Introduction to CFD
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Lecture - 53
Basics of Interface Capturing Methods for Application in Multiphase Flow (continued)

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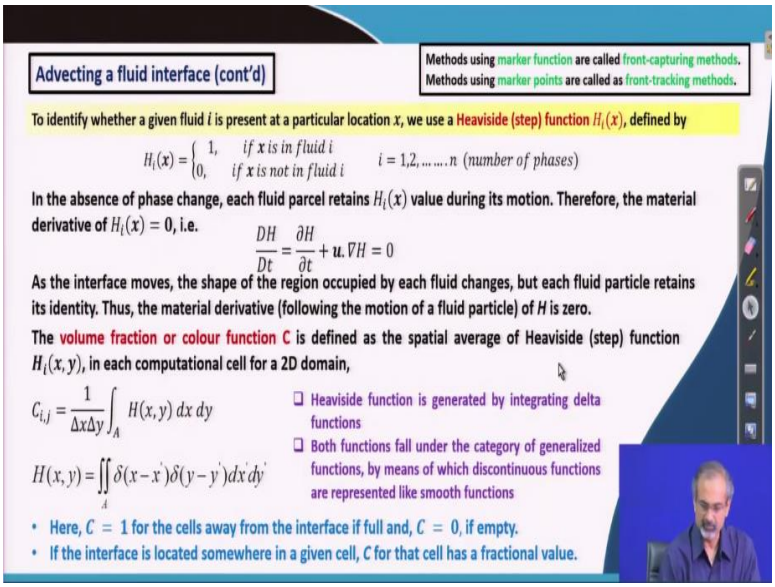

In this lecture, we continue our discussion on advection of the interface. So, in the previous lecture, we had discussed about how we introduced the concept of advection of a fluid interface. And then further we had distinguished two different techniques in the sense that there are a set of techniques called as front capturing, which are based on marker functions and another set of techniques called front tracking which are based on marker points.

So, currently we are discussing about the marker function. So, we already talked about the concept of substantial derivative. And the substantial derivative of the Heaviside function when it is a sharp interface goes to 0 which means, a particular fluid particle contains information about whether it has a marker H = 0 or H = 1 and gets advected in the flow. We discussed briefly about the volume fraction or color function C which is built on the Heaviside function by integrating it area wise in a two dimensional domain.

And then we understood that C also would occupy values anywhere between 0 to 1. And if a cell is empty, then this volume fraction or the color fraction, which is acting as the marker function will be 0. While if it is full, it will occupy a value of 1 and if it is in the interface

region, it will have a value anywhere between 0 to 1. So, we will discuss more in this lecture on how to tackle such advection of color function C.

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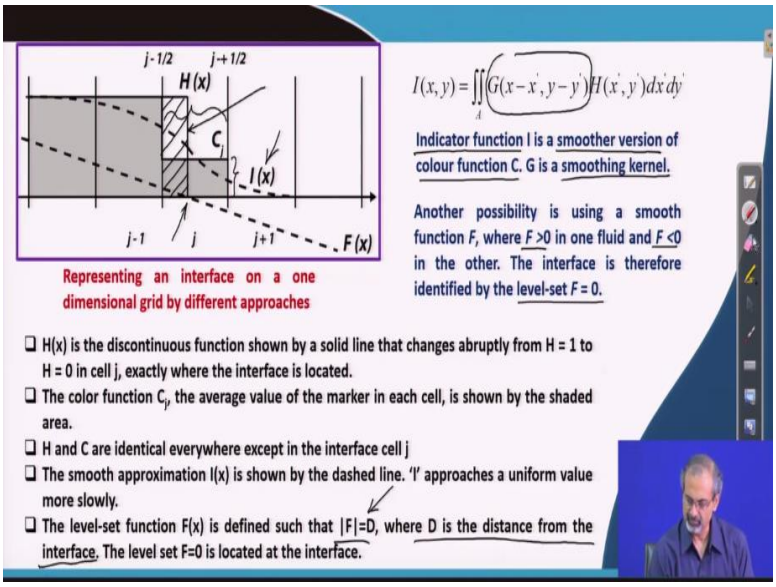

So, here we are talking about an interface region. You can understand this is the interface region where the Heaviside function has dropped down sharply. And you can see that because color function is essentially an integrated effect of the Heaviside function how it is defined within a certain cell. Therefore, the color function occupies this gray region as though the cell is getting filled up from bottom up.

