Computational Fluid Dynamics

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Lecture No. # 39

Unstructured Grid Formulation (Contd.)

We started with our discussions on unstructured grids in the previous lecture and we will continue with that.

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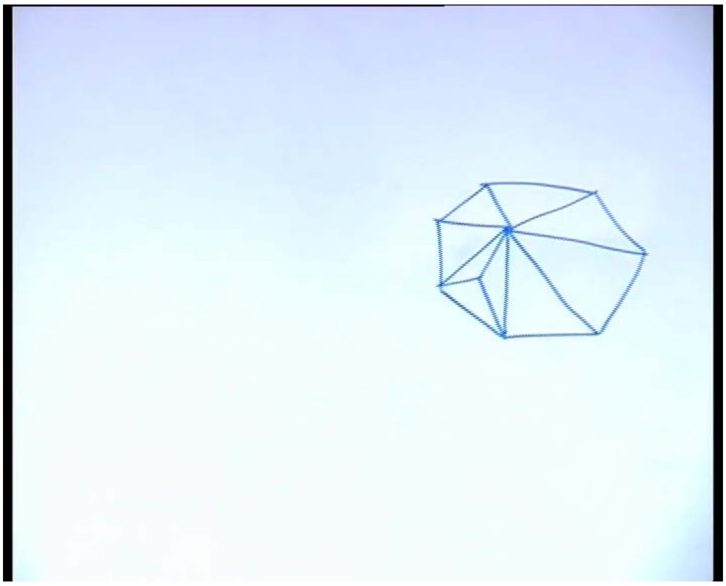

So, what we mentioned is that if you have an unstructured mess, then in an unstructured mess, it is convenient to represent complicated shape domain boundaries with various shaped elements. Here we have shown in an example, a triangular shaped element, but it is possible to use several shapes and the peculiarity is that, the specific characteristic is that one vertex may be connected to different number of neighbouring vertices. So, it is not that one vertex is connected to a fixed number of neighbouring vertices.

Now, there are several shapes of elements that are possible or several shapes of the control volumes that are possible. What we will try to do is to see through an example and demonstrate through an example that how to first generate good quality mess in an unstructured environment and for that, we will assume a triangular shaped mess.

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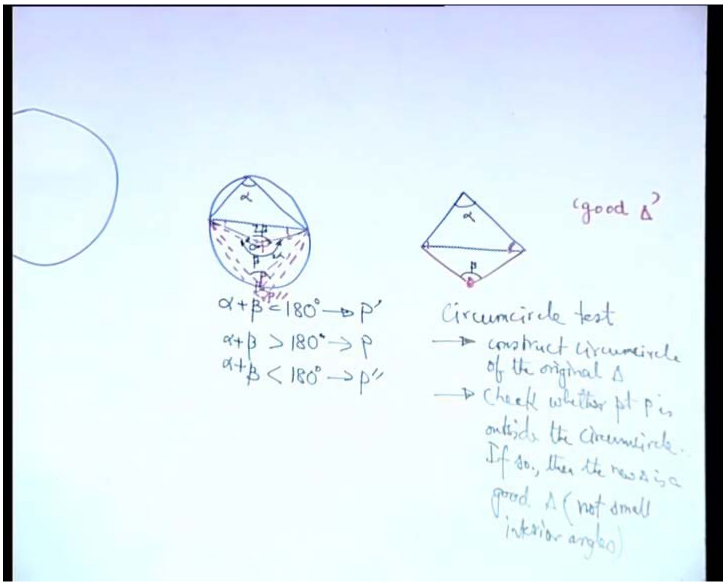

So you have a domain like this or let us take a domain even like this one, which is a regular shape domain. It may be a regular shape domain like this or it may be a regular shape domain like this. Our objective is to divide such domains into a number of sub-domains which are of triangular shape. Now, a systematic way of doing that is called as triangulation. So, how can you do a triangulation? Let us say that you take any point within the domain. Then, say you connect the point with all the corners. So, you get some triangles.

