Computational Fluid Dynamics
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Lecture – 55
Formulation of Finite Volume Method

We are in a module 6, and we are looking at specifically the situation of flow through complicated geometries.

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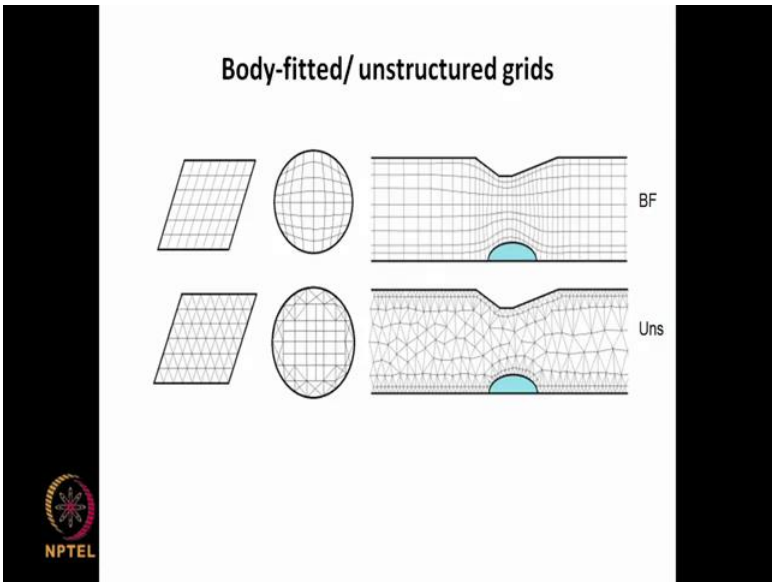

We are looking at the two possible ways of dealing with this one is the body fitted grid the other is unstructured grid.

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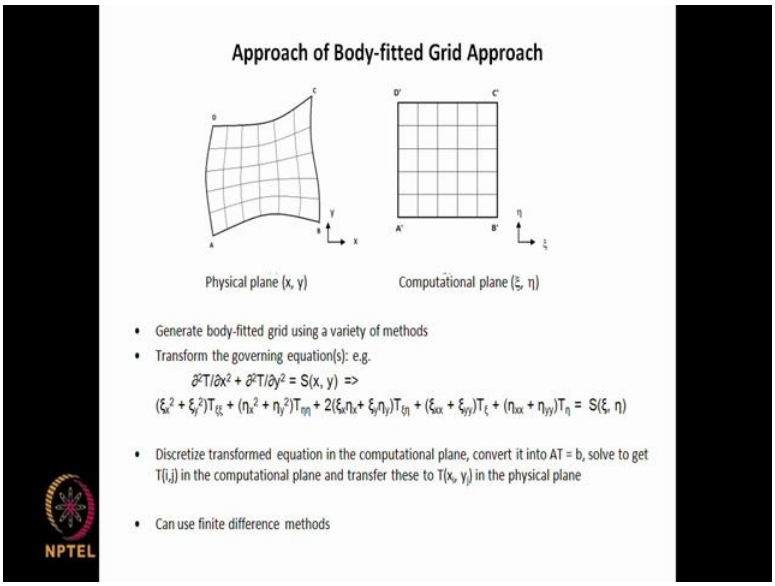

We saw in the previous class that if you were to use a body fitted grid then we would work in the computational plane where you have uniform grid spacing in both psi and eta directions. This psi and eta directions are such that lines of constant eta example this line will be a curvilinear segment here; and some of these boundaries here are such that they fit into the boundaries that are present in the physical plane.

So, instead of working with a complicated grid here like this, we are going to work with essentially Cartesian coordinate type of thing in the computational plane, but in the physical plane, these lines are not linear, they are curvilinear, which is why we cannot make use of the simple Cartesian coordinate system that we have used before.