As the Heaviside function moves into the cell, the color function moves up from the bottom to the top to fill up that cell. So, you can very well understand that there is a area conservation between what is covered by the Heaviside function within that cell and what is covered by the C j function that is the color function within that cell j. Now, there are other ways apart from color function also to indicate the interface.

You can see a function I x which is much smoother than the color function. The color function is also behaving in a piecewise constant manner. But, the function I which we call as the indicator function is a smoother version of the color function. Because we are incorporating a smoothing kernel, it smooths out the step jump. Another possibility is the level set function which we discussed in the previous lecture, which occupies a value greater than 0 in one of the fluids and less than 0 in the other fluid.

And it is exactly equal to 0 at the interface. So, you can understand that this dashed line is crossing over the interface where the function goes to 0. So, you have smoother indicators defined through I and F. And of course, the level set function is defined in a manner where the modulus of the function would generate the distance information from the interface.

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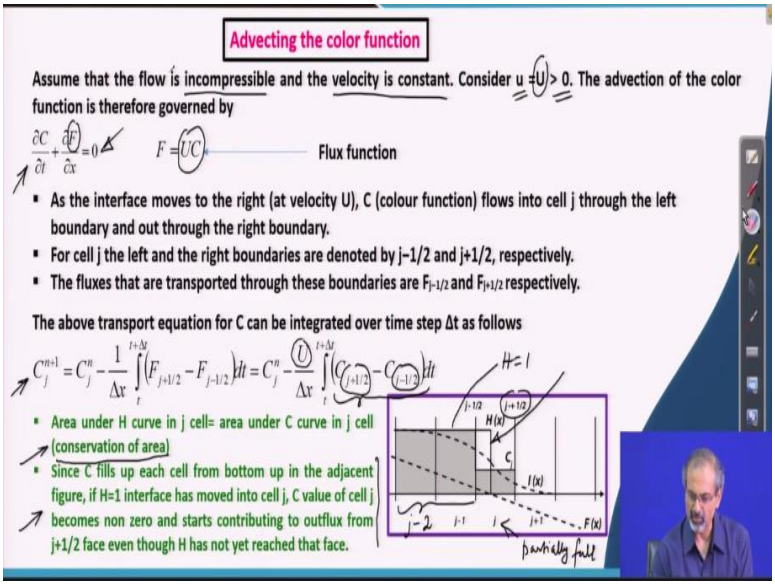

Let us talk about an incompressible flow and where the local velocity is a constant. So, the velocity u, which in general is a variable is set to a constant value here which is called as capital U and it is kept positive. Now, we are trying to find out that under the influence of this positive constant velocity, how the color function would advect. So, the advection equation is written in this manner, where F happens to be the flux function and it is in a conservative form that has been shown over here.

And as you can understand that under the influence of the positive U, the interface would move from left towards the right as time progresses. What would happen as a consequence? That you can already understand that these cells j – 1 or j – 2 have been completely filled up by the color function as the interface moved and the cell j is now partially full. When will it be completely full?

When ideally, the analytical description of the interface which is defined by the H x function would reach the j plus half face of that cell. So, when that happens, then H covers up that entire cell. And in order to conserve the area, both under the H and the C curves, you have to make sure that C also fills up the entire cell. In that case, the gray region will completely reach the top of the cell j.

Now, we have to be careful that this picture is correctly represented when we try to work out the fluxes. If that is wrongly represented, then there will be numerical effects due to that. Now, when you discretize this transport equation, what happens is that it takes up a form of this kind. And then you can understand that when the velocity is constant, it comes out of the integral.

And within the integral you are left with the color function the difference of the color function values between the two faces of the cell which are located at j plus half and j minus half. Now, there are different means by which you can approximate this equation by choosing appropriate values of these color functions at these respective cell faces. Now, the point is that if we do not choose it appropriately, then there may be artificial leakage of flux through a face where the interface has not reached yet.

So, let us look at the point here. So, since C fills up each cell from bottom up in the adjacent figure, if H is equal to 1, interface has moved into cell j. That means, this is the region where H is equal to 1 and that has moved into the cell j. And C value of cell j becomes nonzero and starts contributing to outflux from the j plus half face even though H has not yet reached that face, which means, the interface strictly has not reached the face j plus half.

But because you are filling up the cell already with the color function, you would get a wrong interpretation that the flux has already reached the j plus half face. And this is where the whole problem lies. That means we have to find a way around this problem so that we do the flux calculations correctly.

