Introduction to CFD
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Lecture - 54
Basics of Interface Capturing Methods for Application in Multiphase Flow (continued)

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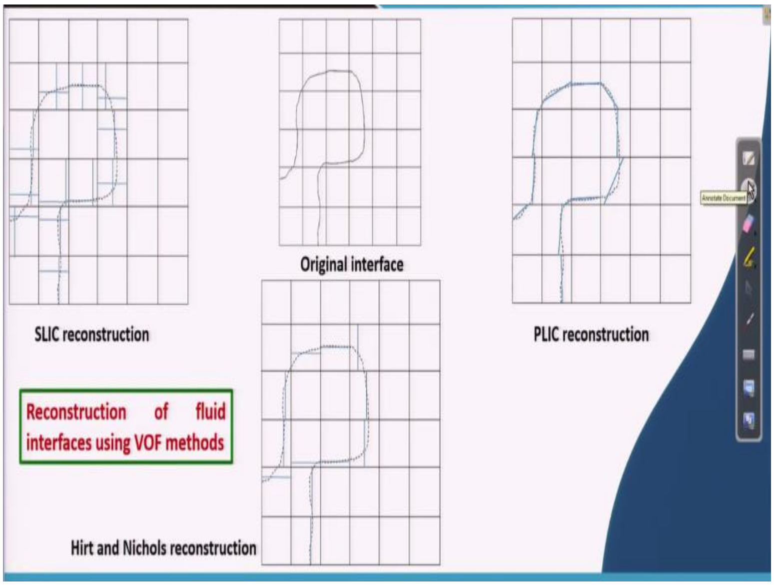

We continue our discussion on interface capturing methods. So, you recall last time we had discussed the volume of fluid method and different means of reconstruction of the fluid interface, under the purview of volume of fluid method. Let us go into the level set method once more.

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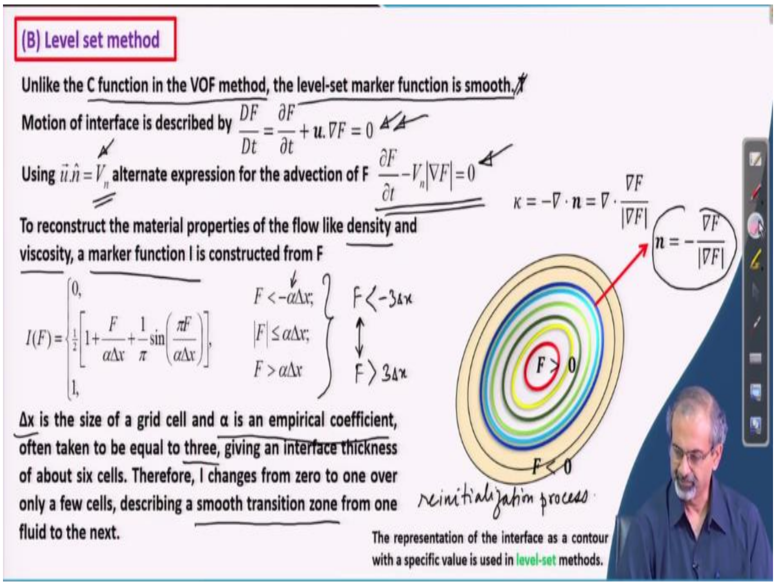

This has been discussed in an earlier lecture in this week. So, just a recapitulation that unlike the C function, the color function in the volume of fluid method, the level set marker function is smooth; is ignore this T. So, the motion of the interface, as we discussed earlier was that the substantial derivative of the function F would be equal to 0. Another alternative definition of this interface would be that the normal component of the level set can be calculated.

That is by dotting the u with the normal vector n which is defined here. So, that gives you the normal component of the velocity. So, if you substitute that into this equation, you get an alternative form of the substantial derivative of F = 0 equation here in terms of the normal velocity. Now, in order to reconstruct the material properties across the level set, let us say you want to find density or viscosity, usually a marker function I is constructed from the level set function.

And it is one possible way of calculating it is shown over here. And delta x here is the grid cell and alpha is an empirical coefficient which is often equal to 3. Now, that basically means that if you substitute that value of alpha into this equation. It gives you a range where F is less than –3 delta x. Here, it is greater than 3 delta x. And this is the intermediate region, which bridges these two ranges, which means that the transition zone is a smooth transition zone between the two phases, and it usually spreads over.

In this case, six cells. So, you could go in for different cell widths. But this could be one possible way of doing it. But usually what happens is, along with advection of the level set, there may be distortions in this distribution. And therefore, you may actually have to impose this distribution freshly after a few time steps so that the transition zone gets freshly disposed about the interface in an undistorted manner as the calculations progress over time.

So, this is inherent complication of the level set function. And it has to be readjusted after couple of time steps. And usually we talk about this process as a reinitialization process. So, we continue to discuss on different techniques using marker function. So, this is the second technique we discussed. Let us look at one or two more.