Next to get new triangles. So, this is not the finest quality mess that you are looking for. So, you need to refine it further. So, what you need to do? You need to insert new points and may be, generate new triangles. In this way, one could arbitrarily generate a large number of triangles out of a given domain shape. The question is once these triangles are generated; do these triangles generated in arbitrary manner work? The answer in no. Any arbitrary triangulation will not work. So, any arbitrary triangulation like this without looking into certain aspects will not work for a good quality mess.

Let us see that what are the conditions that we are looking for a good quality mess with triangles and what are the characteristics of the triangles that are necessary for that. So, let us say that you have already a triangle like this which you assume that is a good quality triangle. Your next objective is to insert a point, so that you can generate a new triangle. So, given an existing good triangle, we will later on see that what is a good triangle or a bad triangle. So, given an existing good triangle, we are looking for a point to be inserted somewhere, so that a new triangle is generated which should be good. What is the characteristic of goodness of a triangle? Goodness of a triangle will imply that the interior angles are not very small. Again question is what is small and what is large. That we have to quantify. So, to do that one possible check is like this.

You consider a circle which is the circum circle of the original triangle. Now, you are inserting a point say P here. Clearly if P is very close to the base of the previous triangle, then you can see that the interior angles will be small. One limiting case is that P is located on the circumference of the circle. So, let us let us consider that limiting case when P is located on the circumference of the circle. If it is located, let us call it P prime. Now, let us say that we have certain angles. Let us call this angle as alpha which is this angle in the figure and this angle beta. In this figure what is alpha plus beta? 180 degree.

So, we can quickly check it. So, if you consider this as the centre of the circle, so angle at the centre is twice the angle at the circumference. So, this is 2 beta. Similarly, this angle is 2 alpha. So, 2 beta plus 2 alpha is 360 degree. So, alpha plus beta is 180 degree. Otherwise, it is a cyclic quadrilateral. From that also, it follows. So, given the angle alpha, alpha plus is equal to 180 degree for the point P dash. Then, for the point P, what is alpha plus beta greater than 180 degree or less than 180 degree? Greater than 180 degree because you can see that if you bring the point inside this angle beta, this angle increases. For a particular alpha, this angle beta increases. So, if for the point P dash it was alpha plus beta equal to 180 degree, for the point P, the beta will be greater than the case with p dash. So, that will be greater than 180 degree.

Similarly, if you consider a point P double dash which is outside the triangle, outside the circle, then this angle will be the new beta. So, alpha plus beta will be what? Less than 180 degree for P double dash. Now, in which of these cases you expect the interior angle of the new triangle to be the smallest one-for P, P dash or P double dash. For the point P because the angle beta is large or largest as compared to the 3 cases. You expect the other interior angles to be small because some total of the 3 angles of a 3 triangles is 180 degree. See one of the angle is large; the others will be very small.

So, what we can see is that if you do not want the interior angle to be small, you can create a smallness or largeness criterion by considering that if you have a triangle, you draw a circum circle, you insert a point. The point P should be inserted in a way that it is falling outside the circum circle of the original triangle. Then, the corresponding triangle, new triangle generated is a good triangle. This is called as a circum circle test. So, in a circum circle test, what you do?

Construct circum circle of the original triangle, check whether point P is outside circum circle. On the circum circle is a limiting case. On is also, on may be also considered as a outside, but in general, check whether point P is outside the circum circle. If so, then the new triangle is a good triangle. So, good triangle will imply that not small interior angles. Why do not you allow small interior angle? Because if you allow small interior angles, then the corresponding coefficient matrix that is generated out of the discretization does not behave properly. So, you try to ensure that through the geometrical considerations, you get rid of unnecessary troubles associated with coefficient matrix of certain types.

Now, how do you assess this criteria? Obviously, every time you do not draw a circum circle and check. So, to assess the criterion, you go for this alpha plus beta criterion. So, you check whether alpha plus beta is less than 180 degree or not. That is possible by coordinate geometry because you are given the coordinates of different points. Because you are given coordinates of different points, you can find out angle between 2 lines using the coordinates of the end points. Like for example, if this angle is alpha and if the slope of these 2 lines are M 1 and M 2, then alpha equal to M 1 minus M 2 by 1 plus M 1 M 2. Plus or minus depending on the sign. So, based on that, so for that to know M 1 and M 2, you require to know the coordinates of the end point, so that you know slope of the lines forming the triangle. So, if you know the coordinates of each point of that each vertex of the triangle and also the new point P, then it is possible to find out the angles alpha and beta from that and then check.