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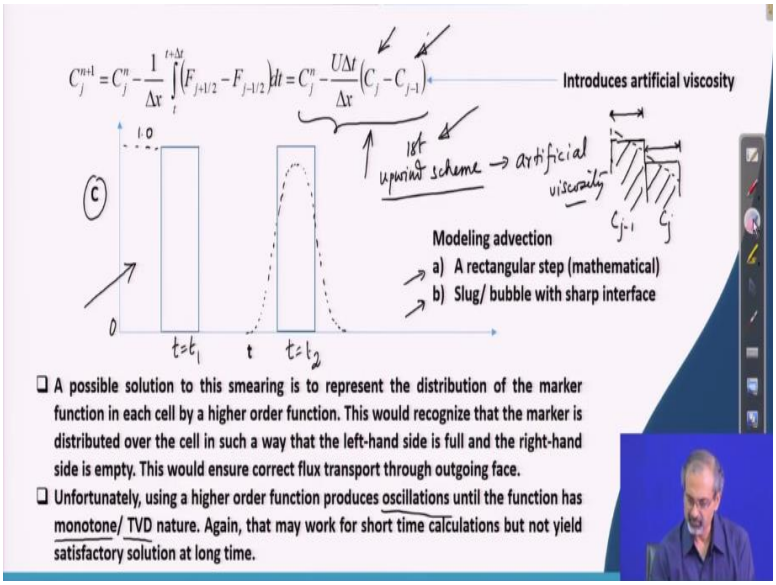

Now, let us say we followed the idea that we placed before that way F j plus half minus F j minus half may be represented in this manner. And if you do that then what happens is that when you are trying to model the movement of a rectangular step like what we have shown over here. Let us say this is at t = t 1. You have defined the step function and the y axis essentially indicates the color function. So, strictly speaking this is 1. And of course, this is 0.

And you are trying to track its nature at some other time t = t 2. Then if you are not accurately monitoring and modeling the fluxes, what it will do to the step function is it will artificially diffuse the step function. And the above discretization that we have written will exactly do that. Because it has an effect similar to what first order upwind schemes do in discretizations we have discussed earlier in the context of say linear advection equation.

And it is essentially an influence of artificial viscosity which comes into the picture. Now, here mathematically we are modeling a step function, but if you talk about a mechanical or application orientation to this problem. This distribution of color function may actually mean a bubble a presence of a bubble or a slug inside the pipe. And that is being indicated by the sudden change in the color function.

Because there is a face change as you cross from the liquid to the bubble and then bubble to the liquid back. Now, if you are modeling it as a sharp interface, and then you find that the numerical scheme is diffusing it artificially what it means is that artificially the bubble will get elongated whereas, physically it should not be according to the modeling law. So, that is

where the numerical scheme plays a major role in predicting the face boundaries correctly as they advect through the fluid.

So, often these advections have to be tracked over longer times and we have to make sure that the errors do not **(()) (11:19)**. Now, possible way out of this is to replace this first order upwind scheme by a higher order reconstruction there. So, here it essentially means that you are taking contributions from each cell in the form of a constant value that means, step wise distribution.

So, instead of doing this step type of distribution say C j – 1 is looking like this. C j is looking like this. Higher order reconstructions usually fit linear distributions which are piecewise that means, in each cell there was there would be a piecewise distribution defined. And there are some geometrical basis on which these piecewise reconstructions are done. So, we will discuss about it shortly.

However, even if you do that the higher order reconstructions often bring along with them oscillations in the solution, which we have seen even in other transport equations that we have dealt with. So, if you are able to incorporate monotone or TVD nature in those reconstructions, then you will not have any oscillations in the distribution of C.

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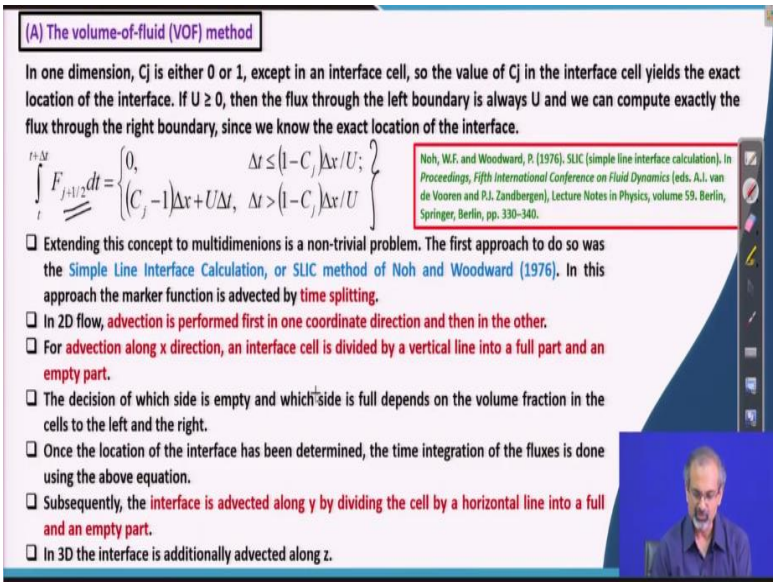

