Computational Fluid Dynamics
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Module no. # 04
Lecture no: 16
Topic

Template for the generic scalar transport equation and its extension to the solution of Navier-Stokes equations for a compressible flow

We have seen how to solve the generic scalar transport equation. We have come up with a certain way of discretizing the temporal term and a certain way of discretizing the advection term which we have said an appending scheme would be the desirable, and also, certain way of discretizing the diffusion term. So, now, we have the means for discretizing a given partial differential equation, according, according to template. Thereby we can generate a recurrence formula, recurrence formula, for converting the given partial differential equation into an algebraic equation at each grid point.

So, now, what we want to see is how we can go from here and apply this method to the solution of the coupled equations, because normally, we do not solve a single equation, but we solve several equations together, and when we consider, for example, the simplest case of unsteady isothermal flow through a three-dimensional geometry, then we have four equations to solve - we have the continuity equation and we have the three momentum equations, and each of these is of the form of the generic scalar transport equation as we have seen earlier.

Now, what we want to see is that given that, we know how to solve a scalar transport equation. How we can apply this to solve all of them together and simultaneously? So, this is what we are going to do, but before that, let us look at some specific case of the generic scalar transport equation.

We know that in the special case, we have, in the generic case, we have three terms - the time the dependent term, the advection term and the diffusion term. For steady flows, we have advection terms and diffusion term. And for steady fully developed flow, for example, in a duct, in a square duct that we saw right in the beginning, we have only the diffusion term that appears in the equation.

So, we can consider three special cases - one is that, one is the unsteady convection diffusion and steady convection diffusion, steady diffusion, and we can also have unsteady convection alone as, as, three special cases of the generic scalar transport equation. So, in each of the cases, we will try to follow the principles that we establish in deriving a corresponding discretized difference formula.

Whenever we have the advection term, we use the up winding scheme so that we follow the flow of the information. If the flow is from the left to right, that is, in the increasing x direction, we use the backward spacing backward differencing for advection term. If the flow is from right to left, that is, in the negative x direction, then we will use the forward differencing for an advection term. This is true of x direction, y direction and z direction.

So, whenever we have an advection term, we follow the flow, and based on that, we discretize the advection term. For the diffusion term, we are assuming that it is isotropic diffusion, and even if it is not isotropic, we can readily encounter it, but in general, diffusion is not specifically directional oriented, and therefore, information goes from both left and right, and we therefore use a central differencing equation. So, by default, diffusion term is done using central differencing and advection term is done using upwind differencing, and the time term, the rate of accumulation term is done using forward differencing.

In each case, we can have any order of accuracy. For example, we can have a second order accuracy in time; second order accuracy in advection term and a second order accuracy for diffusion term or even a fourth order accuracy or a sixth order accuracy as the situation demands, but we have seen that when you want to implement a second order accurate scheme for the time, we have a starting problem, that is, phi at n plus 1 is given in terms of both phi n and phi n minus 1. So, that sometimes raises a problem; we have to see how that can be done, and for the advection term, we have seen that if we make use of we have generally discussed this, this particular issue; we have not explored it deeply, but the point that we are trying to make was that in the case of advection term, if you were to use any differencing which is greater than the first order, that is what have the second order, third order. Then it is possible to give rise to steady spatial oscillations in the flow domain at regions of steep gradients and those kind of things are undesirable, and we have mentioned schemes like the t v d schemes which address this particular issue specifically to reduce or even to eliminate oscillations and still maintain higher accuracy of the discretization.

So, we have to consider, we have to weigh the disadvantages of having a higher order scheme with the advantage that we have for a first-order scheme, and based on this, we will make a choice. So, with this introduction, let us now look at how to solve the set of equations, and what we try to do is that we have said right in the beginning that this particular course focuses on incompressible flows, where density effects are negligible and where the mach number of the flow is less than 0.3. So, we have to come up with methods of solution of the whole set of equations for incompressibility, but before we do that, we will start with the direct extension or the methods of the template that we have already developed for a compressible flow and we show how these methods can be used to solve the set of equations together and then we will see the difficulties that we encounter.

When we want to extend this, the same methods which are even now used for compressive flow calculations to incompressible flow calculations, and we see how these difficulties that we have for incompressible flow require us to pursue a different way of solving the equations from what we have been talking about and we list three four methods for getting the problems specifically associated with incompressible flow, and finally, suggest a couple of methods which are generic and which are still used in many computations for all kinds of incompressible flow calculations. So, with this, this is the overall organization of this particular module on the solution of all the governing equations together; that is the set of governing equations together for the the case of isothermal, three-dimensional, unsteady flows.

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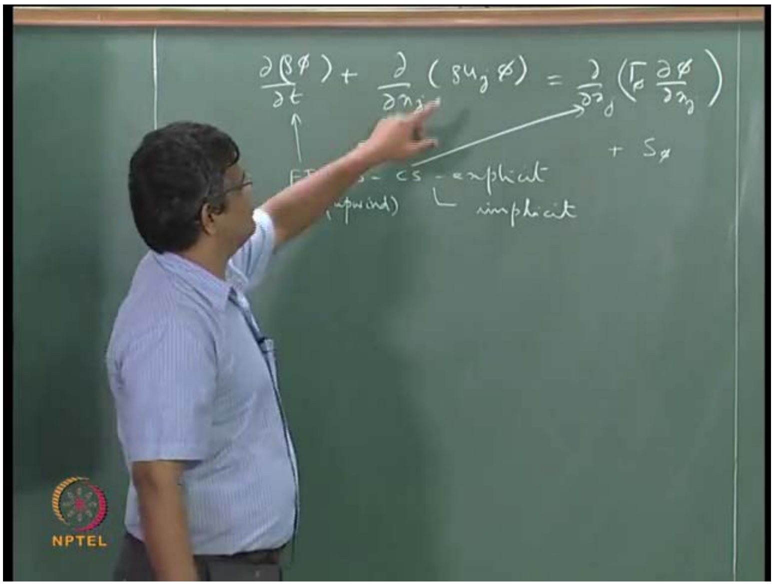

So, let us start with the generic scalar transport equation. We have written it as we are making use of slightly different notation. So, as not to confuse, this is the rate of accumulation of the time dependent term; this is the advection term; this is the diffusion term and we have made use of the capital gamma for the diffusivity of the particular scalar phi, and we know that when diffusivity is equal to 0 and phi is equal to 1, this equation represents the continuity equation.