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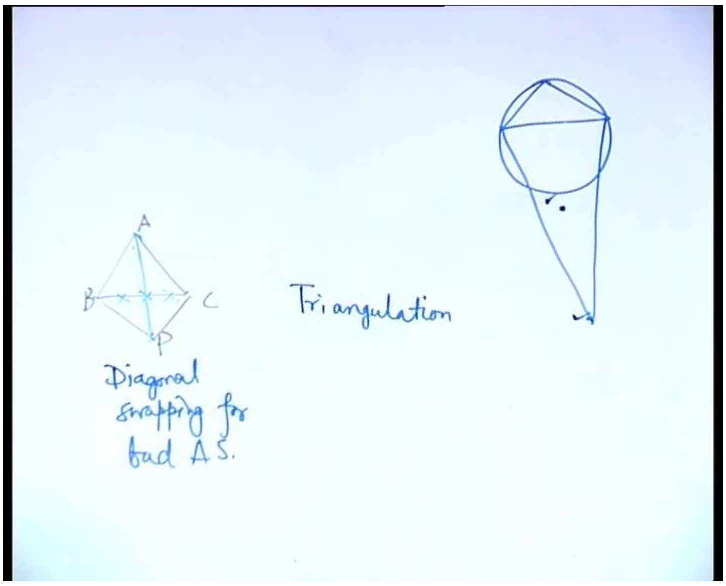

Now, if the check is not successful, then what? So, let us say that you have had a triangle A B C. Now, some what the point P has come. You have formed a new triangle and then, you have made a check whether the triangle B P C is good triangle or a bad triangle. Let us say that the result has come that it is bad triangle, that is, it has failed a circum circle test. Then, what? If it has passed, then it is fine. Always we have to keep in mind that it would have happened if it has failed. If it has passed, it is fine. It should not be a problem. So, if it has failed, then what would you do? Then, one of the easy thing that one can do is instead of making this as a diagonal of a quadrilateral; we would make this as a diagonal.

So, if somehow these angles were small, these angles will be large. So, this is called as diagonal swapping. So what you do is when you consider the new point P introduced, you will have a quadrilateral generate A B P C. It has a common line B C shared between the two triangles, that is, one of the diagonals of the quadrilateral. If the new triangle is a bad triangle, you swap the diagonal. So, what you do is, you do not consider B C as the line, but you consider A P as the boundary line, so that you get two new triangles, A B P and A P C.

If the previous triangle was bad, then these triangles will be good because with the swapping of the diagonal, small internal angle will become a large one. So, this is called as diagonal swapping. So, diagonal swapping for bad triangles. So, these are certain remedial measures. So, this entire process of systematically ensuring that you get good triangles is known as delaunay triangulation.

Remember that next generation is actually a fundamental topic related to computational geometry. So, these are not topics intrinsic to solution of transport equations, but these are auxiliary things which are necessary for good solution of the transport equations, but this fall more into the category of computational geometry. So, if you are more interested in learning this, refer to any book on computational geometry, where you will get more details on delaunay triangulation for example. Here in this particular scope, particular course, we do not have extensive scope of going into the details of computational geometry, but do keep in mind that certain considerations of computational geometry are important for generating good quality measures. How to generate good quality triangles is just an example which we have just highlighted.

Now, next is, let us say that we have generated triangles. We can consider your question is whether we can consider any point far away from the circumference. You will essentially you will never do that. You will never do that because you will let us say that this is the, sorry let us say that you have triangle like this. In principle you can but, you will never do that because what you are doing then is you are keeping a large zone where you are having only single triangle. So, you will try to fill it up with many smaller triangles and therefore, you will not take in one shot away of a large triangle like this, but may be break it up into steps, where each step will confer to a point which falls outside this.

