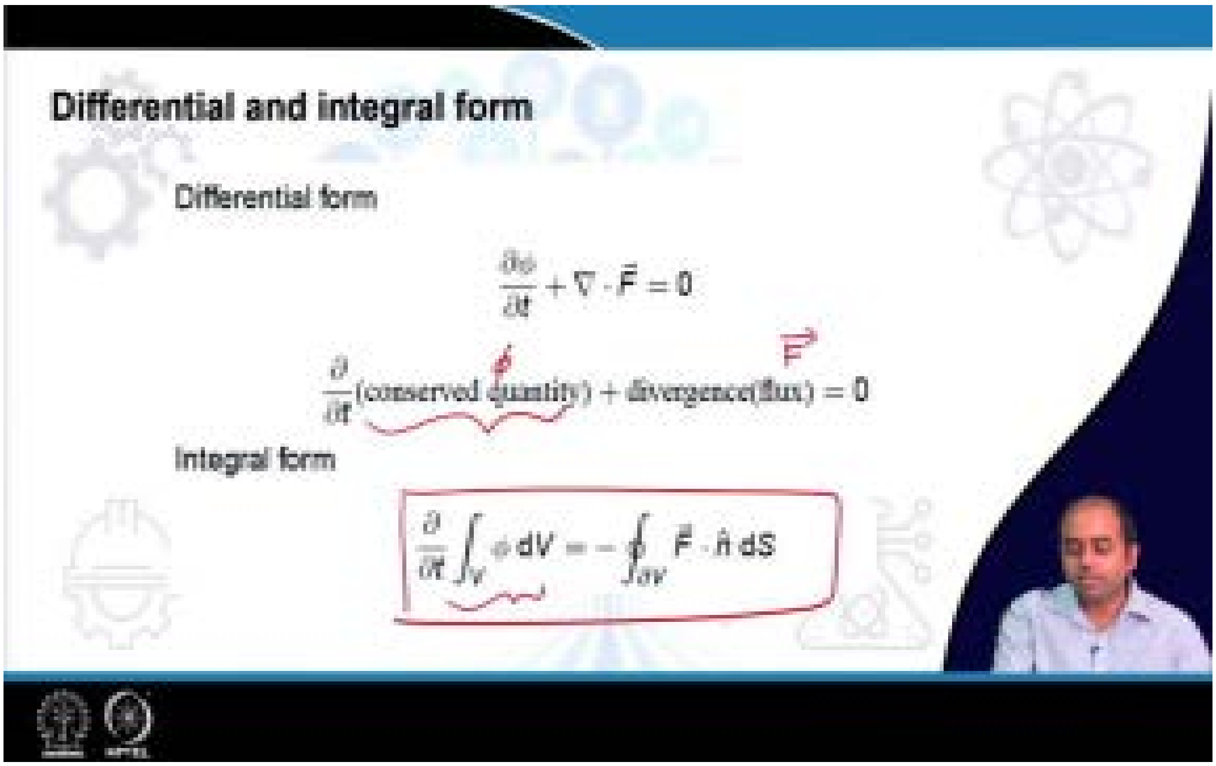

So, the differential and the integral form looks something like this the differential form is the temporal derivative of the conserved quantity, which is this phi and the divergence of the flux is equal to 0 this is the differential formula and formulation or the framework and what is the integral form and integral form is something which we just discussed.

So, this is the computation of (the the) this temporal derivative of (the) this conserved quantity phi over the integral volume is equal to the outward normal flux over the boundary surface of this control volume. So, this is the integral form and it is this integral form which is actually used actually used in the finite volume formulation technique and this is the basis of that whether you go for 1D, 2D or 3D.

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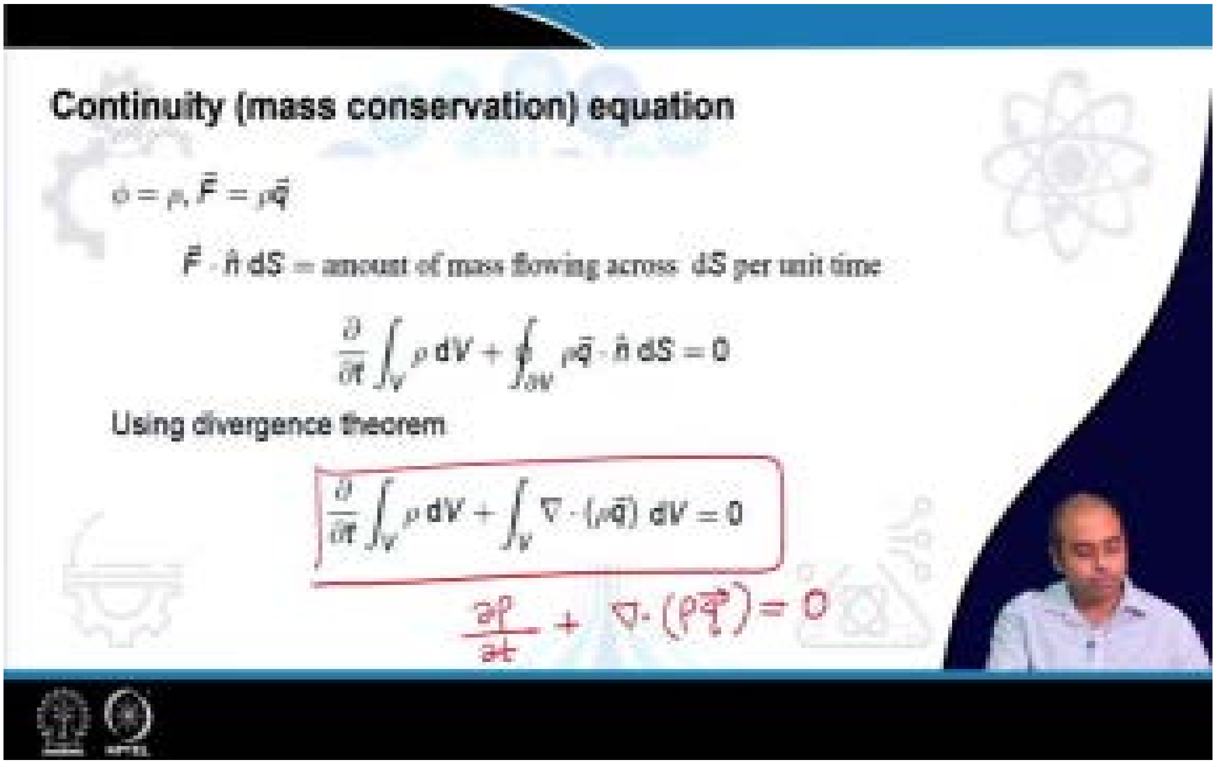

So, based on this idea, if you consider the scalar variable to be let us say to be density and this F you consider it to be rho into q and you can think of this q to be your let us say velocity field that then this u dot or this flux dot n normal vector with dS represent amount of mass flowing across this elemental surface or the or this through this boundary of this volume segment.

And from this divergence theorem, you get this and the immediate consequence of this is del rho del t plus grad of del rho q is equal to 0.