And when diffusivity is equal to mu and phi is equal to u plus a source term and the source term being a negative of the pressure gradient, we have the u momentum equation, and similarly, for phi equal to b and mu here for the diffusivity and minus dou p by dou y, we have the y momentum equation and the z momentum equation like this, and we have said that in the case of for this, we can make use of f t b s c s explicit method for the generic scalar transport equation, where forward in time refers here backward in time in the convection term u is positive or we can replace this with up wind method and central is place for this. We can have the explicit option typically in such a case, we have limited stability and we can also have an implicit option, where we normally have a higher degree of stability if not full stability unconditional stability.

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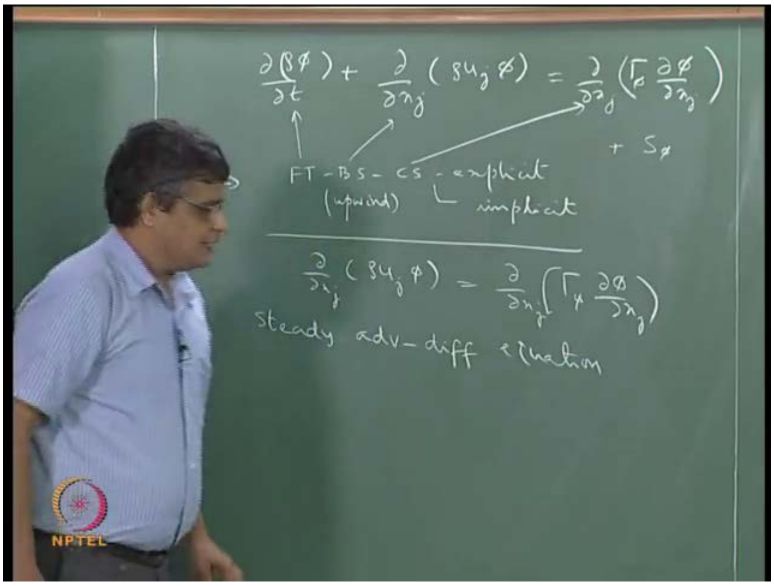

Now, this is for the general case, where the source term is like the pressure gradient which does not depend on the phi value. Now, the steady part of this, we will have this as 0; we will have dou by dou x j of rho u j phi equal to dou by dou x j of gamma phi dou phi by dou x j. So, this is the steady advection diffusion equation and this describes, for example, the steady developing flow in a duct.

If you consider a rectangular duct and you are looking at how the flow develops from an initially uniform profile velocity at the inlet in to the corresponding situation, then this is the equation which describes that, and for which, we can again make use of upwind scheme and central diffusing here, and for example, assuming u to be positive and constant and the one-dimensional form, we will assume that rho is constant; u is constant; gamma phi is constant and we take the one-dimensional form; we can write this as rho u into dou pfi by dou x equal to tau phi into dou square phi by dou x square, and therefore, we can write this as rho u at phi phi i minus phi i minus one by delta x. This is where we have assumed that rho u is positive and we have made use of the backward differencing. So, this is the upwind method and this gives us gamma phi. Here, we make use of the central differencing, so, phi i plus 1 minus 2 phi i minus phi i minus 1 by delta x square.

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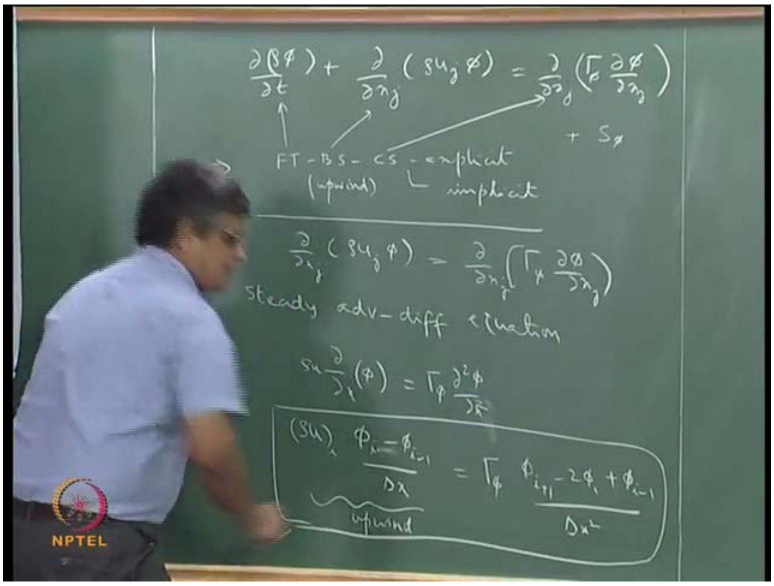

So, this is the discretized equation at space point i - where phi is a sole function of x here. Now, how to solve this together? Here, we have no specific stability problem, because we are looking at a steady condition, but we see from here. Now, we are looking at a computational molecule; we are looking at one dimension.