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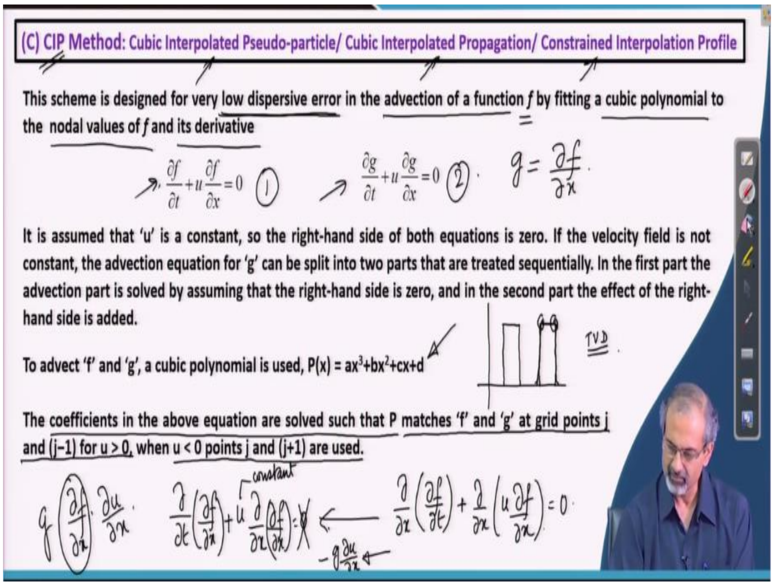

So, the CIP method which has evolved over time, from time to time has got different names, but the abbreviated form continues to remain as CIP. So, initially it was Cubic Interpolated Pseudo-particle. Then, Cubic Interpolated Propagation, and then now more contemporary times Constrained Interpolation Profile. This scheme is designed with very low dispersive error.

As the advection function f is handled, we essentially fit a cubic polynomial to the nodal values of f. And you do not only advect f with the transport equation, but you also advect its spatial derivative using an advection equation. Now, what happens is that if you apply an addiction equation to the spatial derivative of f that means this function g is essentially del f del x.

Now, what that means is that if you were to differentiate the advection equation of the function f, then how will it look like? It will be del del x of del f del t plus del del x of u del f del x. That of course will generate a zero from equation one. Now, this can be written as del del t of del f del x plus u del del x of del f del x, only if u is constant. But if u is not constant then what happens is you end up generating another term.

Because there will be an additional term del f del x times del u del x. So, this will be g. So, g times del u del x. So, essentially, if you send that term to the right hand side it will be minus g del u del x. So, if u is not constant, then the equation becomes inhomogeneous. And it is difficult to solve it also as such, but what is usually done in the CIP scheme is, it is first solved by setting the right hand side equal to 0 to obtain the new form of g.

And with that new form, the right hand side is calculated. And this and then added on, and the effect is just added on. So, that way, both the equations can be solved. Whether u is constant or variable but of course if u is variable, the calculations get more complicated. So, this is accomplished using a cubic polynomial. And it is found that ultimately the scheme would end up giving very low distortion.

And as we fit the polynomial, the coefficients in the polynomial equation match the f and g values at grid points j and j – 1 for positive velocities, j and j + 1 for negative velocities to take care of the upwind direction. And again, we had looked at how a rectangular step function was discretized using a scheme somewhat like first order upwind scheme in the previous lecture.

And we saw the effect of artificial diffusion as advection takes place. In the CIP scheme, what happens is the interface is very well captured with only a minor ripples at the corners. So, the ripples are minimized unlike many of the other higher order schemes. And therefore it is a low dispersion scheme. Of course, you can further improve it, if you bring in TVD properties. We also have discussed what happens when you have overshoots and undershoots of the C function as computations go on.

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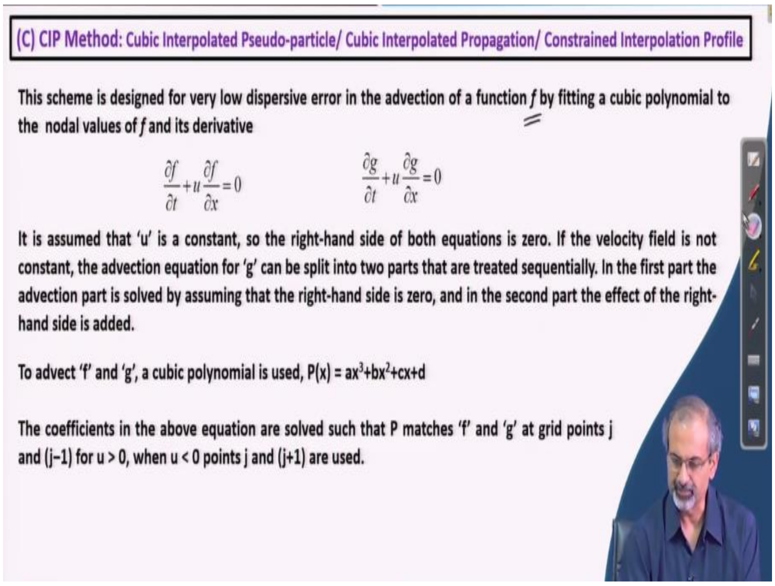

In this CIP scheme, the same function is referred to as f, but the implications remain the same. That means if you have overshoots and undershoots in f, there could be numerical instabilities, and also non conservation of areas swept by the function. So, we should at all cost try to avoid such overshoots and undershoots. Because inherently these methods, ensure volume or mass conservation through conservation of area swept by marker function.