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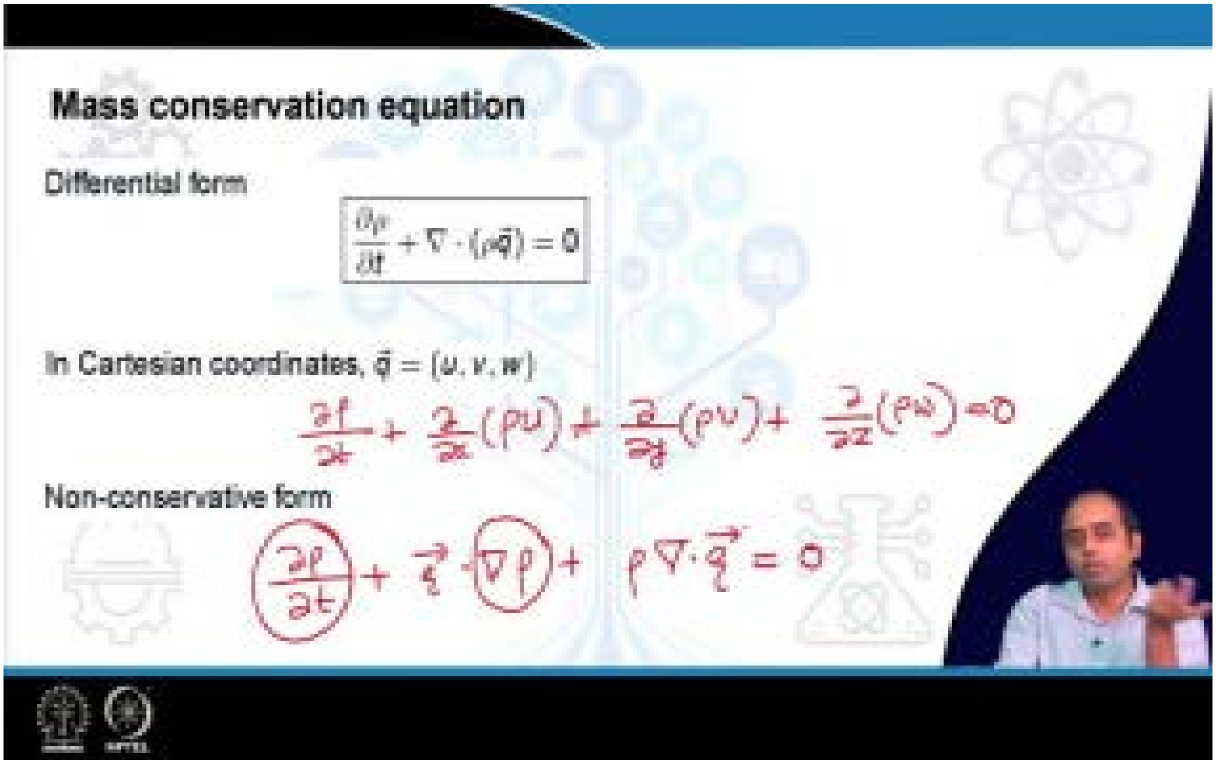

This is the immediate consequence or the resultant of this. So, this is what we write down as the differential form and if we try to expand this in terms of the Cartesian coordinate, so, this will look something like this del del of x of and please note that this is the conservative form of the continuity equation and the non conservative form is and the non conservative form is of course, if you take this row and q outside of this domain, so, it would look something like of course, if the fluid is compressible then this there is the existence of this term this is not 0 and this is 0 in the case of in the case of incompressible fluid in the incompressible fluid density does not change.

So, both these and these two quantities will be close to 0 and it is essentially the divergence of the flux is equal to 0 that is what the incompressible limit tells us. So, always it is this conservative form is a generalized version and that takes into account of the mass continuity.

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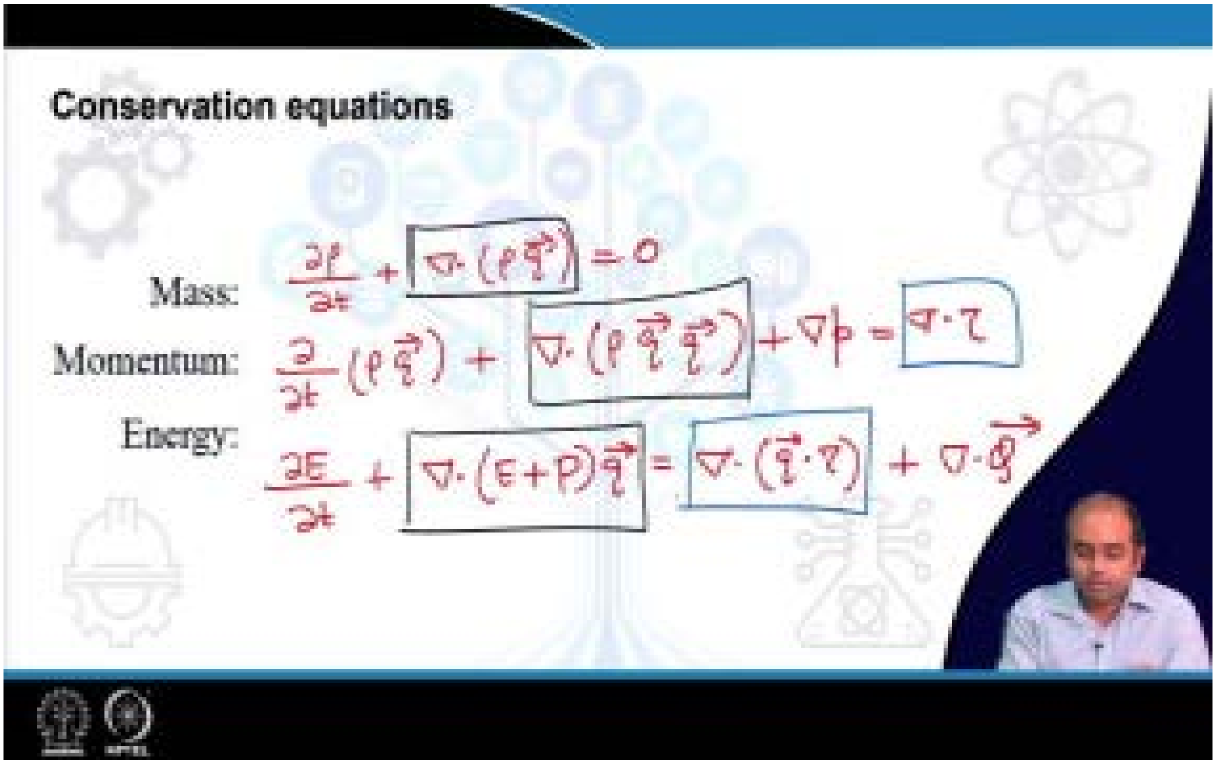

So, using this idea, you can also explore and write down the different conservation equations. So, this is for the case of the mass of the fluid element which is what we represent like this the continuity equation then the momentum equations which is nothing but the Navier Stokes equation in this case can also be written down in the same way.

Similarly, energy equation so, E is the energy variable it could be temperature in this case delta and q is the additional energy source from something like this. Now, please note that in all these equation this part this is the convective part, this is the convective part and this is the diffusive part.

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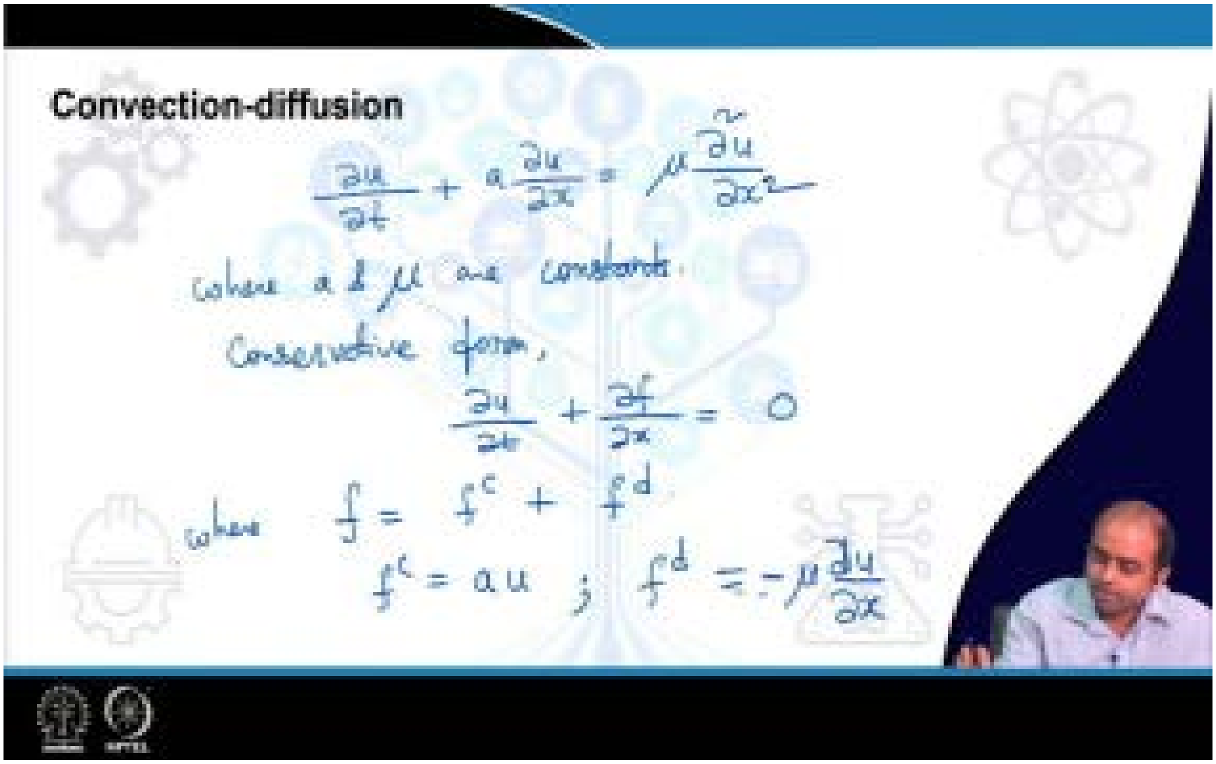

So, if we try to write down a simple convection diffusion equation, let us say based on this fluid velocity or let us say I am trying to write down for a 1 dimensional case so, let us say where a and this mu are constants then the conservative form looks something like this where the flux F has two components - convective component and diffusive component.