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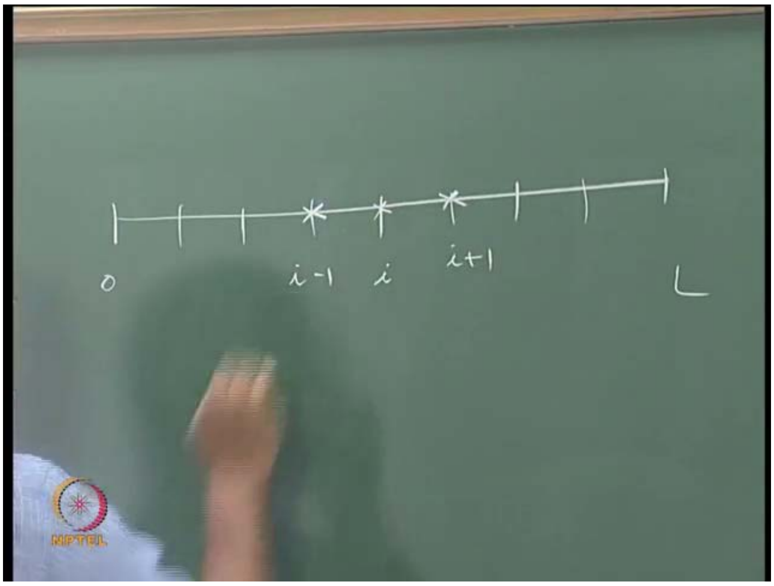

So, this is x equal to 0 to x equal to l, and as usual we will break it up into small number of points. Right now we are considering uniform spacing. So, we have i here and the value at the i th point is expressed in terms of i minus 1 and i plus 1. So, the value here is expressed in terms of this and this. So, this i plus 1 and i minus 1, and what this means is that you cannot march forward in time, because if you want to compute this, you need to know both the left neighbor and the right neighbor. So, marching forward from one end to the other end in either direction is not possible.

So, we have to write this. We have to apply this template to all the points at which we need to get a solution and we will put them together into a matrix form a phi equal to b, where phi consists of, let us say that this is a Dirichlet boundary condition and this is given phi 0 is given and phi l is given. So, this will be i equal to 1 2 3 and so on like this. So, we will have as unknown values 2 3 4 5 phi 2 phi 3 phi 4 phi i minus 1 phi i phi i phi n transpose.

These are the unknowns, these are unknowns which appear in this and we have an equation like this which we need to solve using methods which we can describe; we will describe later on. For example, in the first example that we considered we solve something like this using the Gauss Seidel iterative method and it is a matrix equation. We can also use Cramers rule and we have many other methods to solve in this. We will discuss these methods later on after we come up with a template. So, for the solution of steady advection diffusion case, we have to solve a matrix equation, but if we are solving a time dependent equation which is in explicit form, then we do not have to solve a matrix type of method in order to get the value at phi i and plus 1. If it is implicit, normally we have to solve a matrix type of equation.

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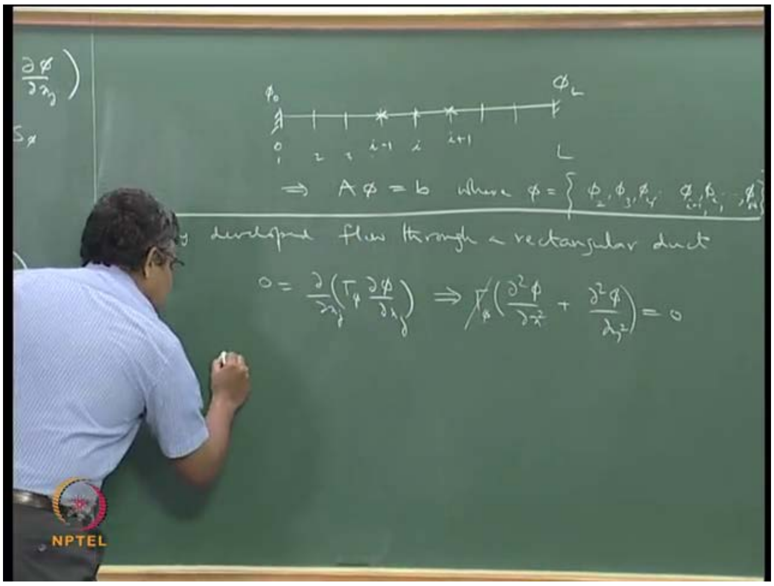

Now, let us consider the other case of only diffusion equation where, for example, a fully developed flow through a rectangular duct, because the flow is fully developed. The advection term goes to 0 and we have only the diffusion term. So, in which case, the governing equation will be 0 equal to dou by dou x j of gamma phi dou phi by dou x j, and if you write in two dimensions, this will be equal to dou square phi by dou x square plus dou square phi by dou y square equal to 0, assuming gamma phi to be constant, and something like this can be readily discretized using central diffusing because this is a diffusion term, and since gamma phi is constant, we can even cross it out.

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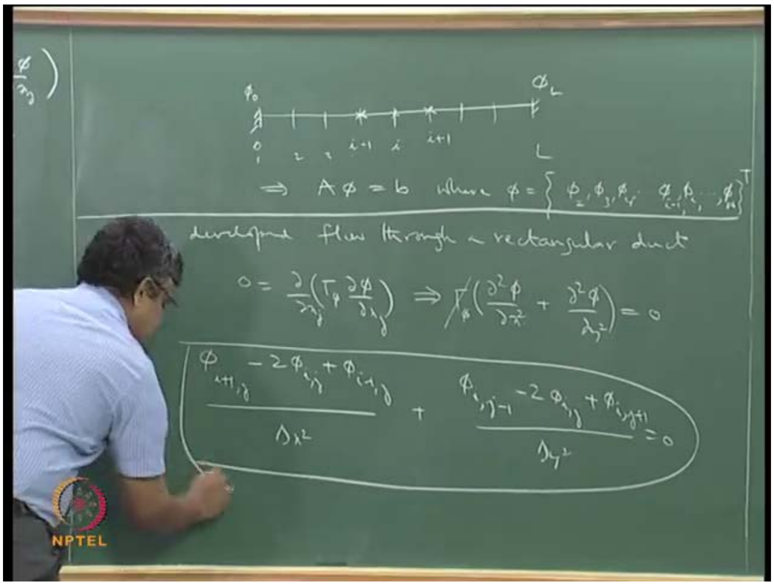

We will have a template at phi i plus 1 j minus 2 i plus j plus phi i minus 1 j divided by delta x square plus phi i j minus 1 minus 2 phi i j plus phi i j plus 1 by delta y square equal to 0. So, this is the template that we have for a pure diffusion term in two dimensions. In one dimension, this will not be there and this will be there, and in both cases, what we see it the value that we want for. So, we need to solve this for phi i, j. So, solution of this will give u phi i comma j, but in order to do this, we need to know i plus 1 j and i minus 1 j. So, that is the two neighboring points.