So, with this introduction of the color function or the marker function, let us go into the description of the volume of fluid method, which is one of the most powerful methods in this category. So, as we discussed earlier that in one dimension the C j value can lie anywhere

between 0 to 1. And in the volume of fluid method, we define the flux at the j plus half cell in this manner, which maintains the advection of a sharp interface. So, it eliminates the problem that we just saw in the previous slide. So, let us try to understand what it actually does. We will talk about two situations.

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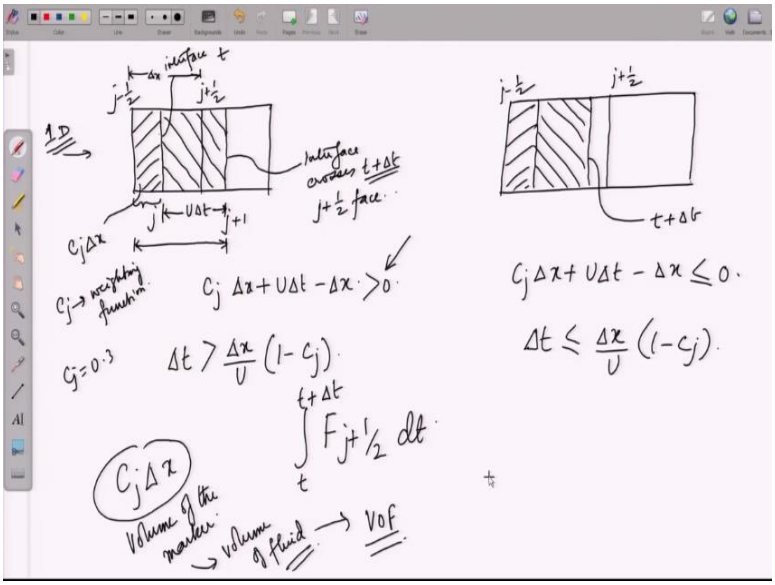

Let us make a small diagram here or rather a pair of diagrams, so, that we can see the two scenarios. So, these are the two cells. Let us say, this is the j cell; this is the j + 1 cell. So, this is j plus half interface; this is j minus half interface. And let us assume that at this point of time the C j has been defined this way that C j times delta x shows the dashed region. Now, remember that C j is essentially acting like a weighting function.

When you multiply it with delta x, what it does is it fills up a certain fraction of a certain of a cell a certain fraction of the width of a certain cell. Again, when it is a one dimensional advection, watch carefully that this time we have oriented the C j distribution in the vertical manner, unlike what we did previously, where it was oriented in a horizontal manner that means it was filling bottom up.

So, here we are forcing it to fill it from left to right rather than bottom up and that makes a difference, you will realize soon. Now, as we said that if C j is equal to 0.3, this basically means that C j delta x gives you 0.3 delta x, which means you are exactly filling up 0.3 times the width of the cell and that is where the interface exactly lies at a certain time t. Now, you are interested to know that with elapsing of some delta t time where the interface will stand.

Now, let us say that with passage of time, the interface moves ahead and the area that is now covered is U times delta t because it is advecting at constant velocity U. Now we will try to work out this expression C j delta x plus U delta t minus delta x. So, this is C j delta x plus U delta t that means this total length that is covered by the **(()) (16:14)** region minus delta x, which is this cell width.

Now, if this is greater than 0, then what happens is that the interface crosses the j plus half face. So, it has filled up the entire cell j and then moved on. Now that is possible if delta t is greater than delta x by U times 1 – C j. So, as long as delta t satisfies this condition the interface will cross that and in that case, we know that how to calculate the flux through that interface j plus half because it has reached and it has crossed that interface over that time.