So, the convective component is this one and the diffusive component is this one. So, individually and if you try to think of the only the pure convection or only the pure diffusion, you can write down their individual counter parts and from there you can get the scalar convective equation and the diffusive equations generally the scalar convective equation is.

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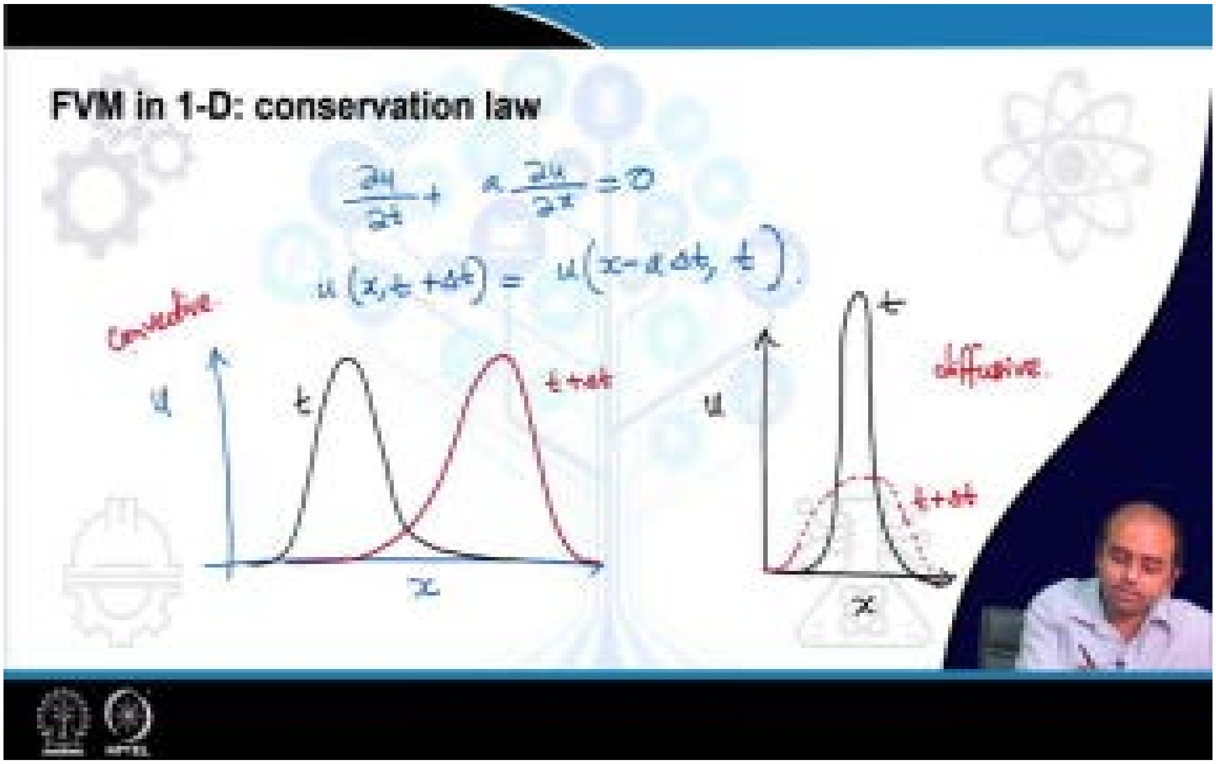

So, if you have only convection to the problem just to give you more on this though if you have only conviction to the problem, where of course, a is constant the solution to this equation can be done or can be obtained by a simple substitution of this. So, if you just substitute your space variable into x minus a t, then you will see that these variables get combined and you can get a solution which does not change its shape.

So, what I mean over time, but it gets only translated so, if I try to do something like u versus x, so, let us say a time at a particular time it is like this then at a later time. So, this is t plus delta t and this is t. So, this is what we generally get from the convection. And similarly for the diffusion the diffusion equation would look sorry I should draw it in a better way. So, let us say at this is a t but at a different t plus delta t it would be expanding like this.

So, this is the diffusive characteristics of the parabolic equation and this is the convective terms and the convective characteristics of this 1 dimensional scalar transport equation. I need to tell you about the 1 dimensional formulation here before we move to the grids.

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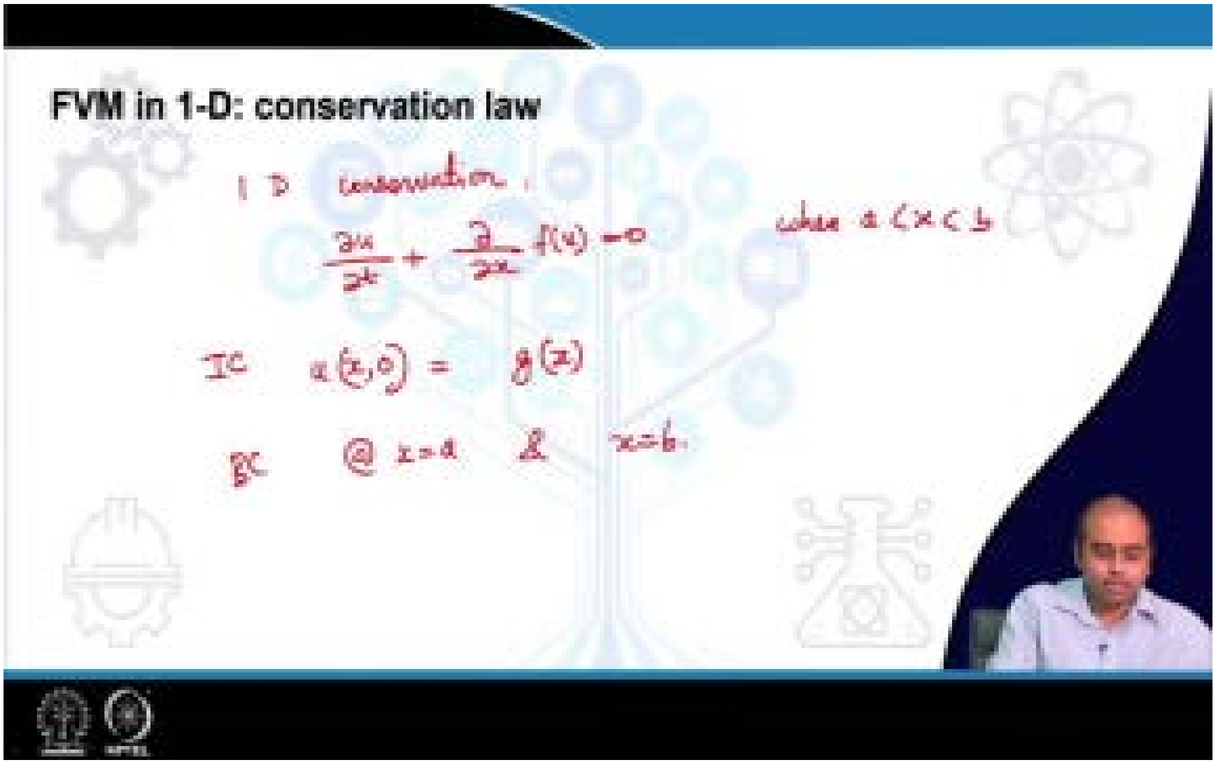

So, so for a 1 dimension mass conservation of scalar transport conservation we can get something like this where it has said the x is bounded within the range of a to b and you have the initial condition of u, x comma 0 thus this is a function g x. So, the boundary condition is also known as x is equal to a and x is equal to b.