So, we move into the computational plane, when we have where we have these Cartesian type of grid here, but as we move from the physical plane to the computational plane, the equation gets transformed into derivatives with respect to x and y from derivatives with respect to x and y, we have derivative with respect to psi and eta. So, this transformation is fairly easily derivable, and we have a transformed equation, which is then discretized using finite difference principles on a uniform mesh here.

And then, that gets converted into AT equal to B type of equation in the computational plane, solution of which will give us the values at the grid points in the computational plane. For every grid point in the computational plane, there is a corresponding grid point in the physical plane so that means, that we get the values at points which are

distributed throughout the physical plane computational domain and that is how we work with the body fitted grid approach. Generation as a body fitted grid is not trivial and that also will require some effort.

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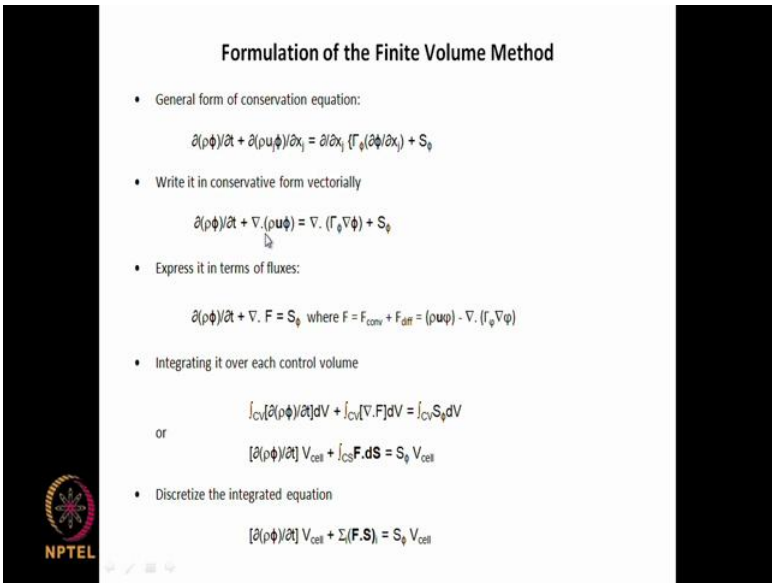

We are looking at we are taking a closer look at the other possibility which is making use of the finite volume method and dealing with complicated geometry in the physical plane itself. The formulation what we started with discussion with discussing last time; and in this lecture, we are going to look specifically at the formulation in the finite volume method for a any geometry for an irregular geometry especially. We have a governing equation as scalar transport equation containing the time derivative the advection term, the diffusion term and the source term. This equation is represented in the form of divergence of these advection and diffusion fluxes.

And finally, it is put in the form of flux dou phi by dou t equal to del dot f plus s phi, where s phi is a source term and f is the convective flux, and diffusive flux which are given by rho u phi minus del dot grad phi here. And we integrate this over each control volume in order to get an equation like this where we are assuming that phi has within that cell it has a constant value. So, we can write this as dou by dou t of rho phi times the volume of cell; and then integral of all these fluxes over all the faces of the control volume equal to the source term in the cell times the volume of the cell. So, this itself is discretized into i number of surfaces that envelop the control volume completely.

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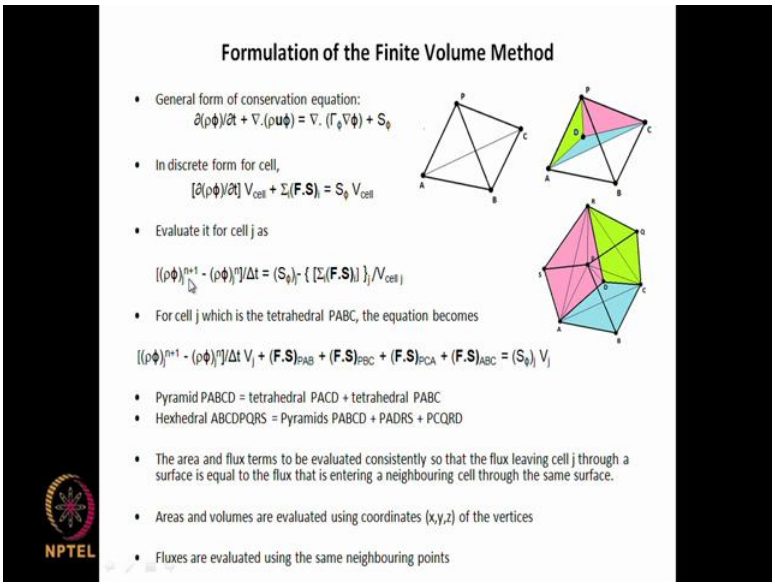