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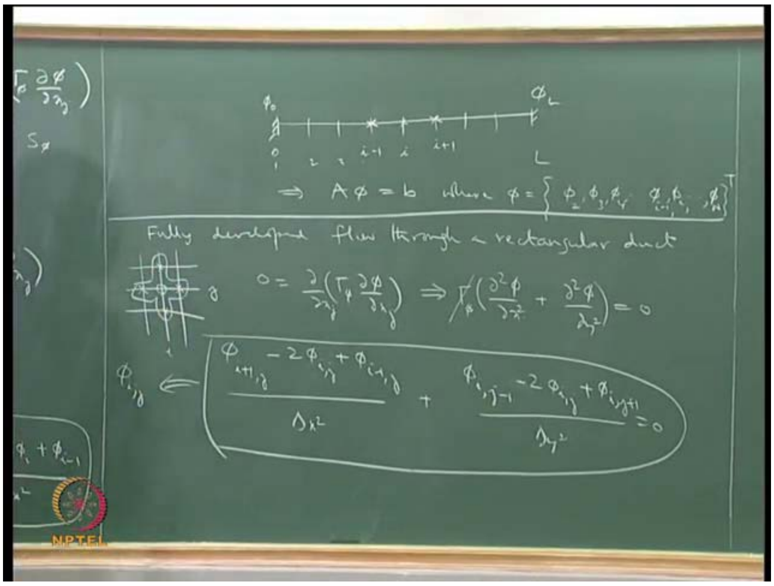

Let us consider a grid here. This is i and this is j. So, we are looking at the value and we need to have i plus 1 j. So, that is this value here and i minus 1 j this value, and similarly, for here we need j minus 1 at i. So, that is this 1 and j plus 1 at i this. So, we need to have the four neighboring points. So, again it is not possible to have a marching forward type of solution to this and we need to apply this equation to all the interior points or for all the values, for all the nodes at which the variable value are not known.

And we will assemble this in to p phi equal to q, and this again is a matrix equation and we have to use methods that are specifically developed for this and solution of this will give us the value of phi at i j. So, again in this, it is not possible to march forward in time; we have to solve a matrix type of equation. So, depending on the generic scalar transport equation may require, march may enable a marching forward type of solution if you have an explicit type of scheme from an initial condition and initial and boundary type of conditions that are specified if the problem is unsteady.

And if the problem is steady, then we would have to solve a matrix type of equation. So, with this understanding of how we can solve a given scalar transport equation, let us now see how we can implement this for the case where we have a number of equations which are to be solved simultaneously, like the case of Navier-Strokes equation where we have continuity and the three momentum equations. So, let us start with the simple case where an extension of the methods that we have looked at is quite possible.

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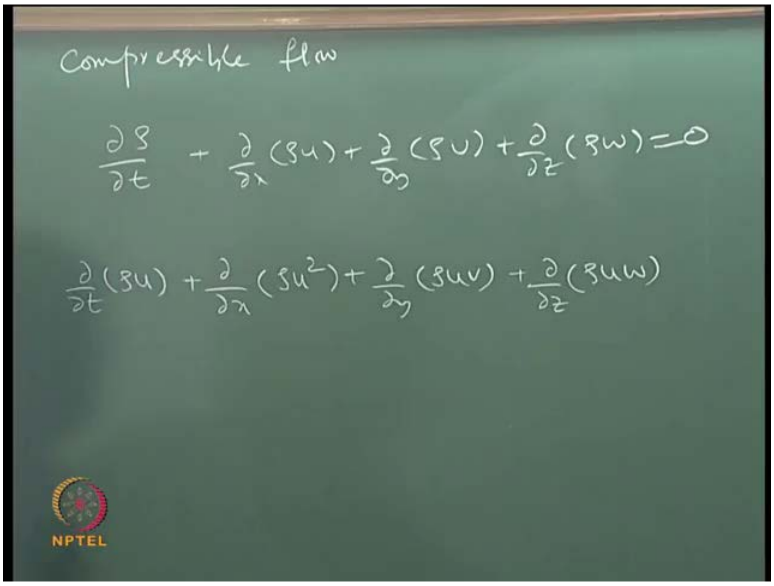

So, we will consider the case of compressible flow. Essentially, we have density will come in to the equations and it is already there in the equations, and so, so we can write down the continuity equation as d rho by d t plus d by dx of rho u plus d by dy of rho v plus d by d z of rho w equal to 0; this is a continuity equation, and the x momentum equation, for example, can be written as dou by dou t of rho u plus dou by dou x of dou u square plus dou by dou y of dou u v plus dou by dou z of dou u w. We have the density term; we will just, we will have the gravitational term which we will neglect for the time being minus dou p by dou x is the is the pressure plus we have the three sheer stresses - dou by dou x of tau x x plus dou by dou y of tau y x plus dou by dou z of tau z x.