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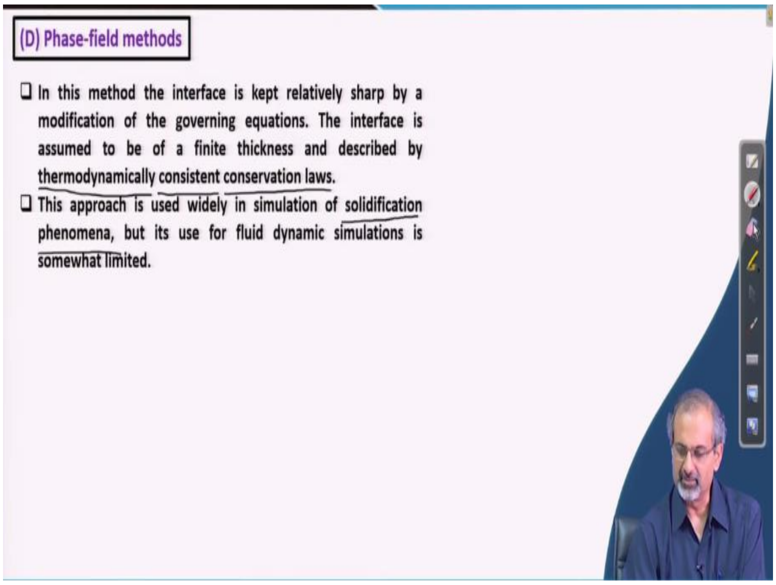

There is another very popular method called as phase-field method where the interface is kept relatively sharp by modifying the governing equations. And usually these modifications are done by thermodynamically consistent conservation laws. And these methods are widely used for capturing solidification kind of phenomenon. They are not all that common in fluid dynamics simulations. So, in the fluid dynamic domain, in general, volume of fluid is one of the most often used methods.

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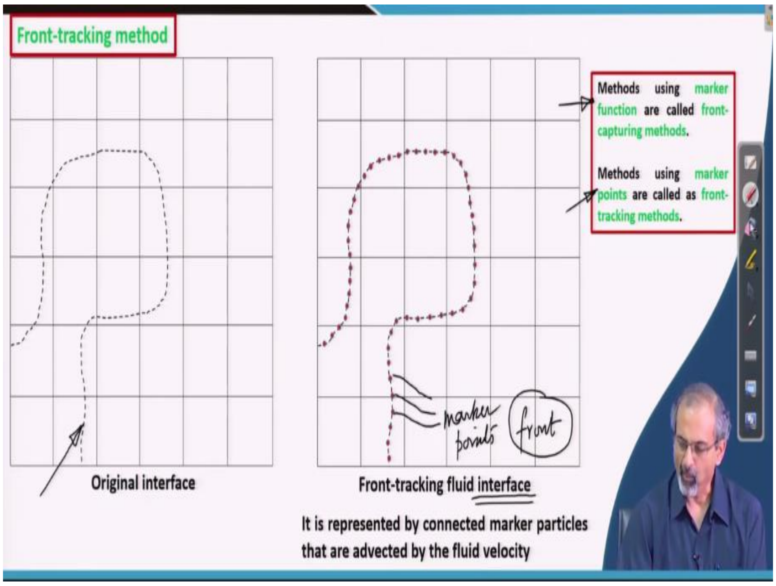

We recapitulate that all this time we were mostly discussing about marker functions and front-capturing methods based on marker functions. We have discussed a number of techniques like volume of fluid, CIP, the level-set method, and so on. Now, we spend a little time on the concept of marker points, and how they apply to front-tracking methods. So, in this slide, we see that the this is the original interface that we have been looking at for some time now.

And in front-tracking method, we try to define a front which tracks the interface, and the front is comprised of marker points. So, these are marker points which are indicated in red, which form the interface, which is also called as a front. Of course this front is also advected by the fluid velocity like the in the front-capturing methods. Let us add on, little more details to this.

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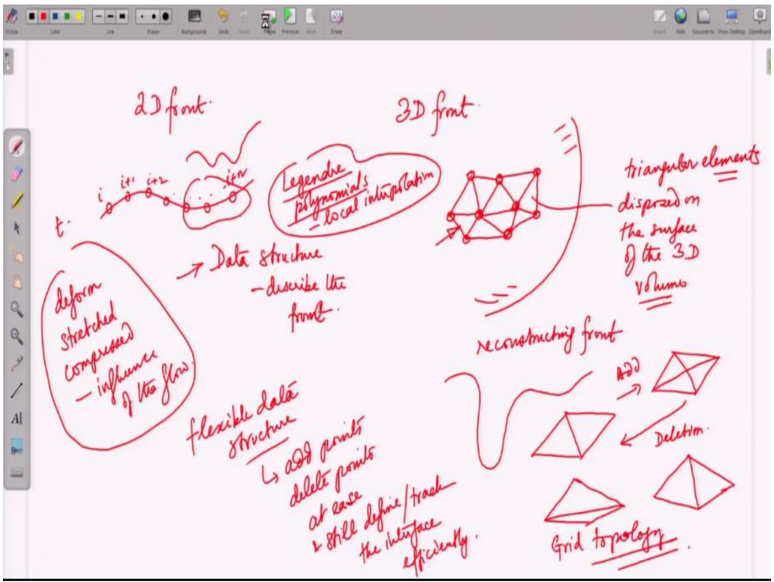

So, in a 2D front, as we saw in the previous slide, we have marker points like this and a curve looking like this. How will it look like on a 3D front? Let us imagine that there is a three dimensional surface like this. Let us say part of a sphere. And then you are trying to build a front comprising of marker points. Usually, we wrap the surface with triangular elements like this.

Triangular elements are better suitable to wrap even complicated geometries. And you assume that this network of triangles are disposed on the surface of the 3D volume. And 3D volume is essentially a volume covered by a fluid and beyond this volume lies another fluid. So, essentially the surface is the interface between the two fields. And we are trying to dispose triangular elements on that surface to identify marker points, which will define the front.