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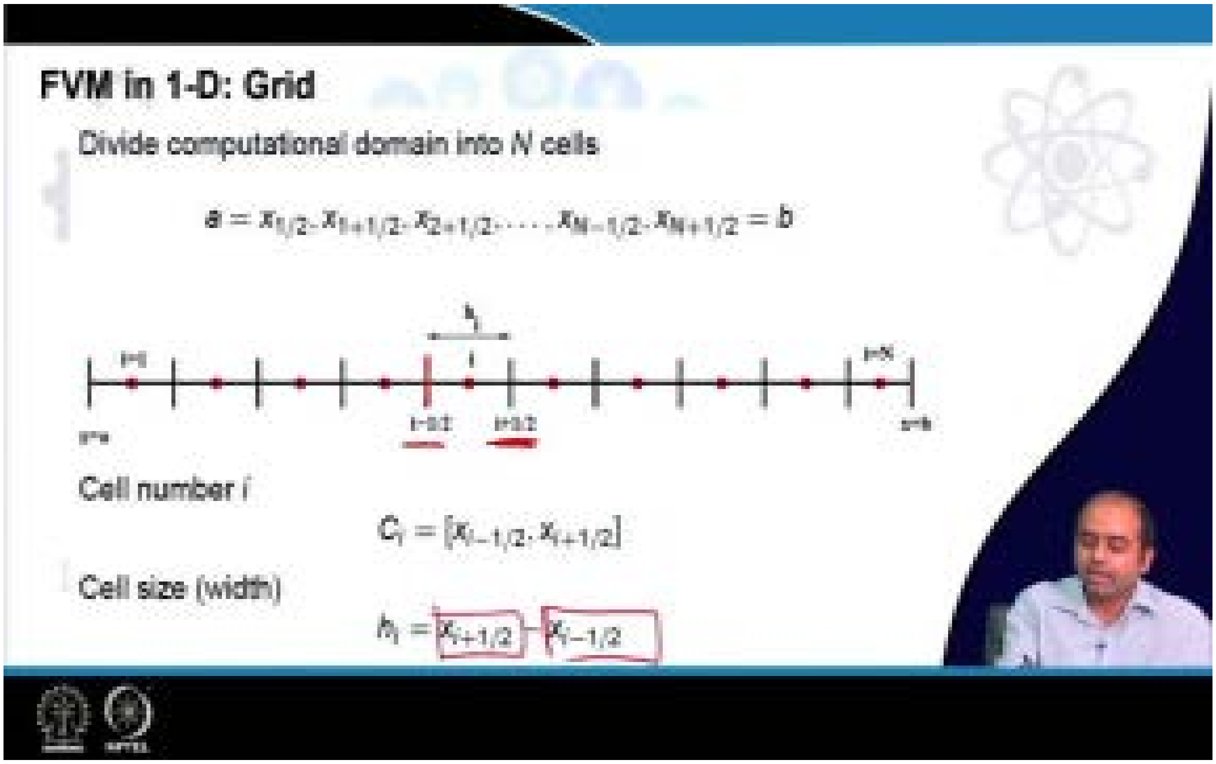

So, for this problem, we try to discretize or divide the domain into let us say n number of cells so, or n number of grids so, each grids are designated the center points of the grid (())(14:53) is equal to 1, 2, 3, 4 like that and the edges of each grids are let us say marked as i minus 1 and i plus 1 half i minus 1 half and i plus 1 half.

So, like that I can discretize my entire 1 dimensional domain into several such this number of grids or number of cells and of course, the cell size or the width in this case can be represented by the x coordinate value at the two edges i plus 1 and i minus i plus half and i minus half and the cell number is denoted at the center of these individual discretized positions.

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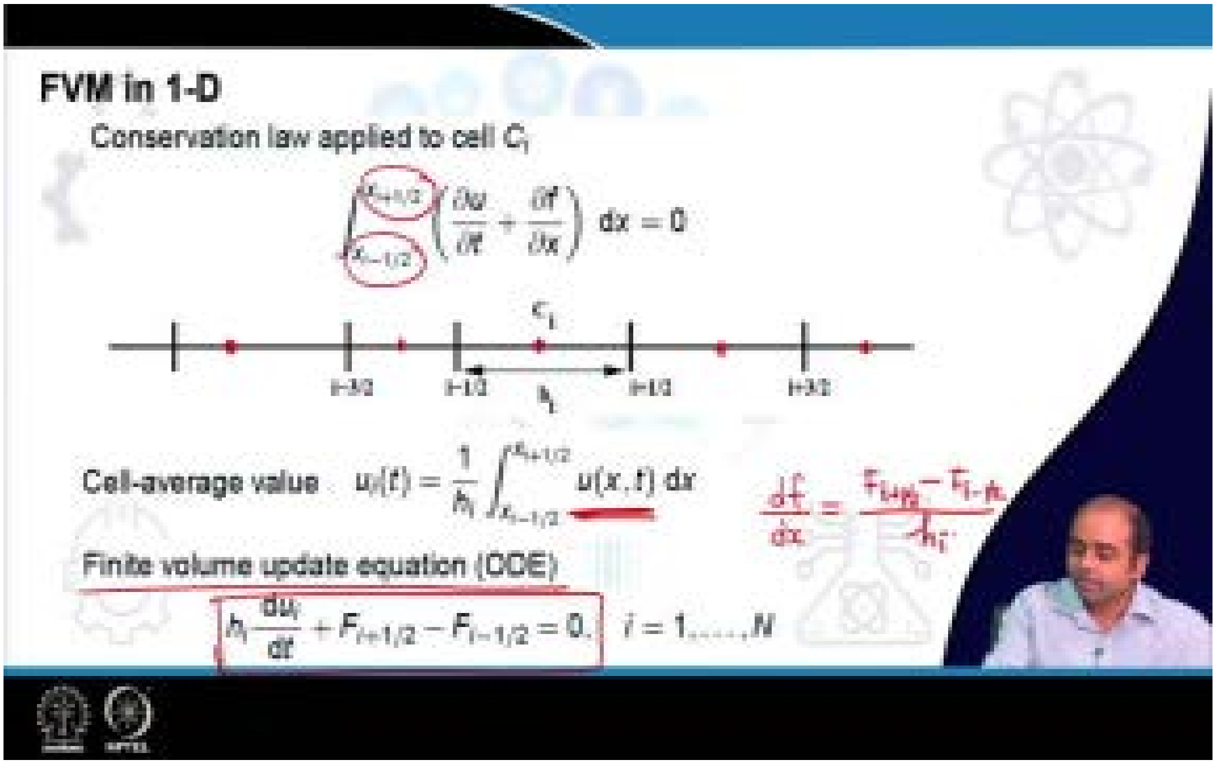

Now, if I try to apply this conservation law to each cell ci so, it is essentially I have to do this definite integral with the limits from x i minus half to x i plus half because these are from the center points these are the i points. So, if I apply this conservation law and try to work out this I will see that at each grid points mass has to be conserved.

So, based on this idea I can calculate out what is the this cell average value like if I know the u once I find out this u x comma t I will find out what is the u average value and this is the finite volume equation to find out my u at a different time. So, this is the generating equation and you can clearly see that this equation is something which we have been discussing so far in the discretization and the method of lines formulation that it came from there only so, d f of x how do I write d f of dx which is nothing but f of i plus half minus f of i minus sorry i minus half divided by h this is how I write my this flux df in this case.