In reality, neither take this point nor take this point. In reality, you take the point arbitrarily. So, it may be at a large distance. No problem. Why? Because even if it is at a large distance, you are not scared of in having a large triangle because you may divide it again into small triangles. So, the thing is the circum circle is not initially there in your mind, you have a triangle. You just insert an arbitrary point and then, make the circum circle test. If the test satisfies, it is fine. Whether it is very close or very far away does not matter because if refinement is required, that you can always do. So, once this point is located outside the triangle, it is fine and once it is inside, then you can make the diagonal swapping to make it alright. So, either way. If it is outside, then straight away it is fine. If it not outside, the diagonal swapping will make it fine.

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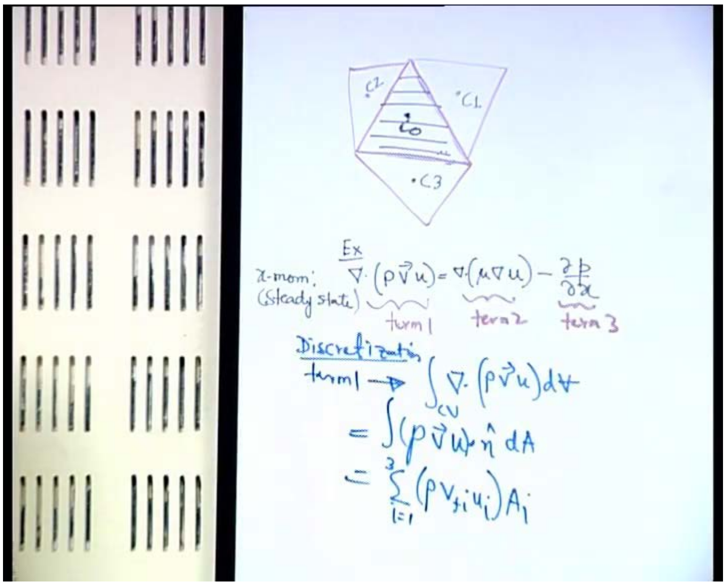

Next issue. Once we have these triangles, how to discretize the governing differential equation based on these triangles? So, let us say that, let us consider that you have triangle like this. Let us draw it somewhere else. Let us say that you have a triangle like this. In discretization we have seen that a control volume, this triangle is a control volume. Till now in structured grid, we have considered rectangular control volumes. Instead of that, just consider that you have a triangular control volume. One control volume is influenced by whom? It is influenced by the characteristics or the transport phenomenon occurring across its neighbours at the most, but not beyond that. So, you can consider how many neighbours? You can consider 3 neighbours. Each neighbour is a triangle with base as one of the sides of the original triangle. We can name the grid points. The grid points for convenience you can choose as the centroid or geometric centre of each triangle. So, this is say C 0, this is C 1, this is C 2, this is C 3.

Now, we have to see that when you are considering the transport equations, how to discretize the transport equation with this as the main control volume and the others are neighbouring control volumes. So, what equation we need to discretize? I mean we can give several examples. Let us take an example that we want to solve the naviest of equations in a steady form.

So, x momentum equation as an example, steady state. The unsteadiness, how it is discretized? It is discretized in the same way. Unsteadiness does not depend on the shape of the control volume. It is a time domain; it is not a special domain. So, that is why we do not want to unnecessarily complicate it by putting an unsteady term. You put an unsteady term and it is discretized in the same way as what we do for structure grid systems. For the special discretization unstructured and structure will differ. Let us see that how do they differ. Let us say that we want to solve x momentum equation, where u is the x component of velocity and p is the pressure, mu is the viscosity and v is the velocity vector for which u is just a component along x, v is component along y and w is component along z.

Now, we can discretize different terms. Let us just do it term by term. Let us call this as term 1, this as term 2 and this as term 3. So, what is the first step that we you follow in the finite volume method. Integrate the governing equation over the shaded control volume. So, let us try to do that. Discretization of term 1. Integral where the control volume is the shaded triangle. So, what will be this?

Where eta is the direction normal to the surface. So, this triangle has how many surfaces, bounding surfaces? It has three bounding surfaces. So, each surface will have a direction normal and we have used the divergence theorem to convert that volume integral into the area integral. Therefore, we can discretize this as sum of rho into v f i, where what is v f. V f for face. So, when we say surfaces in computational geometry, they are more appropriately known as faces. So, you have three faces of these triangle.