So, you may say that what it says of these triangles may act as marker points. Now remember that there is a data structure involved to describe the front. Let us say, in a two dimensional front, it may be stored in an array, it goes on. So, there may be numerous such points which define the interface at this point of time t. Now, as time progresses, this interface will deform, it may get stretched, it may get compressed and all due to influence of the flow.

The interface may even rupture in the sense that there may be a bubble rupturing out of a region of the fluid and getting mixed into the other phase. In that case, the bubble carries along with it a couple of marker points. So, maintaining the data structure to cater to all such positions or all such conditions is one of the major challenges in front-tracking method. And we need to have a very flexible data structure so that in order to accommodate for such physical effects.

You can add points, delete points at ease. And still define and track the interface efficiently. So, this is certainly a challenge in two dimensional case but it is more of a challenge in a three dimensional case as is obvious. In three dimensional situations, there may be numerous issues of reconstructing the front in order to accommodate for effects of this kind in different manners.

Some of them would become obvious to you that sometimes when the locally the interface is becoming very sharp like this. You may actually have to add elements into this network of triangles in order to capture those large gradients without which you will not be able to match the surface well or capture, or represent the surface well. So, very often, you have to have first of all, local interpolation functions operating.

So, in a two dimensional interface, we often use Legendre polynomials. These are having relatively local interpolation provision. And that is very convenient in the sense that if locally the interface in a certain region gets some indentations due to deformation or stretching or compression. Legendre polynomials are good candidates to accommodate those sudden changes or rapid changes.

Similarly, when it comes to reconstructing on a three dimensional sense, then you may actually have to introduce more triangles. For example in a certain region, if you have two triangles, you may have to add more triangles in order to take care of rapid changes in the interface. Whereas, there may be certain flattening of some region in which case it may be just the opposite way through deletion of certain elements.

Also, there may be need for reshaping of elements. So, in some region, the elements have become very awkward looking. And then you need to reshape them. So, without altering their overall area, you just connect them in a different way. So, there is a lot to do with the grid topology in front-tracking methods. In addition to this, there is of course the issue of advection of the moving front.

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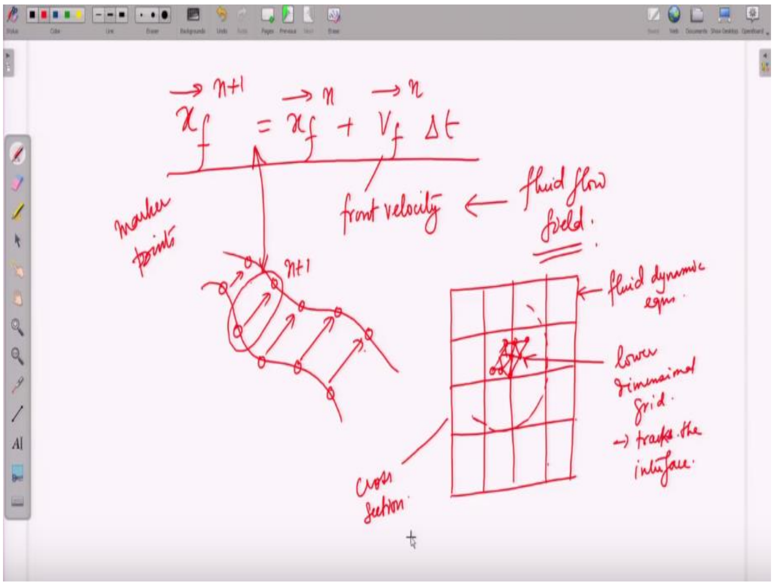

For example, if the front has a certain shape which is given by a vector function x, which can apply to any dimensional problem. So, if you have it defined at the nth time, then you try to progress it to the n + 1th time this way by defining a suitable front velocity which is of course going to be linked with the fluid flow field, which is in the vicinity. So, there would be an evolution equation of this kind which will be applicable to the marker points individually.

So, once you have an equation of this kind in place, what it does is that if the interface is comprised like this with marker points like this. The next time step, it may look like this where location of each one of those points at the new time step is essentially decided through these vector displacements which are again linked with an evolution equation of this kind. So, this is how essentially the front tracking goes on.

And very often in a three dimensional problem what happens is the flow is being essentially solved in a three dimensional Cartesian grid like this. You are just taking a cross section. While the moving front maybe actually advecting through it and on that you have these kind of triangular elements which are defining the marker points. And you essentially have two grids which are functioning simultaneously.

On one grid, you are solving the fluid dynamic equations and another grid, which is essentially a lower dimensional grid that tracks the interface. So, this is a brief idea on the front-tracking method. Now let us move on to a few applications of multiphase flow. And you will be seeing a few videos as well which will add on to your excitement and all these simulations that you will be seeing.

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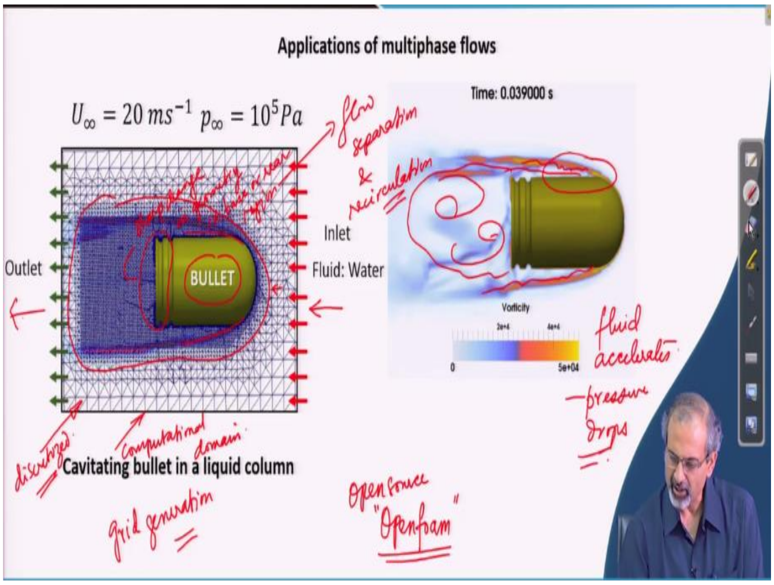