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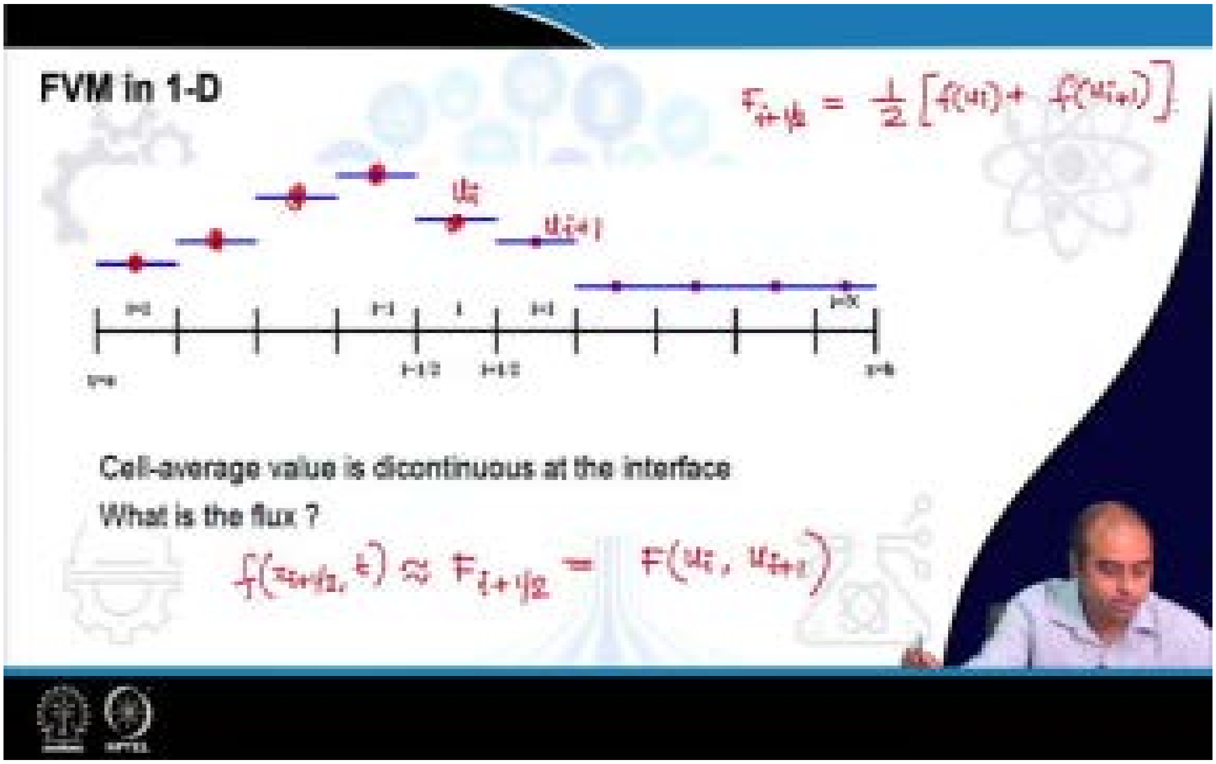

Now, please note or please realize that here (the) whatever the solutions I will be getting will be at these discrete points. So, essentially within each of these cells, my solution u is or the flux is constant within each space domain of each cell. So, now, when I try to take the individual this average value or the value corresponding to the individual locations, I will see that it is a discontinuity and for that you make this numerical approximation that whatever the value of the flux that you get at x half let us say this one is equivalent to f of i plus half and which is a function of F ui and ui plus 1.

So, that is like nothing but the numerical average numerical flux function is nothing but the numerical average of these two a value at ui and ui plus 1. So, let us say this is (my) this is the value at ui and this is the value of ui plus 1. So, I can write so, there are different formulations, but I can write let us say the numerical flux function i plus half is equal to half of these two quantities that F of ui plus f of ui plus 1.

So, this is based on the central difference idea, you can also have a centered flux you can also have appoint flux, let us see we will talk about them.

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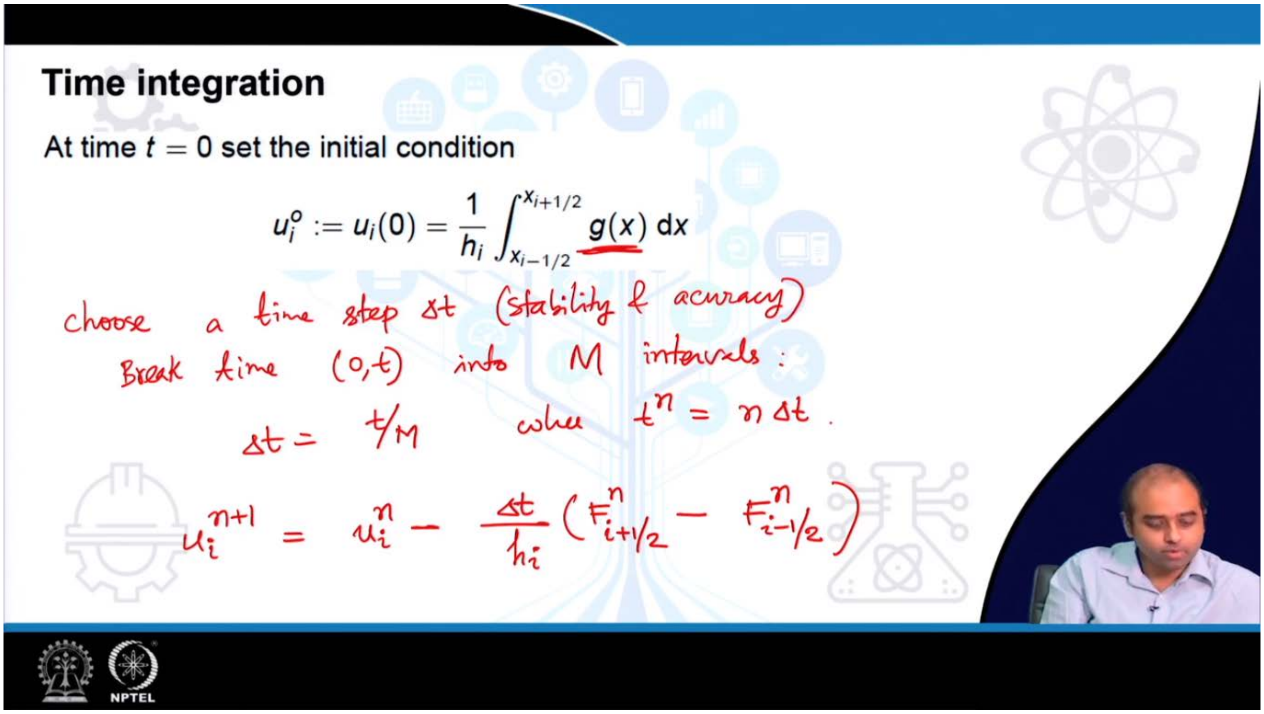

So, what about the time integration now do you have, the time integration tells you that the initial condition is known. So, the initial condition whatever the value that is provided has to be integrated across each of the differential and gx has to be a continuous function. So, initial conditions should be fully known at all the space points.

Now, after this what you have to do is that choose time step delta t based on the stability and accuracy if you want as it is the we are following here in this case for the explicit formulation so, and then you break your time break time this interval whatever you have 0 to 2 into let us say n number of intervals. So, of course, this means delta t is equal to t by M and I can write tn is equal to something like n delta t.

So, for any n I will get back my original equation. So, here that ui n plus 1 is equal to ui n minus delta t by hi, hi is the grid space Fn i plus half minus and you can clearly realize this is the implicit formulation if you want the sorry explicit formulation if you want the implicit formulas and you can replace all these into n plus 1.