Now, what if the other happens? So, this is the interface location at t plus delta t under this condition. And let us say we have another situation where the U is such that the interface does not cross that cell at all. So, this is the j plus half this is the j minus half and interface stands here at t plus delta t. So, that can happen if in the limit the interface can just go and coincide with the cell face but not cross it.

And as long as it does there is no outflux from that j plus half face. So, that is possible if delta t is less than equal to delta x by U 1 – C j. So, if this is the basis on which you are calculating the flux transfer then you will never have any artificial diffusion. And that is exactly what we indicated in the previous equation for F j plus half t to t plus delta t. And another thing that we need to remember here is that the product C times C j times delta x it is essentially indicating a volume of the marker.

And therefore, it is volume of fluid as well which is coming from the gray portion that fluid that face, how much volume has that face filled up of a certain cell and therefore, the technique volume of fluid the name of the technique which comes up. Now, this is somewhat easily done in one dimensional sense. It gets more complicated when you do it in a two dimensional or three dimensional sense.

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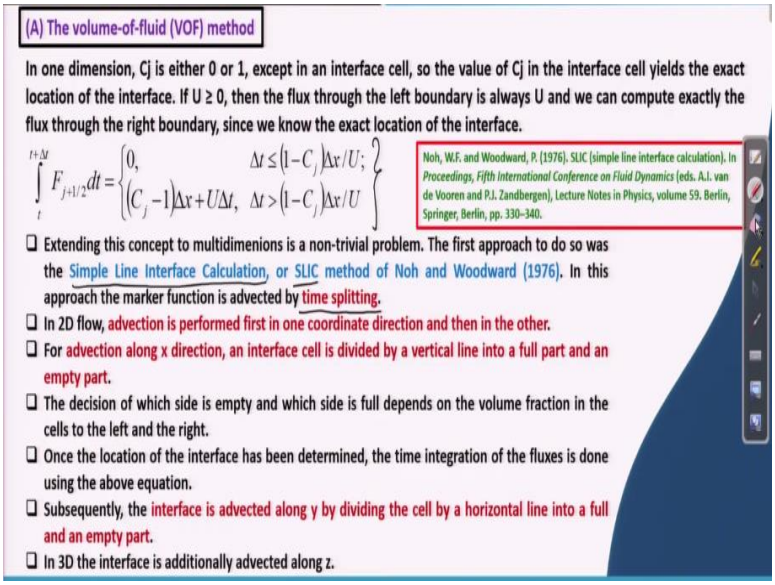

Now, when the interface remains as a straight line like we discussed a few minutes back, then the method that you have essentially is called as the Simple Line Interface Calculation or in brief SLIC. And when it is applied in multidimensional sense, it is done usually by time splitting. That means you take care of advection along x separately along y separately and along z separately in a three dimensional situation **(()) (19:56)**. Again, there were other methods which evolved over time. Let us have a brief look at that.

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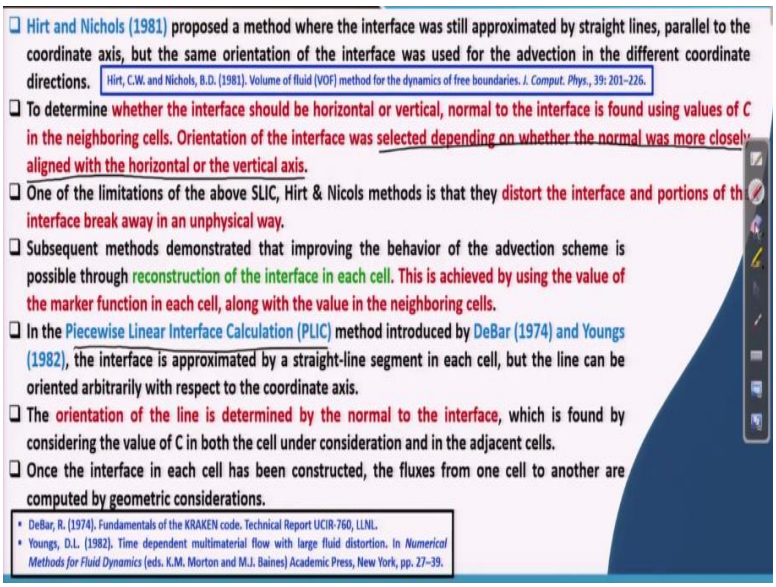

So, there was another technique which was related to the SLIC technique. But somewhat more simpler than that which was proposed by Hirt and Nichols. And there what they did was that they looked at the interface as any one particular orientation, either horizontal or vertical. So, you remember that when we first showed you the gray color diagram, there, the interface was horizontal.