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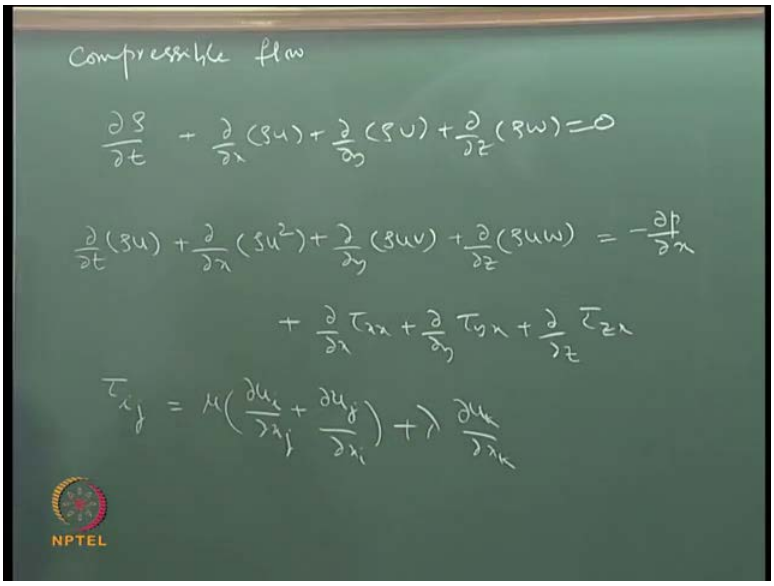

We know what this tau x tau x x and all these things are. We have seen that the general case of tau i j is given as mu times dou u i by dou x j plus dou u j by dou x i plus lambda times dou u k by dou x k. So, this defines the values of tau x x in all these things. And we have said that this is the first coefficient of viscosity or the dynamic velocity which we normally associate and which can be readily measured. And lambda is the second coefficient of viscosity or the bulk viscosity or the bulk modulus of something like that, which is not known and which is also insignificant in a vast majority of the cases. So, for the exposition of the principles here, we will neglect this particular term, and anyway, our interest is in incompressible flows, in which case, this term will be identically equal to 0.

Even in compressible flows, this term plays a role only in a very minor case and even there the value of the second coefficient of viscosity is known only for some simple gaseous molecules. So, it is very difficult to measure and we often neglect it. People sometimes say that lambda is equal to minus 2 3 of mu. It is only in some value and the sanctity of this value is yet to be verified. So, we will not make such assumptions, we will just say that this term is negligible.

So, now, we have these equations, and we have the corresponding y momentum and z momentum equation. What we do is that we will try to rewrite this in the form of the scalar transport equation that we know here and we can write the whole set of momentum equations and the continuity equations as dou u by dou t, because we have a term here plus we have dou by dou x term; we can write this as dou by dou x of e plus dou by dou y of f plus dou by dou z of g equal to, we can write this as 0, where the e f and g will capture. For example, rho u here for the x momentum equation, for the continuity equation, and for the x momentum equation that we, e here will be rho e square plus dou p by dou x minus tau x x. So, in that way, we can rewrite these equations - so, where this e u e f g are column matrices.

So, when we write, we can say that u here for the continuity equation is rho; for the x momentum equation, this is rho u; for the y momentum equation, this will be rho v, and for the z momentum equation, this will be rho w transpose. So, when we list all the equations, we have four terms four components in this u here, rho for the continuity equation, x momentum equation rho u, y momentum equation rho v and z momentum equation rho w, and similarly, we can write the term e which is appearing in this as when we consider the continuity equation, we have only one term - dou by dou x of rho u. So, this, this will be rho u, and when we consider the x momentum equation, we have dou by dou x here rho u square.

Since we are putting on the right hand side as 0, all the terms all the terms on the right hand side should be brought here. So, we have plus dou p by dou x; so, that is dou by dou x is coming plus p and we have this dou by dou x of tau x x with the positive sign is coming from the other side. So, that becomes minus tau x x. So, this the term which is appearing as the term in the x momentum equation for e, and when we consider the y momentum equation, we have v here; this becomes rho u v and rho v square rho v w dou p by dou y tau y x tau y y tau z y like that. So, we can, in the y momentum equation, the terms with dou by dou x will be rho u v and we have dou p by dou y is the y term and we will have tau y x minus tau y y. In the z momentum equation, dou by dou x will have rho u w. So, this will be rho u w, and here, we will have y minus tau z x.

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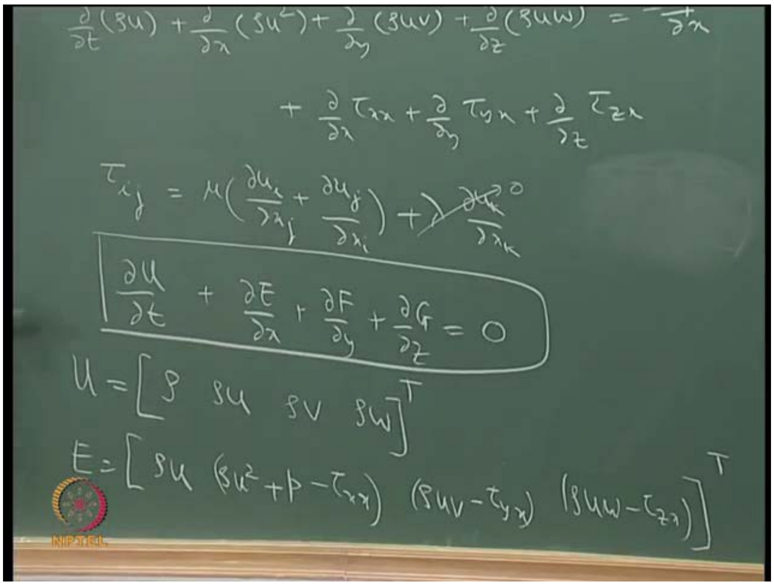

So, what we are trying to do is that we are writing the four equations together into one equation like this, in which, u e f g are column matrices and each term of that will come from each of the four equations. So, for the e matrix, we will have four terms and we are writing the transpose of this. So, from the continuity equation, you get rho u, and from the x momentum equation, we get this term rho u square and this term which is brought to the left will become plus p and this term will become minus tau x x.