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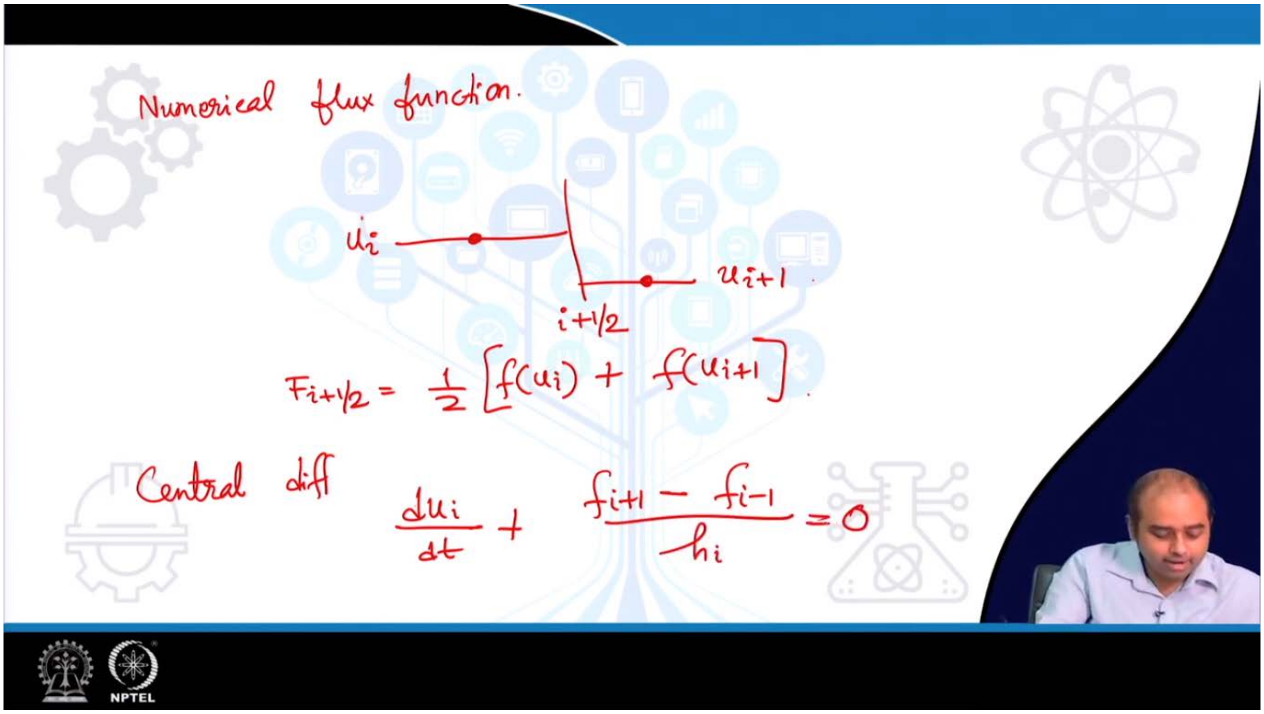

So, let us talk about this numerical flux function as I was talking to you and I was implying that if I have this value and let us say this is i plus half so, this is you i and this is you i plus 1 so, I am going to write my Fi plus half as half of Fui plus Fui plus 1. So, this from the central different scheme tells us that dui by dut should be Fi plus 1 minus F of i minus 1 by hi is equal to 0.

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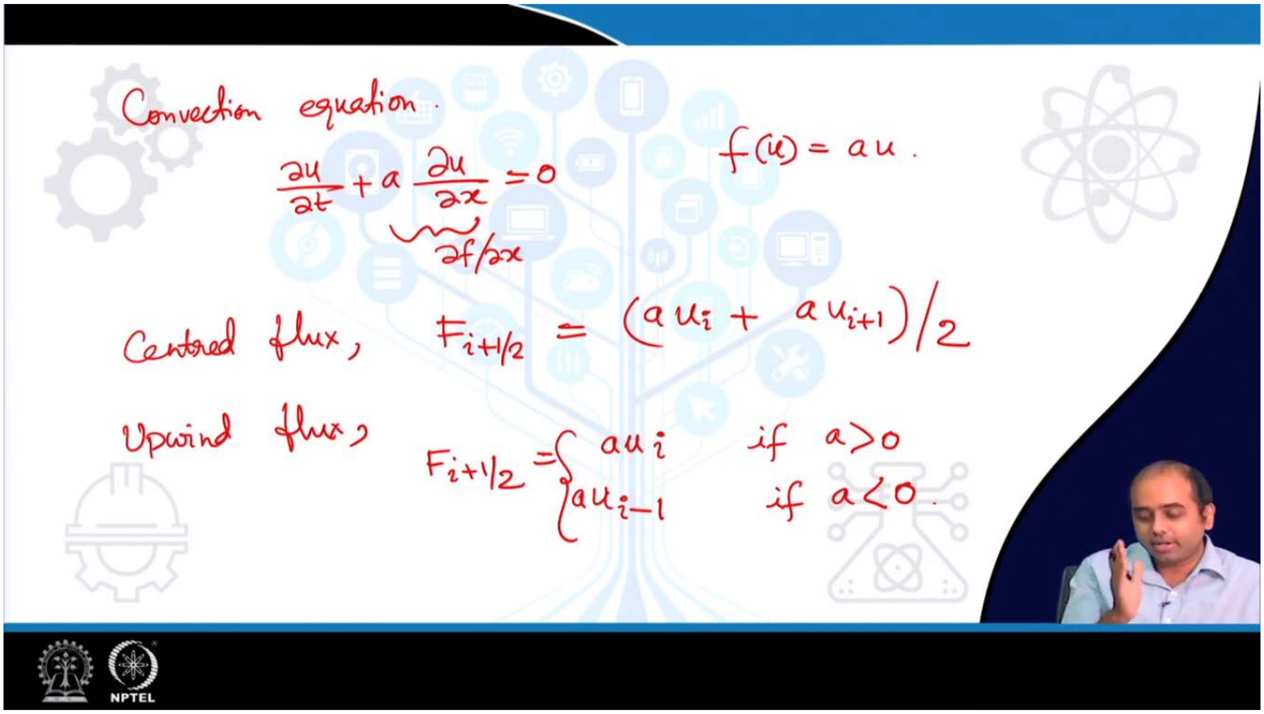

Now, if you have this convection equation, convection equation things are slightly tricky, because you can have a centered flux. So, let us say I have this same convection equation and I write my flux as au. So, of course, this means I can write also as df dx. So, the centered flux there is the concept of a centered flux at f of i plus half is equal to the value at aui plus aui plus 1 whatever the value I get I get the average between the two flux. So, this is the centered flux idea.

In the case of upwind flux. So, what is this upwind idea, in the case of our point flux or what is this upwind idea so, the upwind idea tells you that Fi plus half is equal to aui if a is greater than 0 and it is aui minus 1 if a is less than 0, which means this upwind has a transportive property, how is that, if the velocity or this u whatever this convection is in the positive direction that is greater than 0 if it is positive, then you take the flux value at i plus half to be the value at the previous cell or the current cell, but, so, Fi plus half is the edge.

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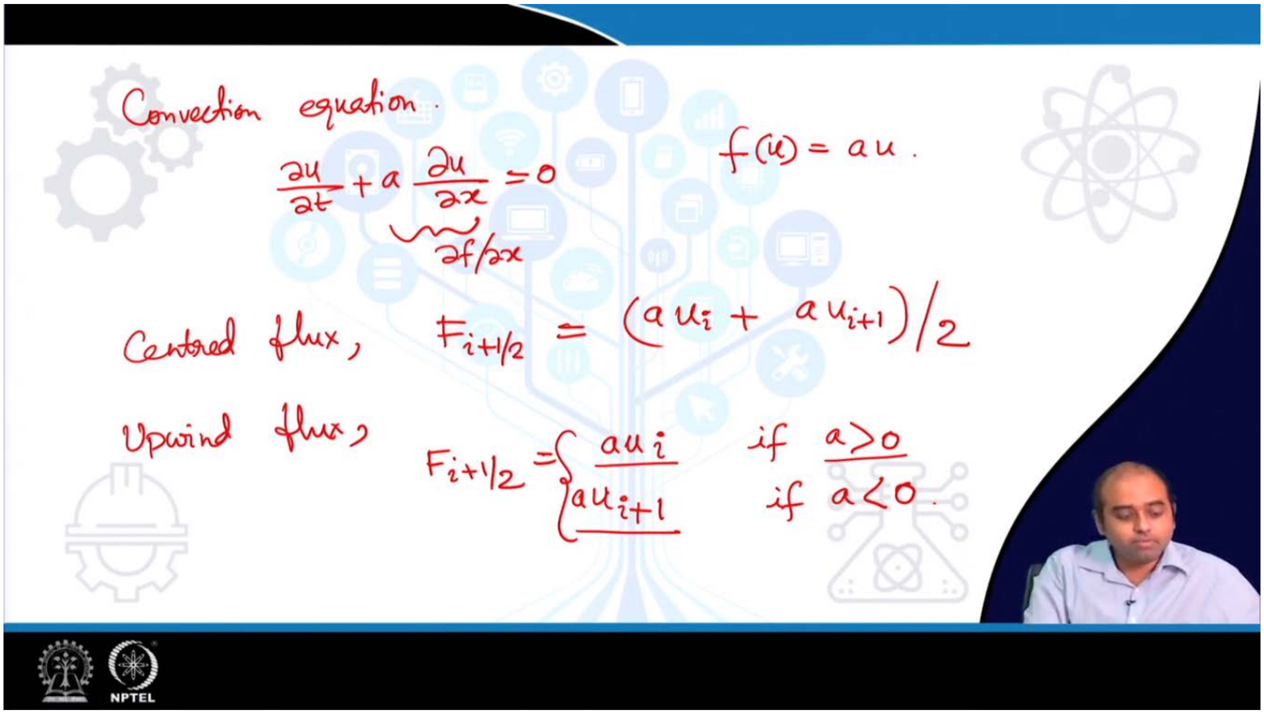