Then in the calculations, we showed that the interface if you keep it vertical, then it is easier to track fluxes when it is a one dimensional movement. So, you can imagine in a multidimensional problem, if it is oriented along y, then it is easier to calculate fluxes along x. If it is oriented along x, then it is easier to calculate fluxes along y and so on. So, SLIC scheme did different orientations, when they did the time splitting and calculation of fluxes along x or y directions.

But in the Hirt and Nichols scheme, they used one particular orientation only to do the flux calculations along different directions. And how was that direction chosen? They selected based on whether the normal to the color function front at that point was lying closer to vertical or closer to horizontal. Based on that they chose how to orient the interface.

Then further came a more sophisticated method which was more accurate than these two previous methods of SLIC and Hirt and Nichols, which is called as Piecewise Linear Interface Calculation and that define the interface as a slanted straight line. That means the slope of the straight line could be other than just purely horizontal or purely vertical, it could have intermediate slopes also. And then that give more accurate calculations of the interface advection. So, we briefly look at a few diagrammatic representations so that these concepts are clearer to us.

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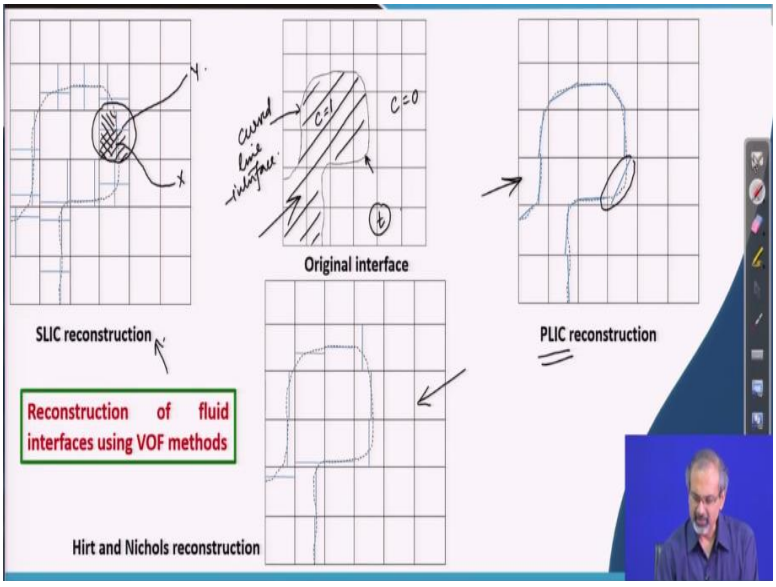

So, this is where we have a brief look at how the different schemes look in perspective. So, this is essentially the original interface as you can understand that this curved line represents

the interface you can say that inside that curved line, you have a certain fluid or a certain face outside that line you have something else. So, you can say that strictly say C is equal to 1 here and C = 0 here. And the sharp jump essentially comes here.

That is how it stands at a certain point of time. As time changes, as you can understand that this interface is going to advect, it is going to deform, it may even rupture somewhere and so on. Now, at this point of time, how are the different reconstructions of the interface working. So, as we defined SLIC reconstruction, you can pick up any one of the cells and you will see a vertical and a horizontal front which is indicated.

So, as you can understand that this vertical front will work better, as we advect along the x direction. The horizontal interface will advect better, will work out better as you advect along y. But in both cases, there are area conservations which are working that you have to ensure.

So, the locations are not arbitrary, if you have a horizontal line that then the amount of area that it fills up should be exactly equal to the area filled up by the vertical line from the other interface. And again should match with the exact area under the interface curve the exact interface curve. So, all of them equate with each other within numerical error bounds. So, this is how the definitions work.

Hirt and Nichols somewhat simplified it by using only one front. And a still better way of reconstruction was shown by the PLIC scheme which is piecewise linear that means, these can be could be slanted fronts or interfaces. Now, there is little more to this PLIC reconstruction. So, let us proceed with a little bit of discussion on that front. So, in the PLIC scheme, let us see how the calculations work out briefly.