The simulation results that you are going to see are generated in the open source platform OpenFOAM which you are encouraged to explore. So, to begin with, we have a slide showing a computational domain. So, as you can understand that this is a rectangular domain which we call as the computational domain. And though, we have not reached the module on grid generation which is coming up in the subsequent weeks.

You can understand that the domain has been discretized. Will discuss more on these issues of discretization and different kinds of grids later on in that module, but you can see that around this body of interest which we are trying to show in this domain, it is a bullet, which apparently is moving through the fluid. We have a very fine distribution on mesh in order to resolve the details of the flow around the body as the flow moves passed it.

So, as you can understand that there will be some kind of a boundary layer formation on this body, and then this body has a sharp change in geometry in the base region. So, there will be flow separation in the base or rear region. So, this often leads to flow separation and recirculation. That is a region of low pressure usually. And we are interested to explore this problem from the multiphase perspective in the sense that in low pressure regions.

There is always a possibility that if you have a liquid flowing passed this body that there would be cavitation phenomena and therefore possibilities of bubbles forming. So, then you have the prospect of two phases coming up a liquid phase and a gaseous phase. So, flow is moving in and out in this manner. So, let us look at the video, which will probably give us more idea about how the flow evolves.

(Video Starts: 24:12) So, as you can see now that the flow is moving past the bullet. **(Video Ends: 24:19)** And as we mentioned earlier, the flow seems to be attached over here. But then, soon after it undergoes separation. So, there are vortices which are moving from those regions, and gradually the flow gets separated. It recirculates here and there is possibility of bubble formation in regions where pressure has dropped quite significantly.

Pressure can also drop in regions where the fluid accelerates substantially. So, in the next slide, we will try to see whether we can have a look at these bubbles that we are talking about. So, this is the slide where we are looking at the body in a kind of isometric sense because those simulations were performed in three dimensional sense.

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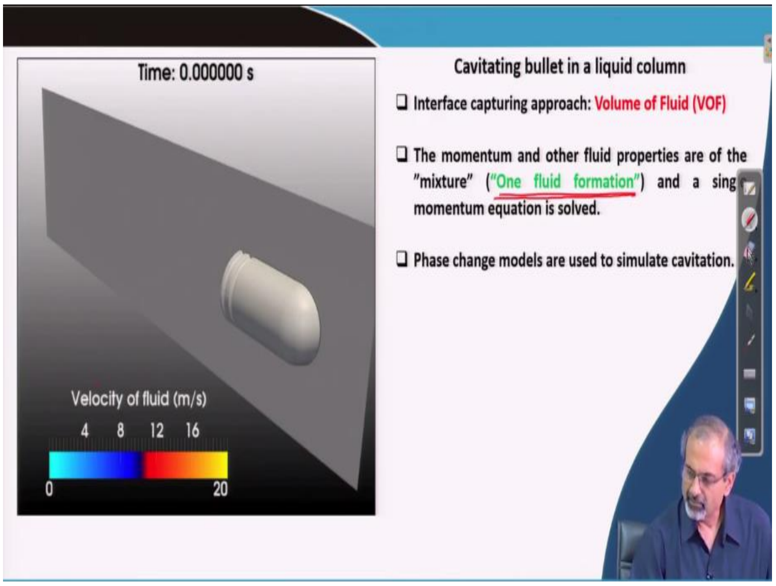

So, in the previous slide we just saw a cross sectional view, we have more complete view over here. And now, interestingly, what you will see is, you will find vapor formation. **(Video Starts: 25:35)** And what you see over here in the wake of the body is that the vapor is colored with the velocity field. So, vapor forms due to cavitation, and the color that it attains is from the neighboring velocity fields.

So, wherever there is larger velocity, it becomes reddish or yellowish, and lower velocities are in the bluer region. So, with the volume of fluid method, you are able to account for the interface tracking and segregation between the liquid and the vapor phases. And therefore you are able to show the region covered by the formation of bubbles and their propagation into the wave. **(Video Ends: 26:28)**

And as you can understand that the velocity field plays a major role in terms of the advection of the features. And we have used the one fluid formation here of course to simulate the cavitation phenomena. Will show the next instance, which is often called as the dam break problem. So, what happens is you have a region of let us say water accumulated in a dam or a reservoir.