If you recall this i plus half are the edges. So, if we are considering the upwind scheme tells us that if flux is if we are having a convection from the in the positive direction that is a greater than 0, then the flux at this intermediate this edge of each cell is taken from the value of the previous cell, if the if the convection is in the negative direction, then the flux is taken from the subsequent cell that is i plus 1.

So, here we see that a is this is for the case when the flux is in in the positive direction or mostly in the rightward direction and this is the case i plus 1, when the flux is in the negative direction that is from towards the leftward direction. So, this is what we mean by the upwind flux or the upwind scheme.

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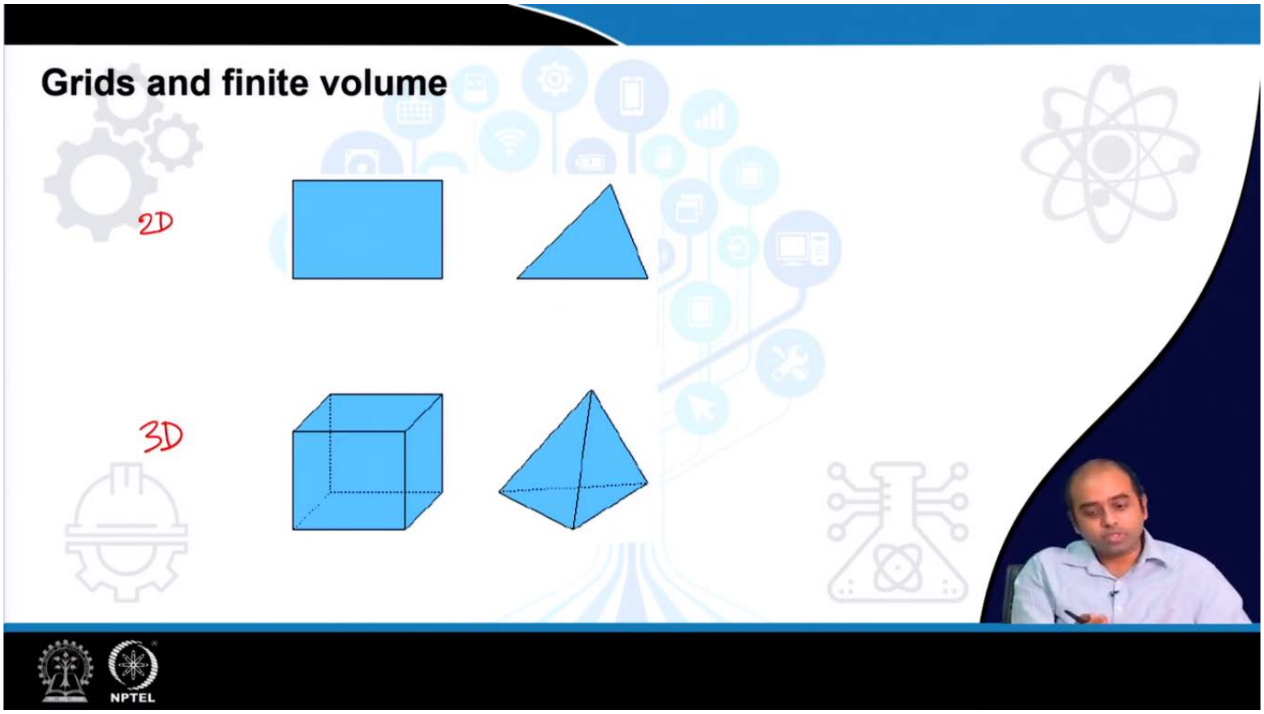

Now, when we move from 1 dimensional space to a 2 dimensional system generally these each of these grid segments is converted to surface a surface segment or a 2 dimensional element. So, this is the case of 2 dimension but when we move to 3 dimensional spaces or 3 dimensional problems, these small sections or the small volume elements are created instead of a line segment or a surfaces segments.

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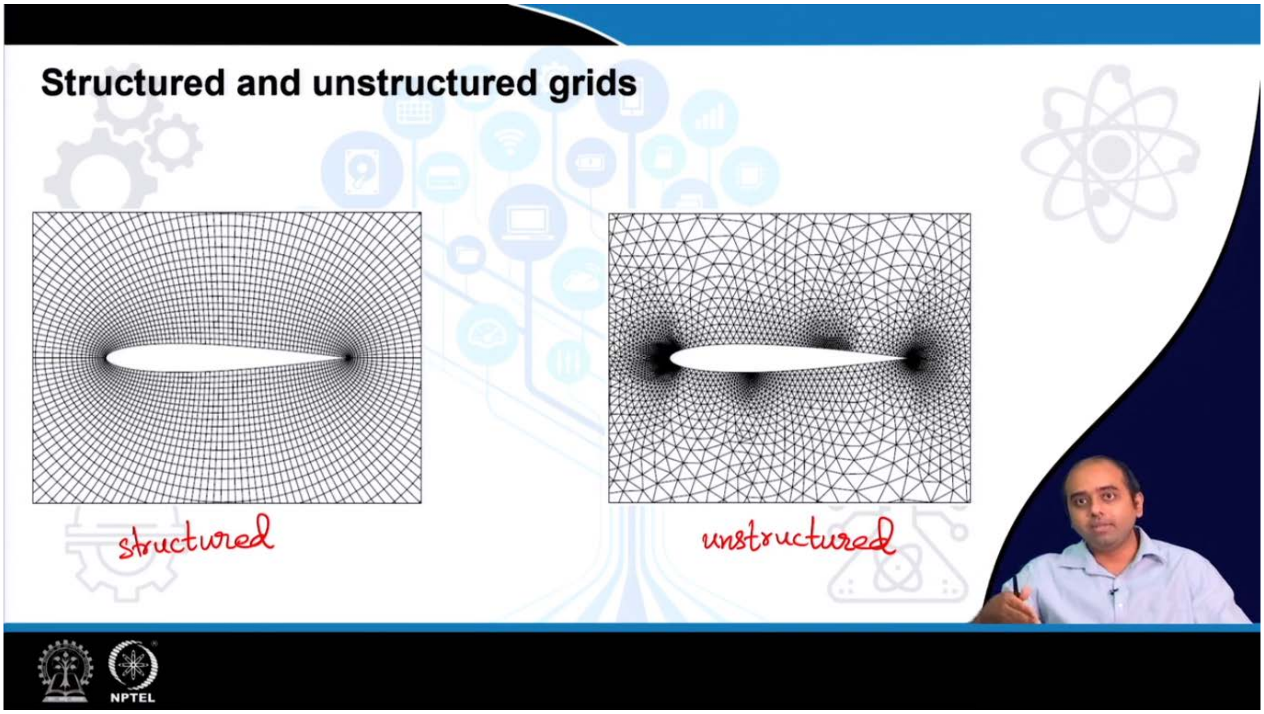

So, based on this idea, you can have a structured or unstructured grid. So, please note that in the structured grid essentially you have a smooth radiation of the grid sizes along with the coordinate dimensions often computationally constant grid sizes are not maintained, because it may be not possible practically to resolve the computational domain adequately for all the boundary layer effects and that is why the structuring whether uniform or non uniform is very important.