So, how does it actually work, we have the general form of the continuity equation discrete form is what we have just now shown. And if you evaluate it for cell j, and if you write this dou phi by dou t in this form, for example, using a first order in time forward in time, so the rho phi rho phi cell j at n plus 1 minus rho phi of cell j at n divided by delta t is dou phi by dou t for cell j. And you take the volume of the cell onto this side, and then so you have s phi for cell j, the source term for cell j, and we have taken this on to the other side minus sigma i sum over all faces of f dot s for the cell j divided by the volume of the cell j. So, this volume is being brought forward here.

For example, if you take this tetrahedral cell which has four triangles as the faces here. So, you have a bottom face which is A, B, C and then you have this face which is PBC another triangular face PAB and another triangular face PAC. So, it has four triangles has its four faces. So, for that, we can write this equation as rho phi j, this is cell j rho phi j at n plus 1 minus rho phi j at n divided by delta t times the volume of the cell j that is v subscript j plus f dot s over for the face PAB plus f dot s for cell side PBC plus f dot s for PCA plus f dot s for surface ABC. So, the over the four sides are equal to the source term s phi in the cell j times volume of cell j. So, this is the discretized form of the governing equation for a specific cell.

So, this is for a tetrahedral cell with four sides here. If you have a pyramid, so now, you have a pyramid is something which has a quadrilateral base and an apex P. So, you can

say that this quadrilateral pyramid can be broken up into two tetrahedral. So, you have this base ABCD quadrilateral, you join one diagonal here and you have two triangles quadrilateral ABCD is now composed of triangle ACD plus triangle ABC.

And if you now take join this thing with apex here then the pyramid is decomposed into two tetrahedral, and if have a hexahedron like hexahedral element, so it is like a rectangular parallel piped. So, you have ABCD here and then we have PQRS, PQRS here. And you join this; you have 6 faces like the blue face bottom and top, the pink face left and right, and the green face front and back.

So, this is a conventional cuboid kind of a control volume which have been considering. This can be broken up into pyramids, so you can take it broken up into three pyramids - p times with this as the base, p with the green one as the base and p with the pink one as the base. And each of these pyramids can be broken up into this tetrahedral and for each of this tetrahedral we have this discretization. So, we can write it in this particular way.

When you have the hexahedral element as the control volume then all these internal faces will not have to be included in the integration, this will just be the external faces which are enveloped in control volume are the ones which come here. If you take the internal ones they in the way cancel out, it is no harm, but this equation here this formulation is for all the control surface the surface, which is enveloping the control volume. So, in this case, there are six faces enveloping the control volume; and each of the faces is divided into two triangles, and you can extend this in a similar way into this.

So, if we now want to evaluate this, because in this case it is still not yet in a solvable form because we obviously have phi j n plus 1, but unless we know what this fluxes are, we are not in a position to evaluate this. This source term is something that needs to be specified and it needs to be evaluated. So, if you look at this, the things that are coming as things to be evaluated are obviously we need to know for each cell the volume and we need to know the surface area for of each of those for example, the triangles. And we also need to take the dot product with the fluxes. So, we need to know the orientation of these triangles and so and we need to evaluate the fluxes.