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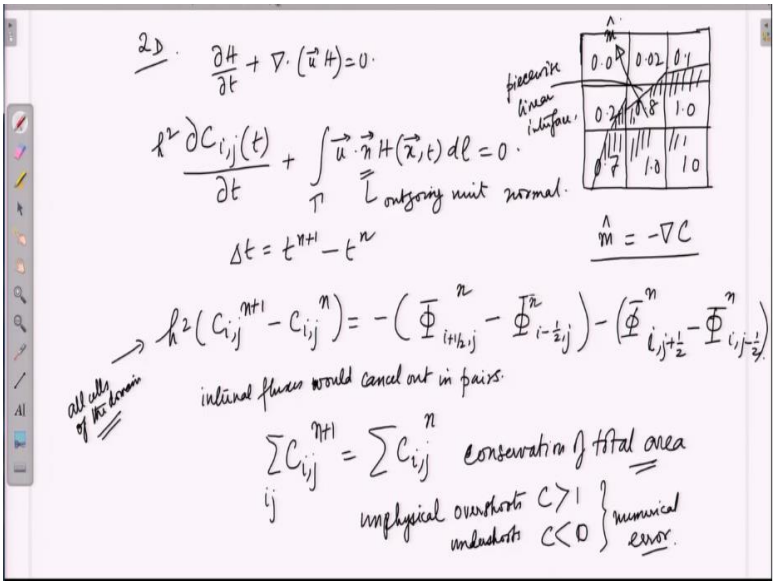

So, in a two dimensional scenario, let us say you are trying to advect the color function and then the original governing equation in terms of the Heaviside function is this. But when you apply it in an area weighted sense for the color function and then you discretize it you will see that the equation works out like this essentially. So, of course, gamma is the cell boundary and the n is the outgoing unit normal.

And then when you integrate this equation over a certain time t which is say t n – 1 – t n. Then you will be able to show that this equation becomes like this. Remember thus that h is the grid spacing which is equal along both sides both x and y and the capital phi's essentially they are denoting the reference face areas which are crossing the different cell faces. So, they are essentially the fluxes.

Now, if you introduce this equation to all the cells of the domain and sum them up over all the cells with appropriate boundary conditions, what happens is the internal fluxes would cancel out in pairs. So, flux going out of the face i plus half j from the cell j is flux going into the cell j + 1 let us say through that face. So, that is how they cancel each other. So, then finally, you will be able to show that when you sum it over all the cells then you are able to maintain conservation of total area.

And this is a very necessary constraint which needs to be filled up fulfilled sorry. So, this ensures conservation of volumes as well. Remember that whatever numerical algorithms we are using in order to approximate these fluxes should not ever ensure any unphysical

overshoots like C going beyond 1 or undershoots where C goes below 0. This might lead to numerical error and therefore non satisfaction of the conservation.

So, these can trigger numerical instabilities. Now keeping this in mind, remember that in the PLIC approach what we were talking about was that instead of having straight lines indicating interfaces, you have curved lines. Let us give an example that in a local two dimensional region you may have a distribution of color functions. Let us distribute them in a manner like this.

Then you will see that the PLIC method may construct the interface at a certain instant in this manner. So, these are the filled up reasons. So, this is essentially the piecewise linear interface. And then we are interested to know the outward pointing normal. Let us call it say as m. So, it is known that this outward pointing normal will be equal to minus gradient of C. So, if that happens.

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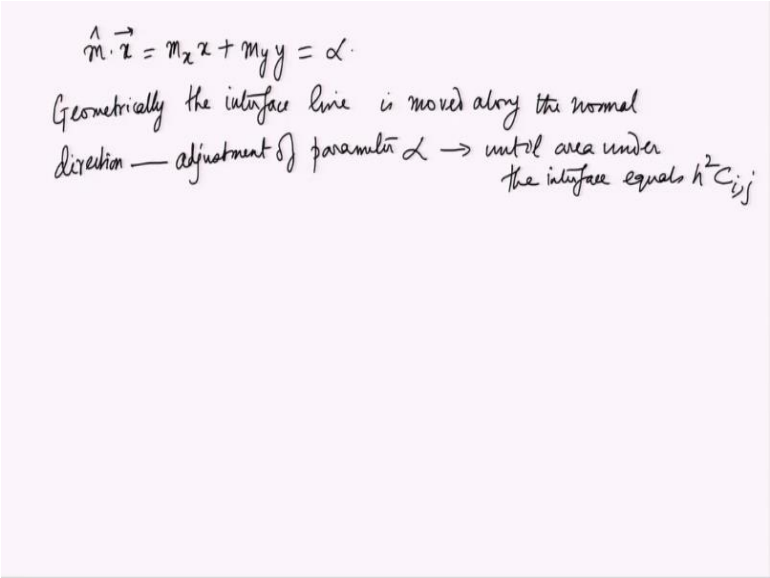

We can define the interface in this manner. So, what happens is that geometrically the interface line is moved along the normal direction through adjustment of parameter alpha. Until when, until area under the interface for that particular cell equals h square C i,j. And that is for the new time. So, what we are trying to mean is that we have shown the discretized equation which indicates the new time C i,j.