So, if you were to rewrite this equation, you can write this as plus dou p by dou x minus tau x x minus dou by dou y of this minus this is equal to 0. Now, we can club this, this and this together and put as the term e in the x momentum equation, and similarly, in the y momentum equation, the corresponding e term here, this is all e will be rho u v minus tau x tau y x and, the, the term coming in the z momentum equation is rho u w minus tau z k. We will also write the terms for f and g and that will complete the set of equations that we have to solve for unsteady compressible flow in a three-dimensional case.

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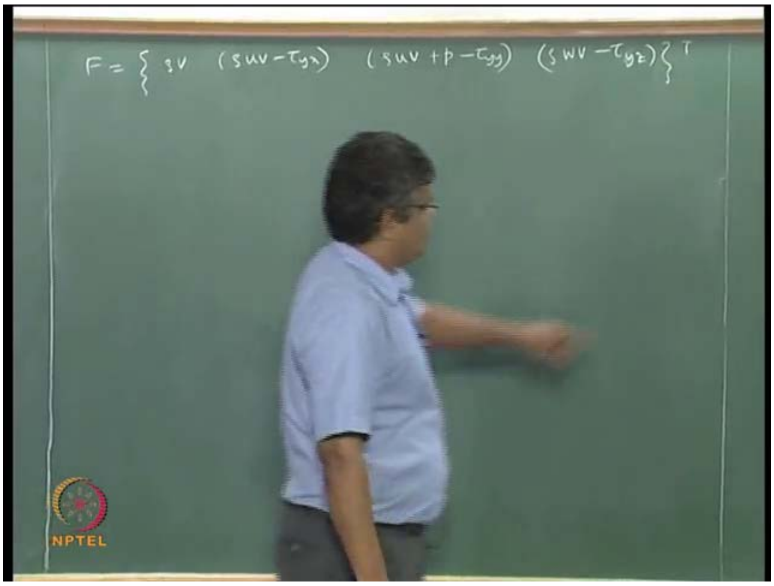

We have written the four components in the term e. Now, let us look at the components appearing in f here; f terms are those terms with a derivative - first derivative - in the y direction. So, we can write f. When we look at the continuity equation, we have rho v as appearing with the first derivative with respect to y; so, this is rho v. In the x momentum equation, this is dou by dou x; dou by dou y, we have rho u v, no y derivative, no y derivative, no y derivative. Here, we have minus tau y x; so, this will be rho u v minus tau y x. This is the f term in the x momentum equation. In the y momentum equation, we have v here, v here, and here, instead of rho u v, we have rho v square and that appears with the first derivative. So, we have rho v square here; this is z derivative, and here, we will have dou p by dou y. So, that gives us rho v square plus p. Here this is x and here we will have rho y y.

So, we can say rho u v plus p minus tau y y. These are the terms that appear in the y momentum equation for the f column vector, and finally, in the z momentum equation, this will be w here; this will be rho u w with an x derivative rho v w, this is with the y derivative, and here, we will have rho w square and the pressure gradient will be in the z direction. So, that is dou by dou p by dou z. So, you have rho w square plus p and here we have z x z y and z z. So, that is minus tau z. So, we are considering only terms with the y derivative. So, in the w momentum equation, this term would not appear; this term would not appear. Here we will have rho v w and this is the z direction, z direction, z direction, and here, we will have tau z x.

So, we will have, so, let me just, so, this will w here; this will be v w; this will be v w; this is w square dou p by dou z for the z momentum equation, and here, this will be tau z x tau x z tau y z and tau z z.

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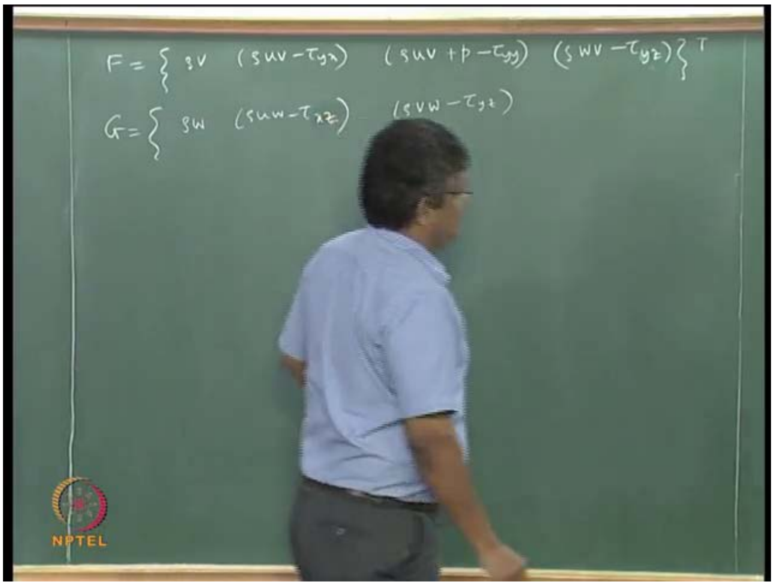

So, those are the things and those with y derivative are rho v w, we have here, and this is minus tau y z minus plus minus y z. So, let us just rub out these extra bits that we have put here. Now, let us look at the final term g again will have four terms; it is a column matrix, and this represents all the z derivatives in the four equations; z derivative in the continuity equation is rho w. In the x momentum equation, we have rho u w minus tau z x. In the y momentum equation, this will be rho v w and this will be rho w square.