So, the area and the flux terms also they are needed to be evaluated consistently, and what we mean by consistently is we are looking at one cell, but your control volume is made up your computational domain is made up of number of cells. So, for example, if

you take this tetrahedral element this PAC triangle that surface is likely to be shared with a neighboring tetrahedral element or hexahedral element.

Now when you write this type of functional equation form, we are talking about a flux which is entering through the face or leaving through a face. Then when we talk about a flux which is leaving through this particular face, it has to go into the neighboring cell, and the amount going through into the neighboring cell must be the same as the amount which is leaving this; otherwise, we have a problem with consistency.

The consistency in the sense that if more is going into the neighboring cell then what this cell is giving, and then where is that extra flux coming, you will have spurious fluxes which are not really physically true. So, those fictitious fluxes need to be avoided and the only way to avoid that is to evaluate the fluxes in a consistent way at the discretization stage itself. And what we mean by consistency is that if there is a joint face, common face between two cells, then the flux leaving one particular control volume must be the same as the flux entering that particular control volume.

Now, how can we make that? If when we are evaluating flux through a control volume through a face for example, F dot S PAB is the flux, which is leaving through this particular face this has an evaluation of flux and evaluation of the surface area and orientation corresponding to this PAB. So, in the evaluation of fluxes and in the evaluation of surface for this PAB, if we make use of the same information for this cell and the neighboring cell in which this is shared, then and if you make use of the same formulas then we can make sure that the consistent evaluation of flux is there.

So, in that sense the consistence is something what we should do. So, in this sense, the areas and volumes are evaluated using the vertices that are that define this control volume and the control surface. For example, we have these four vertices identifying this tetrahedral element, and they also identify the individual areas here; and fluxes are evaluated using the same neighboring points. So, we will elaborate on this now, so that we have a good understanding of this.

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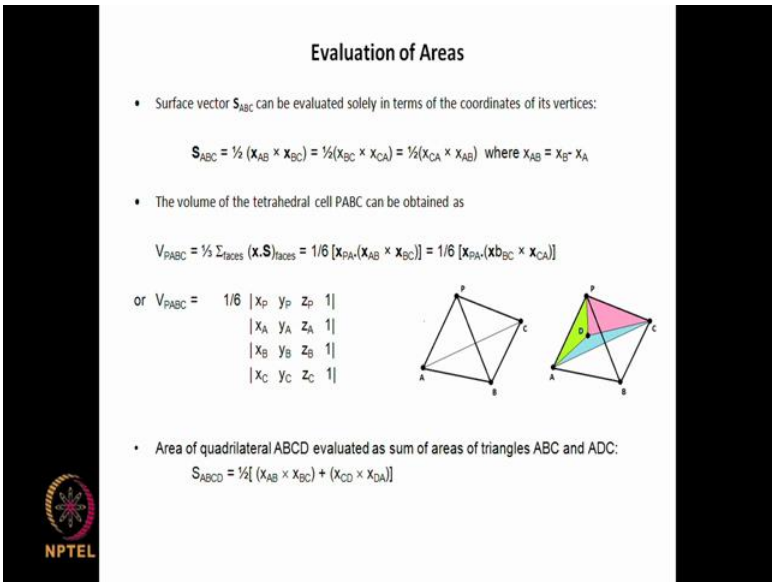

So, evaluation of areas surface area of vector S ABC can be evaluated solely in terms of the coordinates of its vertices. So, S ABC is given as half of the cross product of x AB and x BC, it is also the same as x BC and x CA. So, you can see that and x BC or x AB is x B minus x A, where x is the vector consisting of the three coordinates x, y, z coordinates of point B and x, y, z coordinates of point A.

So, this evaluation of the surface vector for the surface S ABC involves only the three coordinates. So, the when you are evaluating for cell j and the neighboring cell k, and if S ABC is a common surface then the same three points ABC will be coming there. And if you make use of the surface area making use of these formulas here then the area of that particular AB C surface is the same whether you evaluate it for this cell or for the neighboring cell. So, this becomes a consistent evaluation of the surface area vector in the form of this cross product of these vertices.