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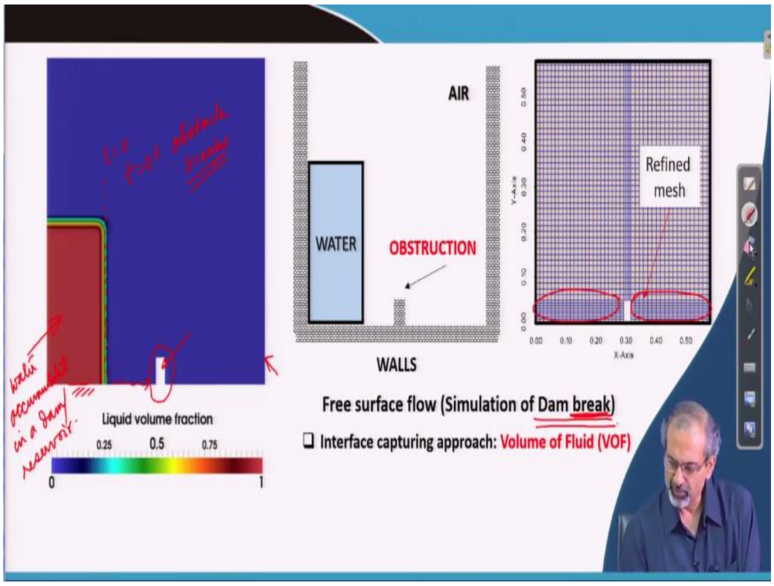

And there is as if an artificial obstacle over here at this point of time say t = 0. And then, at t = 0+ the obstacle breaks. So, that is where from, you are talking about a break. So, we are not seeing the obstacle here but it is numerically imposed over there. And then after the dam breaks, obviously, the intuition tells you that the water is going to rush toward this direction. And then you have another obstruction waiting there.

So, we are interested to see how the water reaches that obstructions spills over it, and then reaches the other end of the domain. And therefore, you know, there are multiple boundaries which are confining the movement of water. So, we will try to look at the time evolution of the whole dynamics. As we do so, we also keep in mind that there are regions where large gradients are expected.

Because as the water starts moving, of course, this is a solid surface on which it moves so there will be boundary layer formation. There will be rapid changes in gradient. Again as it reaches this obstruction, there will be rapid changes because of the effect of the obstruction on the water spillage and so on. Therefore, having a refined mesh in the indicated regions would be a very rational way of doing the simulation.

So, let us try to remove these so that we can see the features well. **(Video Starts: 29:01)** So, as we discussed earlier, we are seeing that the dam breaks and the water rushes towards the right, and then spills over the obstruction reaches the other end of the domain and comes back, and there is a lot of agitation before it tends to settle down. And the colors essentially indicate the liquid volume fraction.

So, what you have is air on top in the blue region, and the colored regions multiple colored regions is essentially the liquid regions. So, the liquid volume fraction is indicated through the color distribution. And as you can understand that wherever the grid gets coarser, the interface is also likely to become more and more diffuse while if it is finer which is true in the lower regions, it tends to be better captured. **(Video Ends: 30:01)**

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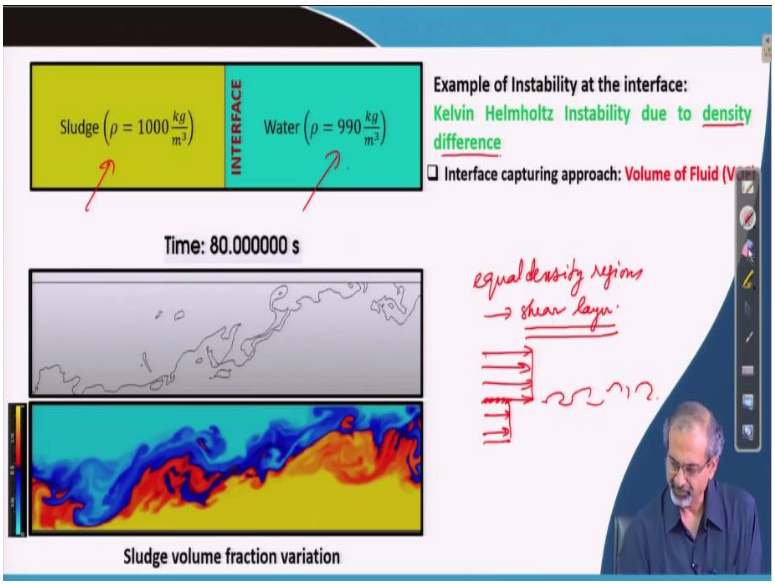

(Video Starts: 30:03) So, we will move on to another problem where we look at the instability of a fluid interface. We talk about this problem as Kelvin Helmholtz instability which is due to density difference. **(Video Ends: 30:20)** So, as you may be knowing that Kelvin Helmholtz instability also shows up in situations where you have equal densities regions which are interacting in the form of shear layer.

That means you have a region moving with a velocity distribution like this. Another which is moving like this. And there is a jump in the tangential velocity at this surface which makes that liquid region or fluid region unstable. So, as this interaction goes on, you will see that some structures will form in due course at the interface. So, that is also Kelvin Helmholtz instability, but that is purely due to shear layer effect.

Here we are talking about instability due to density difference because there is a heavier fluid here, and a lighter one here. As they mix there are instabilities at the interface till they reach an equilibrium where the heavier one settles below and the lighter one on top. These kind of situations also arise in atmospheric flows. So, let us try to look at the simulation once again. Sorry. **(Video Starts: 31:45)** So, we just look at the bottom picture.