And but the idea is that in the structured case this radiation of the grid sizes happens uniformly with the dimension in the case of the unstructured grids which is the right hand side scenario, it does not follow the sort of uniform variation of the grid spacing or the grid sizes with the dimensions of the with or with the coordinate dimension of the problem.

And most computational softwares based on this finite element or finite sorry finite volume or finite difference scheme can quite nicely handle these unstructured grid formations or mesh formations. There is a whole lot of research involves with the unstructured or generation of these unstructured grids and which is more computationally efficient and a good way to define these grid elements, there are several grid parameters and these comes in the picture when we talk about 2 and 3 dimensional problem is about the quality of these mesh or the grids or the skewness factor of these grids, because we do not want these grid elements to be abnormally skewed that they should not be very long elongated in 1 dimension.

So, the ratio of the area of each grid to its perimeter is a factor which determines the quality and we do not want it to be very small or that is something that will make it too skewed if the ratio of this area by perimeter, if it is too small, it means it is either elongated in 1 direction and that is not something good for the problem, because the flux variation in 1 direction will be completely too much compared to the flux variation in another direction that is how you can determine the quality of the grid.

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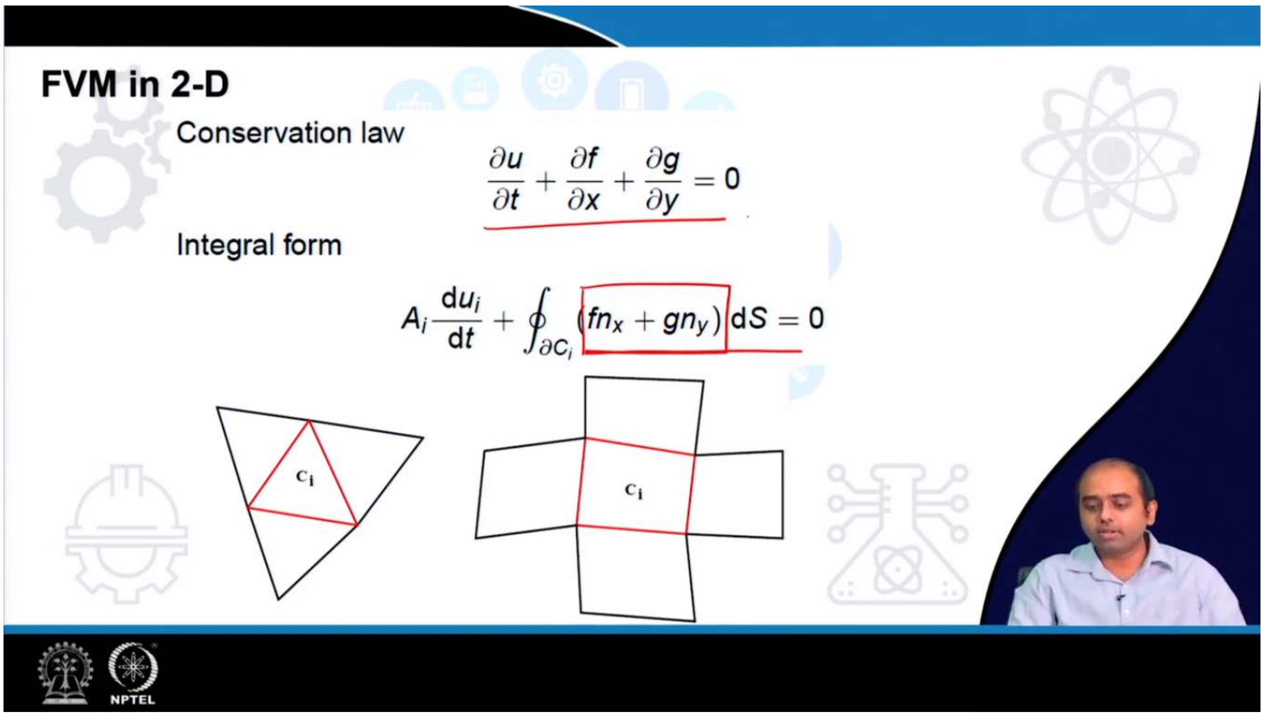

So, in the 2 dimension case, we write the same conservation law and you can see that the integral form can be represented in this way and it is essentially this part that the integration of these fluxes within this surface element instead of the line element now, we have the surface elements so, the surface element could be either triangular space it could be quadrilateral space, each one of them has their own merits and that is something beyond this lecture. So, you can look into some of the reference books for this case.

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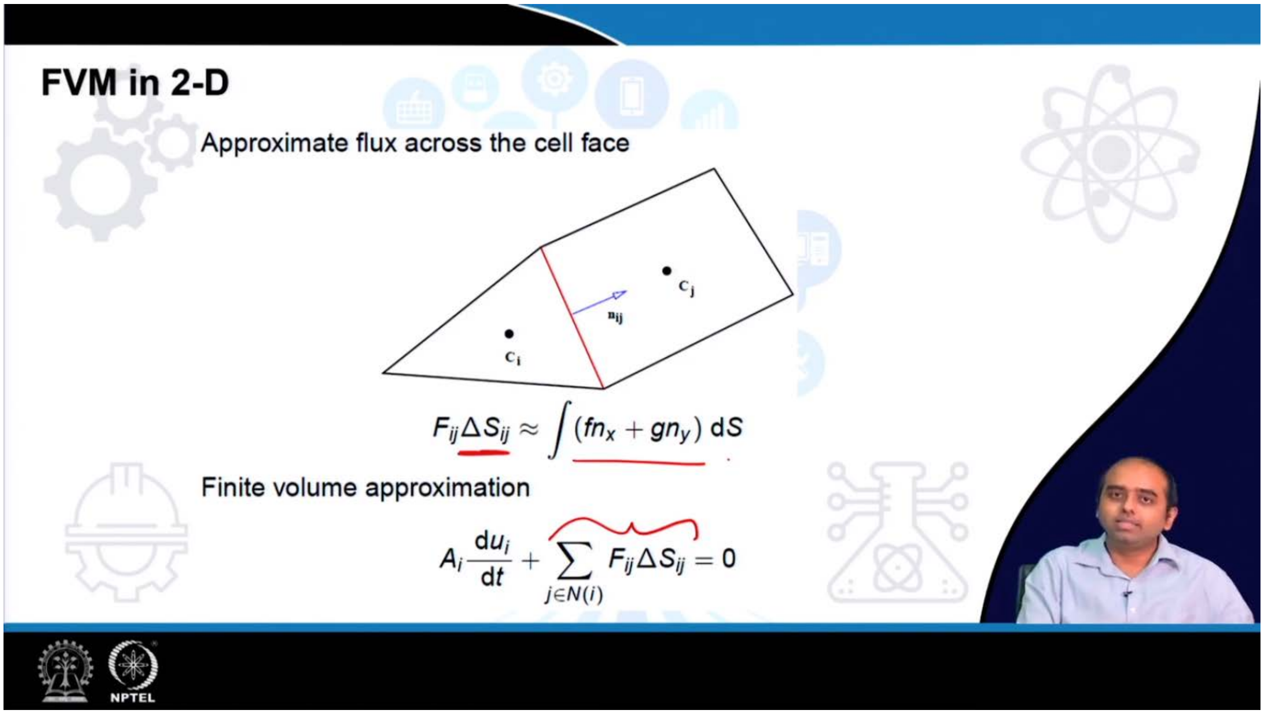

And these calculations of this flux in this surface element is actually made by an approximation, which is just stated here and which is the basis of the finite volume approximation, that this is represented as instead of this and this integration of the over the surface element is made at the is written down in the discretized form as the numerical approximation of F at the center point flux value multiplied with the surface area of the surface element.

So, with this the integral is represented by this summation down here and that is how you do again you do this same idea of writing the temporal derivatives of u and go on to calculate the values of u with forward marching in time.

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So, these are some of the reference books which you can find useful for further reading about this topic or these finite volume particularly for 2 and 3 dimensional systems and domains. I hope all of you really liked this introduction to the finite volume technique and based on which there are several computational tools which are available both open source as well as commercial tools are available for example, ANSYS fluent is based on finite volume method.

And this will help you really to understand more on the background of these software applications as well as realize the basics of the finite volume methods in solving problems involving partial differential equations, which has convection and diffusion. Thank you. I hope you find this useful.