The volume of the tetrahedral element PABC that is this one can be evaluated as a one third of sum over the faces of x dot S face. So, this becomes one-sixth of x PA dotted with x AB cross x BC also x PA dot x there is a mistake here x BC cross product with x CA. So, again the point is we can make use of the coordinate points to evaluate the volumes. So, this is the determinant of x p, y p, z p, 1 and x a like this. So, you can see that if you know the vertices of the tetrahedral element, we can compute the corresponding area here.

And similarly, if you have a quadrilateral as a face then the quadrilateral can also be evaluated in terms of x AB cross x BC plus x CD cross x DA. So, if you know the coordinate positions x, y, z of the four corners, then you can and if it is a triangle you can make use of this; if it is a quadrilateral, you can make use of this; if it is a volume, you can make use of this. And you can evaluate all these things from the vertices only. So, if you do this then for whatever cell you are evaluating these things for the same vertices, which are making up that particular plane or that particular surface or particular volume, you will always have the same surface area vector and that is necessary for the for a consistent evaluation of the fluxes.

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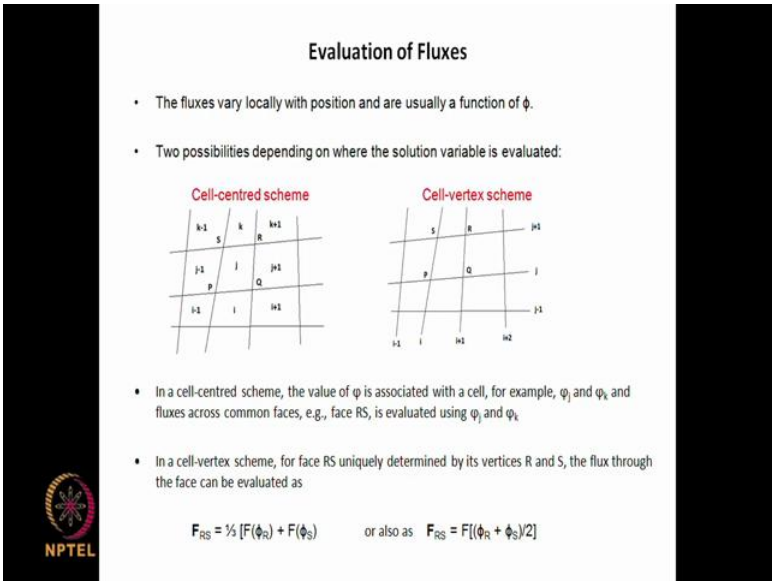

Now, flux is F dot S, we have seen how the surface area vector can be evaluated from the coordinate positions of the vertices. Now how can we evaluate the fluxes and fluxes very locally with position and they are usually function of phi.

For example, if you are looking at the fluxes you have the advective flux which is rho u phi, and the diffusive flux which is a function of the gradient of phi, so that means, that diffusive flux depends on the phi itself the gradient and the advective flux also depends on phi. So, when the function f itself is the flux itself is a function of phi, then if phi is changing from position to position, then how can you make use of a consistent evaluation, how can you do a consistent evaluation because for cell j phi has some value for cell m you have a different value. So, there is a possibility of inconsistent evaluation.

So, here especially in the finite volume method, we can have a cell centered scheme or a cell vertex scheme, where a cell you are breaking up it into number of cells, and you can say that a cell value is characterized by the value at its center geometric center or whatever center. And throughout this cell you have the same value that is a cell centered scheme. A cell vertex scheme is where a cell is characterized by the vertices, for example, the PQRS, and the value of phi at PQRS at these four corners can change, it changes and any value anywhere in between is to be obtained by interpolation.