Again, you can make over that the volume fractions are indicated through the color distribution and the sludge the heavier one the yellower one is gradually settled down, settling down at the bottom. And the upper portions are getting more and more filled with the blue region which is the lighter liquid which is incidentally water. That means mud settles below the water the clear water is seen on top. This is a commonly seen phenomena in many instances in nature. **(Video Ends: 32:27)**

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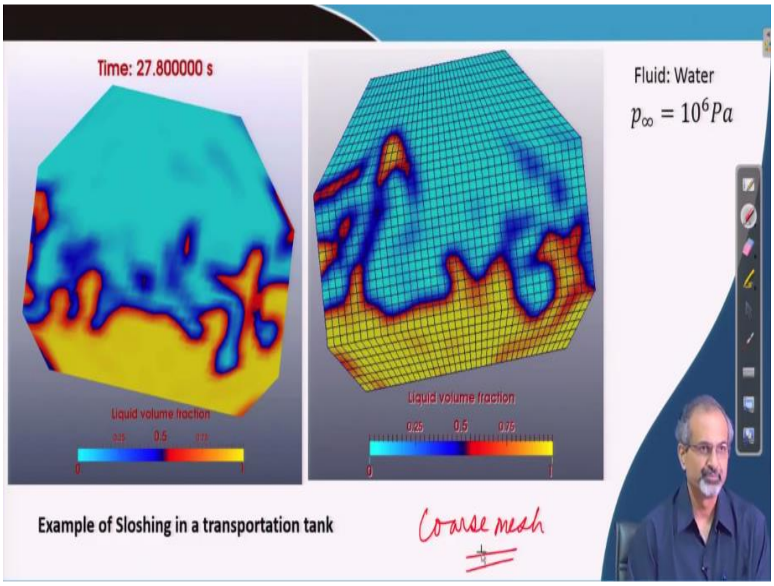

We look at an instance which is very practically important. **(Video Starts: 32:44)** That means you have a vessel which carries some liquid some water, heavy fluid and the vessel tends to move. It may be a truck which is carrying some kind of fuel. And the truck is moving over a very rough road. So, you can imagine how the fuel gets agitated inside. And this simulation has been done with a very coarse mesh as you can see. **(Video Ends: 33:07)**

And coarse mesh essentially means that the interface will be heavily diffused. This problem is also of enormous interest of aerospace community because you can have sloshing of propellants inside rockets which have just lifted off and moving through the atmosphere. And if there is very heavy sloshing in these propellant tanks that may make the vehicle unstable at points.

So, you have to take corrective measures in order to make sure that you have opposite control forces generated so that they negate that effect. Also, there is often an interaction between the fluid and the structure that means the container itself, making the structure to oscillate deform beyond safe limits. So, this is a very important problem in fluid structure interaction. And then we have another problem where you have sudden contraction and expansion of floats when orifice.

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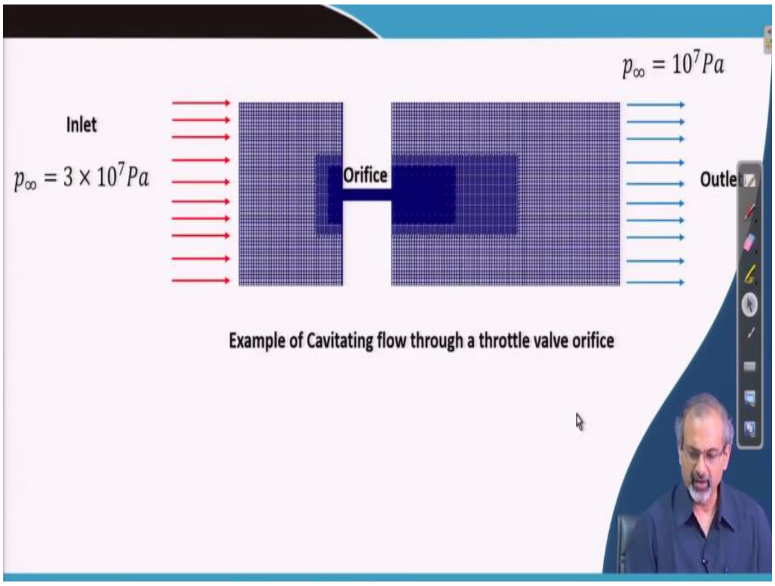

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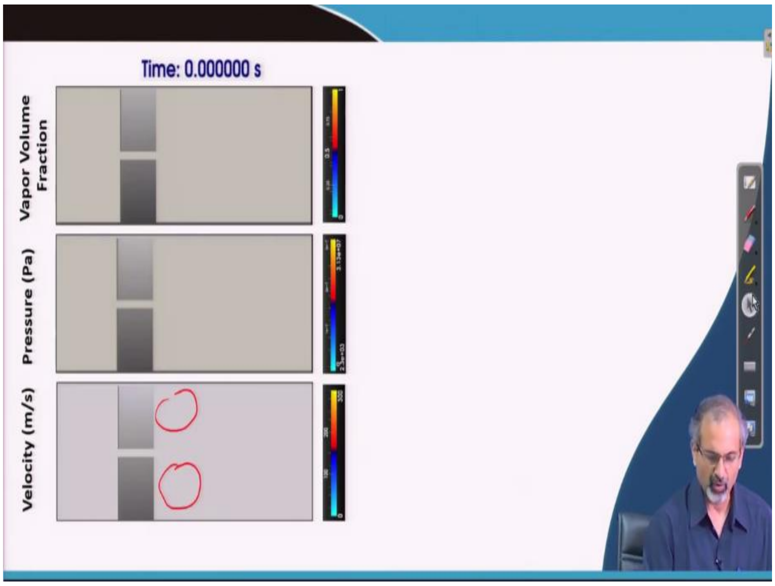

(Video Starts: 34:20) So, you can see how the velocity field is distributed, and you can make out that there is some kind of a flapping instability. That means the high velocity regions sometimes tends to move towards the bottom, sometimes tends to move towards the top.

(Video Ends: 34:39) Accordingly, the recirculation regions which are formed at the corners tend to oscillate between upper and lower sides, and what is the consequence.