So, through each face, you have a velocity normal component of velocity. What is that? v dot eta d a, that is v f i, u we are keeping as the same v dot eta d a is a v f i into a i. So, you can keep different. The nomenclature is not important. You can use different names. What we are basically doing here? We are writing the normal component of the velocity across each face as v f i that multiplied by a i is v dot eta d a integral over that face and for each face, i we are having the corresponding u as u i and rho remains rho and we have did for three faces. This is just one way of representation of this particular term. This term may be represented in several ways, but this is just one way of doing that, ok.

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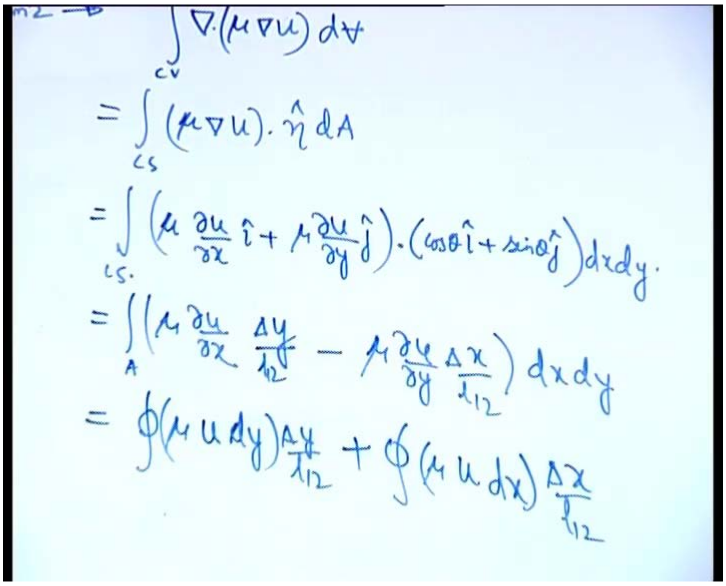

Now it is not difficult to represent this term. It is bit more integrate to represent this term 2. That we will see now. This integral of d v will be by divergence theorem. So, what is a eta? For example, let us let us give some numbers to indicate the vertices of this triangle say, 1 2 3. So, if you do that, then this is the edge 1 2, which is a face. If you consider the triangle as a volume with unit width, then this is the normal direction. Let us say that the coordinates of 1 are x 1, y 1, coordinates of 2 are x 2, y 2. So, let us try to describe the unit vector, unit normal vector eta in terms of these coordinates because the coordinates are the information that you have in your hand. Let us say that this angle is theta, so that this angle is theta. So, angle between the vertical and 1 2 is theta, so that angle between the horizontal and eta is also theta. Remember eta is perpendicular to 1, 2. So, the eta in a vector form is cos theta i plus sin theta j, where i and j are unit vectors along x and y.

Now, from the right angle triangle that we are, we can form, we can make out that what is cos theta. Cos theta is in terms of the y coordinates. What is cos theta? Y 2 minus y 1 by the length of 1 2. So, let us call that the length of 1 2 is l 1 2. That is the length of the edge. So, y 2 minus y 1 by l 1 2. So, in short hand, let us call it delta y by l 1 2, where delta y is y 2 minus y 1. What is sin theta? Sin theta is x 1 minus x 2 by l 1 2. This is x 1, this is x 2. So, the difference between 1 and 2 is x 1 minus x 2. These are positive x direction. So, this is equal to minus delta x by l 1 2 if delta x is x 2 minus x 1. By short hand symbol, delta y is y 2 minus y 1 and delta x is x 2 minus x 1. Now, you can expand this integral as mu, grad u is del u del x i plus mu dot with what is eta cos theta i plus sin theta j. D a is like d x d y. Remember that d a is equal to d x d y. That is fine but, we have to keep in mind that that elemental area is located on each of the faces. It is not inside the domain. It is located on the faces which which are boundaries of the triangle.