So, in the cell vertex scheme, you are saying that I am evaluating the cell the value of the variable at these corners PQRS. In a cell centered scheme, you are saying that I am evaluating a value for this cell, if I need to know the value at SR PQRS then I will get by interpolation from these cell values cell centered values. And here you are saying that I evaluate the variable value only at this vertices if there is any need for any evaluation of phi at any other point, I do by interpolation.

So, in a cell centered scheme, the value of phi is associated with the cell, for example, phi j and phi k here. And a fluxes across common faces, for example, you have R, S is a common face for cell j and cell k. So, the flux through this is evaluated using phi j and phi k, which is on both sides of which are the cell values which are in the two adjacent sides of this.

In a cell vertex scheme, if you want to determine the fluxes, then it has to be evaluated using the values, for example, if you are looking at a cell vertex scheme, where you know the very well value at R and S, then you can say the flux through this R, S is evaluated as one-half, it should not be one-third, one half of the flux value based on phi of r and phi of s. Because in general flux varies with phi so that means that if it is the flux evaluated based on the value of phi here is different from the value flux evaluated from this.

So, you take the average of these two to be this. And something like this will require two evaluations of fluxes. So, you can say that instead of that I will take an average of phi here phi r and phi s and use that average value of the variable here in the flux expression to evaluate this. So, you can have either of these formulations. So, the point that we are making is that flux depends on the value of phi; and in a computational domain phi will

vary specially, so that means, that phi for this cell is different from phi for this cell; phi from this vertex is different from the phi from this vertex.

In such a case, how do you evaluate consistently the surface fluxes through the face? So, that something that and something like this either making use of the two vertices that together define this surface in this case; and in this case, the two cells which share this common face if you make use of those things to evaluate that then it will be correct.

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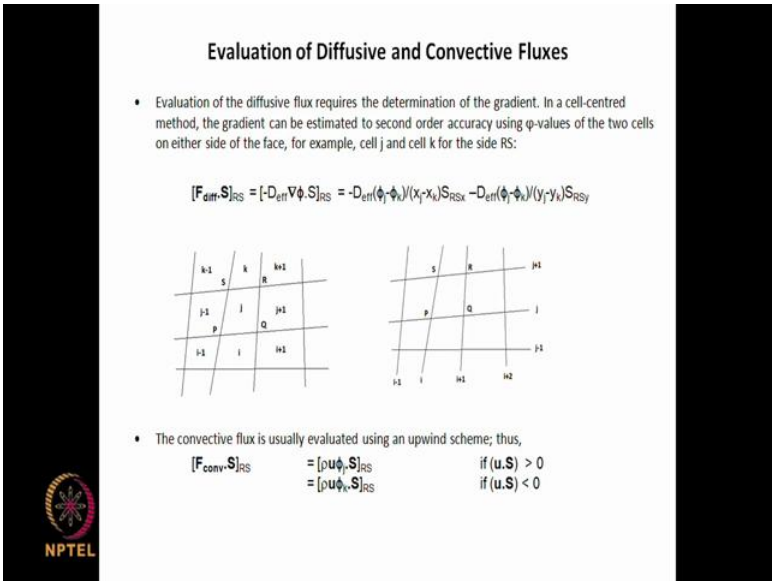

So, there is another aspect to fluxes, fluxes have the diffusive component and the convective component. Diffusive component will introduce the gradient of flux; convective components will involve the value or the flux itself, the absolute value of the flux and not the gradient. Now how do we do this? The diffusive flux requires the determination of the gradient in a cell centered method like this; the gradient is evaluated using the cell value here and the cell value here.

For example, the diffusive flux of f dotted s can be given as minus D effective that is the diffusivity times the gradient of phi dotted with S, you know how to evaluate this S; we are looking at how to evaluate the gradient here. How to evaluate the gradient, in such a way that, it is consistent? So, we are saying that because we are evaluating this thing here and because we know the value of phi at this point and value of i for this cell then we can say that gradient of phi is phi j minus phi k divided by x j minus x k. So, times S RK, component of the surface vector and diffusivity times phi j minus phi k times y j

minus y k this is the coordinate here times the y component of this. So, this is this can be used for evaluation of the diffusive flux.