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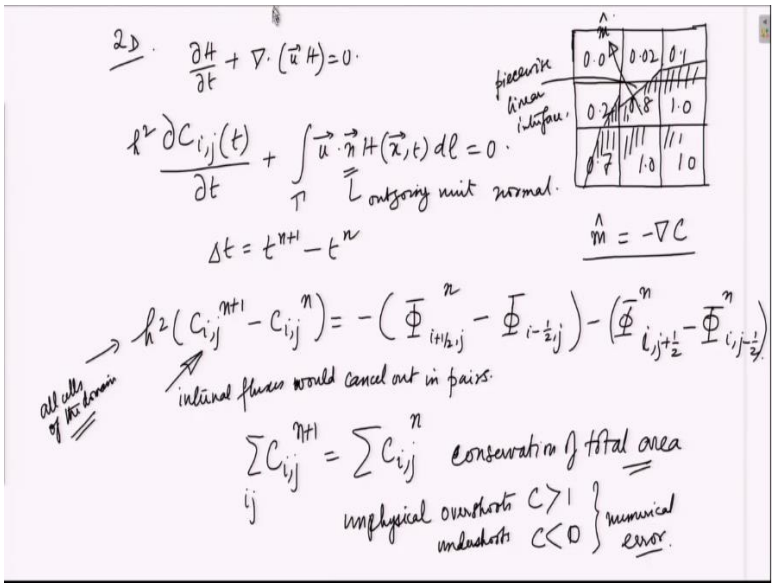

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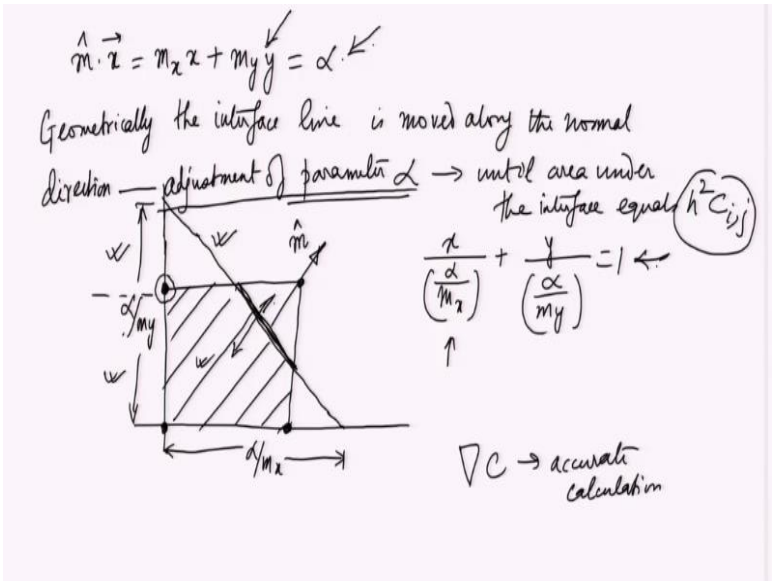

And we are trying to figure out how to reach there. So, we are saying that it can be reached by adjusting this parameter alpha. And geometrically how it is done can be shown through a small diagram. Let us say, we have a certain cell here. And let us say the interface lies somewhere here. And this is the marker filled region. So, the straight line is the one which we have indicated here.

This straight line will move in or out according to how you set alpha. Because this equation can be written like. So, this equation has on top can be rewritten like this in the form of intercepts along x and y directions. So, this is the x intercept; the other is the y intercept. And so as you change alpha these intercepts are going to change and basically the interface here within the cell will change.

So, you are trying to find out an appropriate value so that it matches with this value. As soon as you reach that you are going to get the new location of the interface. Again remember that when we calculate the gradient of C it is better than by doing some averaging calculations. For example, we try to find out the value of C at different corners by incorporating the effect of neighboring cells.

For example, C over here will be influenced by a cell here, by a cell here, this cell and this cell and likewise. And therefore gradient of C can be more accurately calculated. So, accurate calculation of the gradient is very important because that decided decides the accuracy of the direction of the unit normal vector. We will discuss more on advection of fluid interfaces in the subsequent lecture. Thank you.