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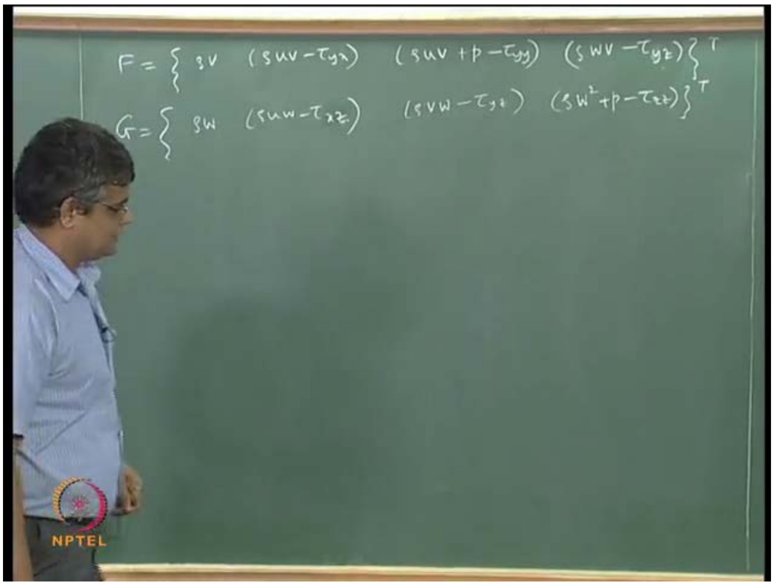

So, we have rho w square and this becomes dou p by dou z. So, rho v w square plus p here, and then, this is z x; this is z y and z z. So, the terms, we are looking at the y momentum equation; so, this will be rho v w and this term will become rho by rho y z rho x x z here, and finally, when we come to the z momentum equation, we have z derivative rho w square plus p minus tau z z.

So, let us just verify that these are consistent. When we want to get the continuity equation, we take the first terms of each of this. We have dou rho by dou t plus dou by dou x of rho u plus dou by dou y of rho v plus dou by dou z of rho w equal to 0. For the x momentum equation, we have, we have to take the 2 terms in each of this. So, that is dou by dou t of rho u, which is this term by dou by dou x of rho u square plus dou p by dou x, which is this term here minus dou by dou x of tau x x, So, that is this.

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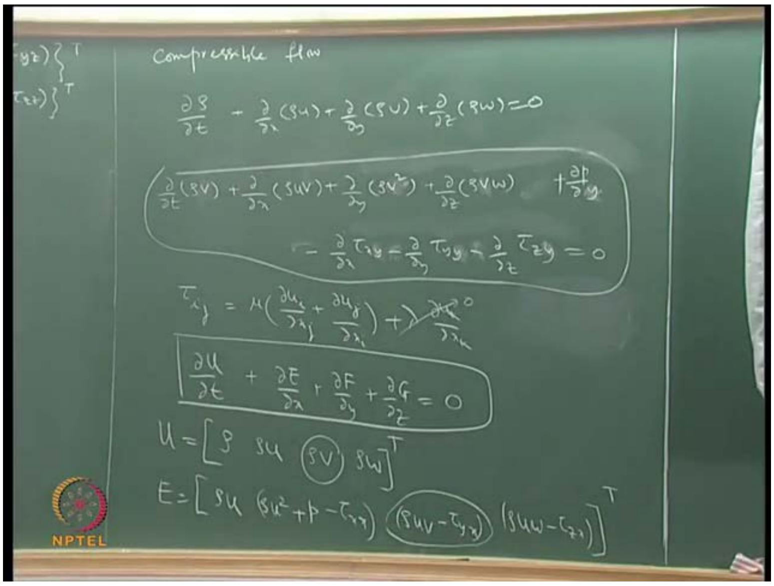

So, we have got these three terms plus dou by dou y of rho u v, so, that is this term, minus dou by dou y of tau y x plus dou by dou z of g term, that is, z plus dou by dou z of rho u w which is this minus dou by dou z of tau x z this is x z x. So, in that sense, we can get this, and let us just for the sake of without scribbling too much, let us just convert this in to the y momentum equation rho u v; this will be rho v square; this will be dou v w plus dou p by dou y dou by dou y of x y y y and z y. So, this is the y momentum equation. Let us just write down the y momentum equation as per this formula here. So, for the y momentum equation, here we have to take the third term. So, we will have to take this term and this term, this term and this term.

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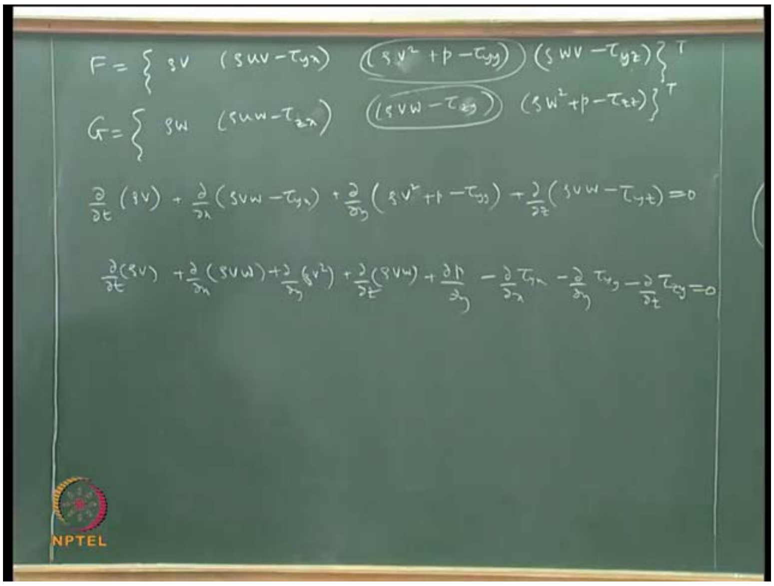

Let us just do that. So, we get dou by dou t of this term rho v plus dou by dou x of this here plus dou by dou y of this term rho u v plus p minus tau y y plus dou by dou z of this term here equal to zero and let us put in the standard format. Let us put all the sheer stresses together and all the velocity terms together plus dou by dou x of rho v w plus dou by dou y of this, I think we have made a mistake here, this is dou v square, dou v square plus dou by dou z of rho v w plus dou p by dou y and then we have minus dou by dou x of tau y x minus dou by dou y of tau y y minus dou by dou z of tau y z is the same as z y, but to be consistent, we have to put this as z y equal to 0, and if we compare this with this, we have the first term and we have, I have made a mistake in writing this too many mistakes, dou by dou x of rho u v and dou by dou y of rho v square and dou by dou z of rho v w plus dou p by dou y minus dou by dou x of tau y x. We will just attend to these x x and y x; x x is tau x y is the same as tau x y, and here, we have tau y y and tau z y equal to 0. So, we have recovered the equation by doing this. So, that is what we want to do but let us just attempt to examine each of these terms here.