Now, for the convective flux is usually evaluated using upwind scheme. So, as to not to have the problem of artificially numerically induced oscillations. So, convective flux can be over this face RS is given as rho u phi j dot S RS, where phi j is the cell value here if u dot S is greater than 0. So, if flow is going in this direction which is given by u dot S being positive then you takes the convective flux which is rho u phi you take the value of cell value of phi here. If u dot S is negative, so that the flow is coming in this direction then you take the phi k value here. So, if you do this then again you have a consistent evaluation.

So, we have seen how to evaluate the convective flux over a particular face, and how to evaluate the diffusive flux over a particular flux. And we have also seen how to evaluate the surface area vectors, and the volume of the cell. And if we put all those things together, then we will be able to fill all these four things. Again depending on the source here we can again need to make a consistent evaluation here and then that will give us the right hand side term. So, now, you can put this as phi i j n plus 1 is equal to this whole thing take into the right hand side; and phi i j n plus this whole thing and then you will be able to evaluate phi j n plus 1, and then you can move on like this.

So, this is a generalized finite volume method. A generalized finite volume method talks about variation of phi in a particular cell of any arbitrary shape. We are looking at a cell shape which is bound by linear segments in case of 2-D, and by plane segments in case of 3-D. For example, this is a plane triangular segment here, this is a planar quadrilateral segment, it is not necessary for this ABC triangles ABC and triangles ADC to lie in the same plane with this particular thing; in general we may have this ABCD as a as being one plane.

But in real complicated geometries ABCD can also be a points ABCD may not be coplanar, but we can divide this into two triangles in such a way that ABC is one plane and the ACD and it is another plane and we can evaluate the volume of that using this formula here.

So, in all these cases we are writing the conservation equation as change in rate of change of the particular variable value of phi as a result of the net flux going through the

bounding faces and as a result of any sources of phi lying within the control volume. So, with this, we can write a generalized form and by evaluating each of these fluxes and areas and all that we can come up with an overall formula in which the phi value at a particular cell is affected by the neighboring values through the fluxes and you can see that you have phi r and phi S.

So, those are phi j and phi k are coming here, and then here also phi j and phi k are coming here. So, these bring in the influence of the neighboring coefficients and you will end up with a compact computational molecule where the value of phi j is influenced by the value of the neighboring cases, neighboring cell values as in the cases that we have seen earlier.

So, this is the general formulation of the finite volume method. And this is applicable for any arbitrary shape thing. What we need to do more is that we should be able to describe that general irregular shape and computational domain in terms of quadrilateral hexahedral elements or pyramidal elements or tetrahedral elements. If you do that over each of those elements, we can then apply this formula here and then we can get a value of we can get an algebraic expression for the cell value in that particular cell in terms of the neighboring cell values. So, we will able to convert this equation into something like a phi equal to B for this.

All it now requires is how to find this vertices how to make it, how to make up, the how to divide the control volume into small number of a bricks of these kind of a planar and a hexahedral shapes, so that is part of the grid generation. So, we are going to next class look at some generic approaches for the grid generation as part of which you will be identifying the vertices or the points that which you would like to make the evaluation of the variable values. So, and we are going to look primarily 2-D, because that is something that can be easily followed.

So, we are going to look at generic algorithms, which can break up an arbitrarily shaped computational domain into small cells, and since we are looking at 2-D and since we are found of these triangles, we are going to look at triangulation of an irregular geometry into small number of triangles. So, if we can do that then essentially we are set because from those triangles and from those vertices, we can come back here and make up volumes, we can make up planes, and we can make up hexahedral elements, and once we

make that up then we can go ahead and solve the cell value here. So that is in the next class.

Thank you.