So, mu del u del x into cos theta delta y by l 1 2 minus mu del u del y delta x by l 1 2. Now, these are area integrals. We can convert this area integrals into line integrals. So, first we converted the volume integral into area integral. Then, next step will be to convert the area integrals into the line integrals. That we can do by using Green's theorem. So, let us write that somewhere.

So, the contour integral of f d x and g d y, where f and g are two functions is same as this area integral, where this contour is bounding this area a. Now, this contour is around the area. This contour is a line. It is a line which is around the area a or completely encircling the area a and this is equal to del g del x minus del f del y d x d y. So, if you consider this g here as u and f equal to 0 as one of the examples, so g equal to u f equal to 1. So, this will become del u del x d x d y, like del g del x d x d y is contour integral of g d y. So, g is equal to u. So, mu u d y that times delta y by l 1 2. This is one contour integral.

Then, for the next one minus del u del y is like minus del f del y. So, u equal to f equal to u and g equal to 0. So, that will give you contour integral of f d x, that is u d x. So, we have now converted all the integrals into contour integrals, a line integrals. So, what are these contours? Let us now consider what these contours are.

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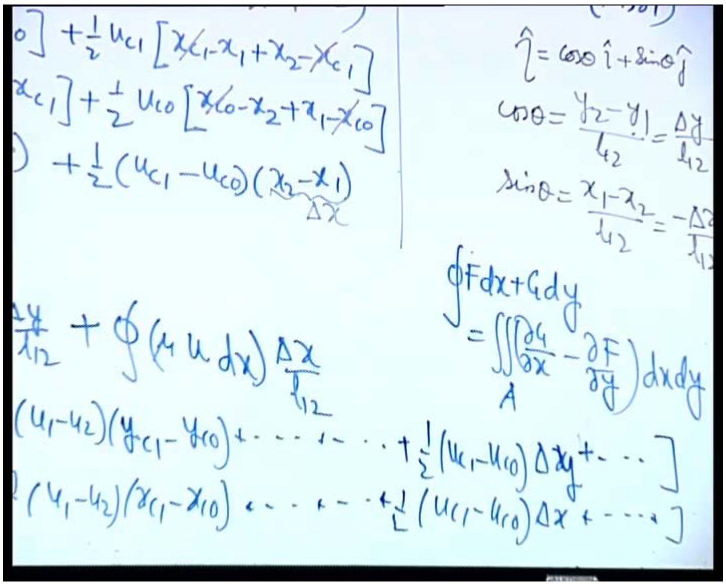

Let us just draw the triangle again 1 2 3. C 0 there are points, c 1, c 2, c 3. So, one of the area integrals is considering the area of the face 1 2. So, you have to consider, you have to construct a contour that totally encircles 1 2, right. So, there are many ways in which such such a contour can be taken. One of the ways is like this.

See this is a contour which totally encircles 1 2. This is one of the examples and it is a convenient example because by constructing this contour, you consider only those points which form the geometrical basis of the triangles and their neighbours. The second important thing that we have to keep in mind is that because directions are important, we have to give orientation to edges. So, when you consider a closed contour, you start with a point 1 and travel the contour in a counter clock wise direction to end up at 1. So, when you evaluate a contour integral, the direction in which you are moving for evaluation of the integral is important.

Now, let us try to write what is integral of say, u d x over this contour. Now, there are 3 such contours. One is for the edge 1 2. So, for 1 2, another for 2 3, third for 3 1. So, we are just giving example for one edge considering that similar thing can be written for the other two edges. So, for edge 1 2 integral of u d x. What is that? Of course, you have to keep in mind that u is not known as a function of x. That is what you are interested to solve for. So, you have to make a numerical approximation of this integral. So, let us say that you have some u as a function of x that you numerically approximate. So, you can use any rule for numerical integration for doing that.

One of the simplest, but not so bad rules is a trapezoidal rule for numerical integration which we will demonstrate through example. You can use Simpson's rules or whatever. Any of the Quadrature rules also that you can use, but just for simplicity in demonstration, we will consider the trapezoidal rule for numerical integration that can be used here. So, for doing that what we are doing? We are piecewise we are considering that this profile is a piece wise linear profile and for each piece, the integration is represented by the area under the corresponding trapezium. Area of each trapezium is half of sum of the use into the distance into the x difference between the two.