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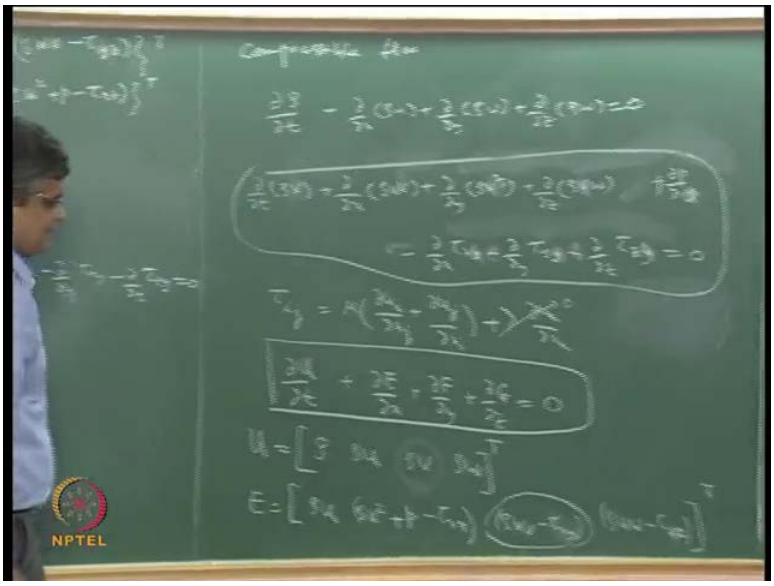

So, there is no problem with, with, the u terms, and here, this is the time dependent term and this is the x component of the advection term plus p and this is the stress acting on the x face in the x direction and this is the y component of the advection term and this is still a force balance in the x direction, but this is appearing in the y momentum equation; y momentum equation must have all the terms acting in the y direction. So, this should be x y on the x face in the y direction, and similarly, this must be the stress acting on the z face in the…

So, this is the term appearing in the, y, z momentum equation. So, the stress must be acting in the z direction. So, this is z, and because it is a derivative with respect to x, this is must be stress acting in the x face. So, that is the formulation, and similarly, when we come to the f terms continuity equation and this represents the advection term in the y direction and this is the stress acting in the x direction on the y face. So, that is, yes, we have changed this. So, that is why this is dou by dou y of tau by x. So, that is correct. This is y momentum equation, momentum equation, in the y direction for and this is the derivative with respect to the y direction.

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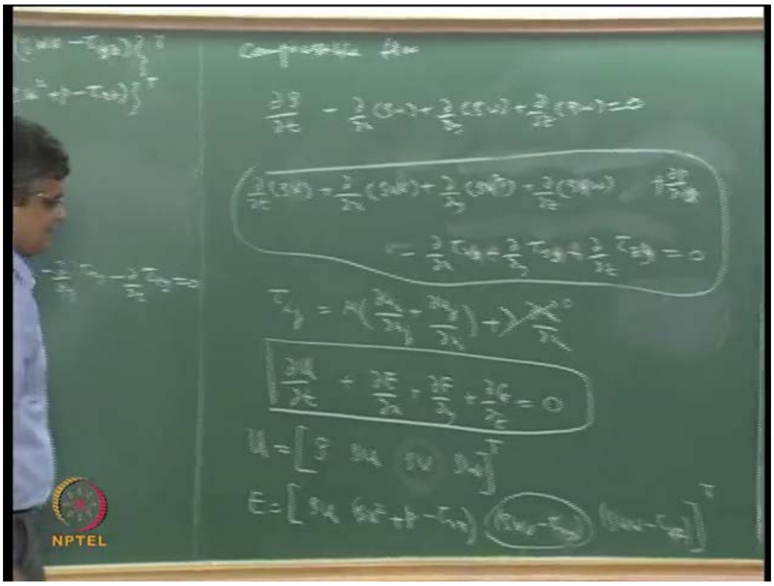

So, this we have dou by dou y of p square plus p and tau y y, and this is the derivative in the y direction from the z momentum equation. So, this is the, this is the, stress acting in the z direction. This is not right.

So, now, what we see as a structure that we should note is that when we have dou by dou x, in the x momentum, we have rho e square plus p. For dou by dou y, we have the y momentum coming here - dou v square plus p, and dou by dou z will have z momentum rho w square plus p, and then, dou by dou x of normal stress appears in the first term here and in the second term here and the third term here, and all the terms appearing in the g, direction, term are stresses acting in the z face. So, you have tau z x tau z y and tau z z and all the stress terms appearing in the f vector are those stresses acting are acting in the y face. So, that is why we have tau y z, and similarly, in this, these are acting in the x direction x face. So, you have tau x x tau x y and tau x z. So, this is the kind of verification we can do. So, essentially what we have written here is that we have written the conservation equations, the four conservation equations in this form. So, now, is the discretizing this so that we can solve this. So, there are many methods for discretization we have seen many methods, and instead of looking at all the methods or a generic method, w will look at a specific method that has proved to be very popular and we will talk about the MacCormack method, and we will first see how it is applied to the one-dimensional case, understand it, and then, we will apply it to the three-dimensional case.