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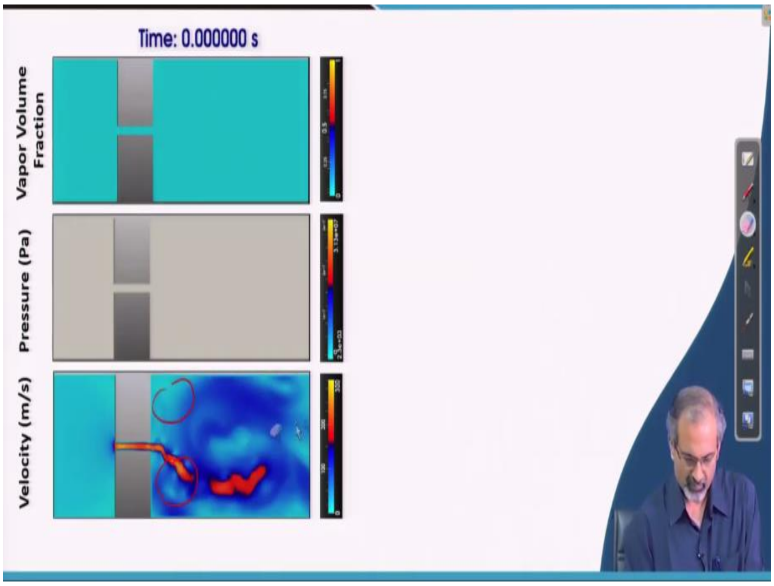

(Video Starts: 34:47) The consequences will be better seen in the vapor volume fraction where you will find that the vapors are accordingly generated that means through the cavitation phenomena the bubbles are generated wherever the pressure is dropping significantly because of the recirculation effects. **(Video Ends: 35:05)**

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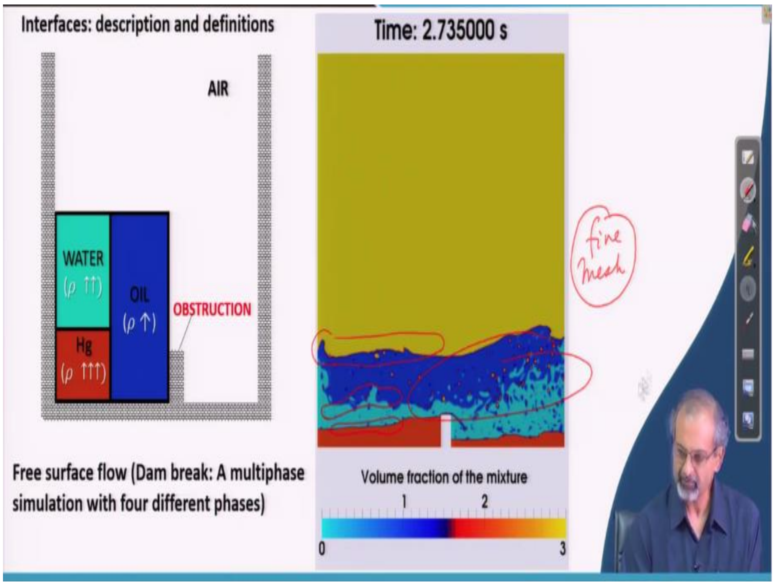

(Video Starts: 35:11) This is another dam break problem which is more interesting in the sense that you have multiple fluids, and the heaviest one is Mercury, then comes water than oil. And you can understand that the heaviest one is settling down at the bottom the red portion, followed by the lighter blue which is water, followed by the oil which is still lighter, and then the yellow region is essentially air. **(Video Ends: 35:36)**

Incidentally, you can find that the features are very well captured over here with a sharp definition of the interface, sharp definition of the multiple interface regions between the multiple liquids. This is of course due to a very finely disposed mesh. And therefore you understand that in multiphase simulations it is not only important that you deploy very accurate tracking methods for the interface, but also deploy, very high quality measures.

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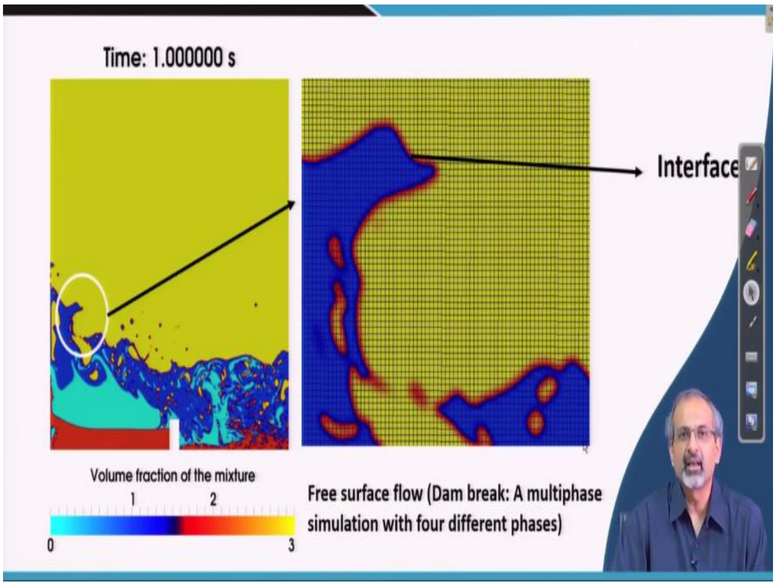

And we learned here by saying that we discussed a number of techniques by trying to track interfaces between different phases in a multiphase flow. And our main emphasis was on trying to explore methods which are accurate enough to track interfaces both in the sense of marker functions as well as marker points. Thank you.