So, here from 1 to c 1, let us say this point is 1, this point is c 1. So, what is the first area? Half into u c u 1 plus u c 1 into x c 1 minus x 1. That is the first area. Then, after c 1, the next point is 2, then the point c 0. That is all. Here, there is no other point and from c 0, there is 1. So, this is the first area. Then, the second area is half of u c 1 plus u 2 into x 2 minus x c 1 plus half of u 2 plus u c 0 into x c 0 minus x 2 plus half of u c 0 plus u 1 x 1 minus x c 0. You can simplify this. Let us say, you take common half u 1 x c 1 minus x 1 plus x 1 minus x c 0. This is u 1. Then, u c 1 x c 1 minus x 1 plus x 2 minus x c 1 plus u 2 x c 0 minus x 2 plus x 2 minus x c 1, then half u c 0 x c 0 minus x 2 plus x 1 minus x c 0.

So, we have just isolated the velocities from different terms. So, certain terms will get cancelled out. So, you can write half into u 1 minus u 2. You can take common, then it will be x c 1 minus x c 0 plus half u c 1 minus u c 0 into x 2 minus x 1. So, this by your notation is delta x. So, similarly, there will be contour integral of u d y. Remember this is for edge 1 2. So, you have u 1 minus into u 2 into this. Then, there will be some u 2 minus u 3 plus u 3 minus u 1 for the other 2 edges. So, similarly, how many total terms will be there? So, these 2 terms for each edge. So, there there will be totally 6 terms. I am not writing each and every term. You should be able to write other terms based on one term for one edge. It is just very very similar. There is no difference at all.

So, finally, when you write this term 2 in its integrated form, then what you get? So, mu delta y by l 1 2 into contour integral of u d y. So, half into u 1 minus u 2 into x. In place of x, it will be y into y c 1 minus y c 0 plus 2 other terms plus half into u c 1 minus u c 0 into delta x, sorry delta y plus 2 other terms. Similarly, for integral u d x, just replace x with y. So, mu delta x by l 1 2 into half u 1 minus u 2 into x c 1 minus x c 0 plus 2 other similar terms. Then, plus u c 1 minus u c 0 into delta x plus 2 other terms.

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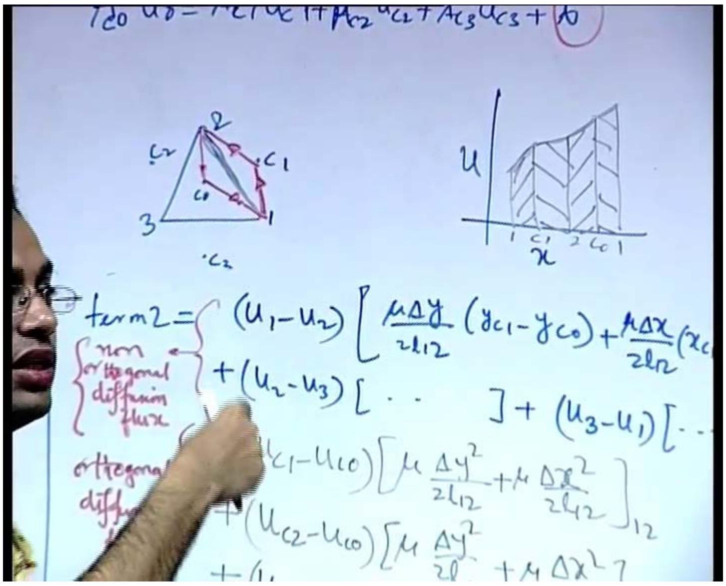

So, term 2 you can write. You can take u 1 minus u 2 as common that, then you have mu delta y by 2 l 1 2 into y c 1 minus y c 0 plus mu delta x by 2 l 1 2 into x c 1 minus x c 0 plus similar terms with u 2 minus u 3 into something similar to this, not same, but similar plus u 3 minus u 1, this one. So, this is one type of term. Then, the other type of term plus u c 1 minus u c 0 into mu delta y square by 2 l 1 2 plus mu delta x square by 2 l 1 2 for the edge 1 2 plus u c 2 minus u c 0. There will be a similar term for example, if it is very convenient to write it delta y square by 2 l, what will be this? l 2 3 plus mu delta x square by 2 l 2 3 of the side 2 3. So, this delta y corresponds to y 2 minus y 3. This delta x corresponds to x 2 minus x 3, sorry x 3 minus x 2 and this is y 3 minus y 2. So, delta y for 1 2 is y 2 minus y 1. So, delta y for 2 3 is y 3 minus y 2. So, we have to follow that order. Similarly, plus u c 3 minus u c 0.

Essentially, what we are writing by term 2 is nothing, but diffusion flux, right. What you can see is that diffusion flux has two different categories. One is this category, where the diffusion flux is driven by the difference in value of the properties of the neighbouring grid points like this is u c 1 minus u c 0. Similarly, u c 2 minus u c 0. Then, similarly, u c 3 minus u c 0. So, this is just like the structure grid formulation, equivalent. Not exact, but conceptual equivalent where the diffusion flux is proportional to the difference in the variable difference in the values of the neighbouring grid points. So, this we call as orthogonal diffusion flux and interestingly, the diffusion flux also has components which are not driven by the difference in values of the neighbouring grid points, but difference in values of the vertices. This we call as non-orthogonal diffusion flux.

So, if it was a structured grid, only the orthogonal type of diffusion flux would have been present, but because of unstructured grid, the non-orthogonal flux terms arise. Then, there is a pressure gradient term. Let us quickly see how we can discretize the pressure gradient term. If we want to make use of the divergence theorem, what we can do? We can write this as divergence of p i, right. So, we can write this as minus of divergence of p i d v and for this, we can write it in terms of the corresponding area integral. So, minus of p i dot eta d a and i dot eta is cos theta. So, minus integral of p cos theta d a. Each edge has a constant length. Cos theta is delta y by l 1 2 for edge 1 2 and sum of the total d a is l 1 2. That l 1 2 gets cancel from numerator and denominator. What is the net P? So, consider this surface 1 2. From this side, you have the pressure p c 1 acting and from this side, you have the pressure p c 0 acting. So, it is the net pressure on 1 2 is p c 1 minus p c 0.

So, this you can write as minus p c 1 minus p c 0 into delta y. This is for edge 1 2. Similarly, you have p c 2 minus p c 0 into delta y 2 3 plus p c 3 minus p c 0 delta y 3 1. So, this is how you discretize the pressure gradient term. So, what you see is that the structure of discretization is again the same. You still, you are again having a 0 c 0 is equal to a 1 c 1 plus, sorry not c 0 u 0, a 0 u 0 is equal to a 1 or a c 0 u c 0 better to say is equal to a c 1 u c 1 plus a c 2 u c 2 plus a c 3 u c 3 plus b. You can see that why this b term is necessary. Even though there is no source term as such, one is to accommodate the pressure gradient term. Other term is to accommodate the non-orthogonal diffusion flux.

In the non-orthogonal diffusion flux, you have u 1, u 2, u 3 instead of u c 1, u c 0, u c 2, u c 3 like that. So, this term you dump it in the form of the source term. So, the non-orthogonal diffusion flux, this is one of the key steps, that is the non-orthogonal diffusion flux, you do not consider separately, but dump in the form of the source term. Then, when you have u 1, u 2, u 3 like that, you can interpolate these values based on the values at c 0, c 1, c 2, c 3 just by using some interpolation technique, but those terms you do not consider in the main terms and you write that in the form of a source term. That is the first thing.

The remaining terms get structured in the general convection diffusion formulation and you can use the convection diffusion formulation that we have learnt in our previous lectures. To write that, combine advection and diffusion flux. So, here you have the advection flux, here you have the orthogonal diffusion flux. You can combine the advection flux and that orthogonal diffusion flux to write the convection diffusion coefficient. That we have done for the structured grid also.

So, we have studied what is the difference and what is the similarity in conceptual paradigm for discretization of the various governing equations in an unstructured grid formulation as compared to the structured grid environment. We stop here today. Thank you.