Introduction to CFD
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Lecture - 52
Basics of Interface Capturing Methods for Applications in Multiphase Flow (continued)

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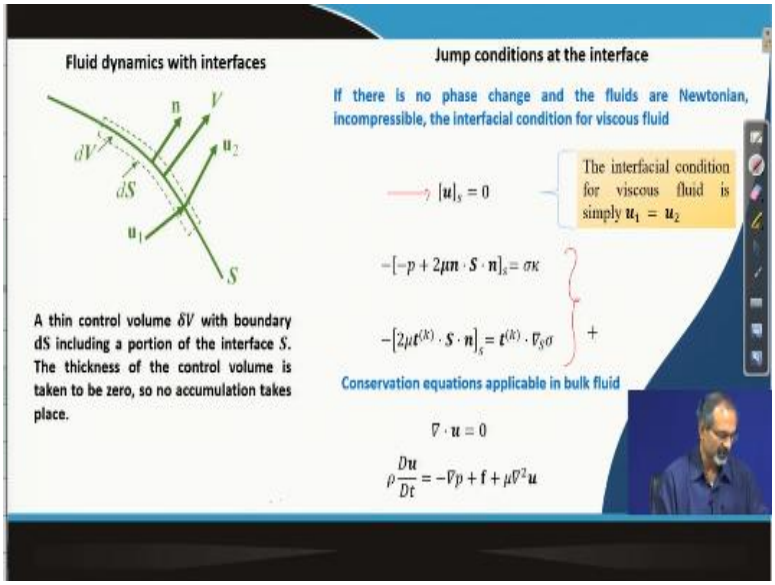

In this lecture, we continue our discussion on interfaces. So, in the previous lecture, we had discussed about the interfacial condition for the mass flux across the interface. And we showed that in the case of viscous fluid, it is simply equal to u 1 = u 2. Now, we also mentioned that we have to look at the stress tensor part in order to look and explained the next two equations.

And we also remember that surface tension plays a role in defining how stresses are going to occur at the interface.

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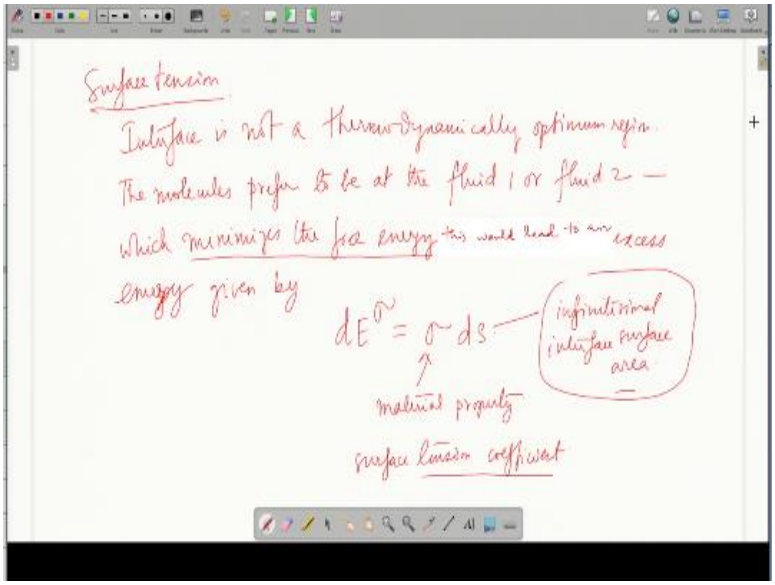

So, we briefly introduced the concept of surface tension in the previous lecture, where you will recall that we introduced the concept of the minimization of free energy. And that expression included the surface tension coefficient and the infinitesimal interface surface area. So, let us proceed with expanding this concept a little further.

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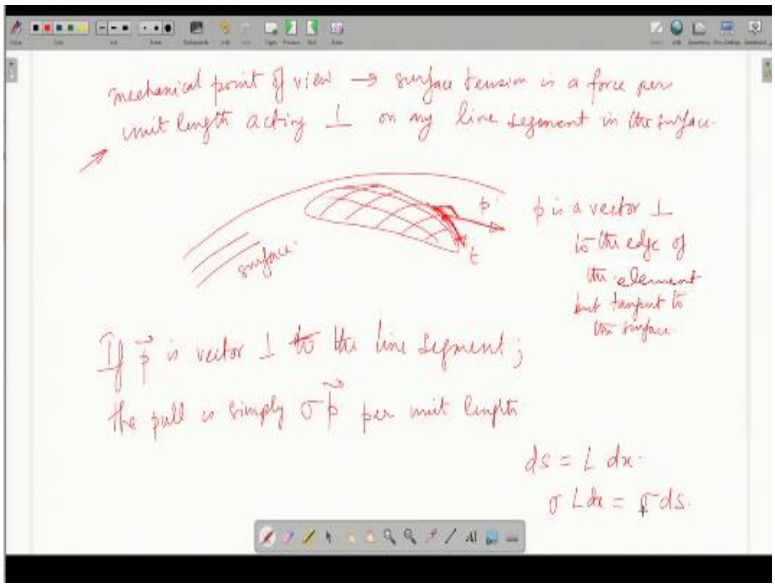

So, if we try to look at the mechanical viewpoint, from a mechanical point of view, surface tension is a force or unit length acting perpendicular on any line segment in the surface. So, last time you may recall that we had drawn an elemental surface in order to define the surface tangents in a three dimensional sense. So, if you just recall that three dimensional surface that we drew with u's and v's drawn on it.

Then if you look at the periphery of that surface on any point located on the periphery, you will have a p and say at t defined on the surface p is a vector perpendicular to the edge of the element. But, tangent to the surface essentially means, that this is part of a bigger surface. So, the p is perpendicular to this edge in the sense that it is making a right angle to that edge. But it also remains tangent to this surface.

So, this is how p is defined. And so, in the context of surface tension, we can say that if p is the vector perpendicular to the line segment. Like it is perpendicular to the edge of the element here. The pull felled by the line segment is simply sigma p, remember p is a vector per unit length. So, this is the idea. So, this would have an effect of stretching the surface when this pull is acting.

And suppose that if you are pulling in the x direction and the surface has an extension say L in the other direction. So, in the case stretching it increases the area by some amount ds is equal to say L times dx. And this would happen at the expense of some work done. So, that work done will be sigma times L dx or sigma ds and this increases the interfacial free energy.

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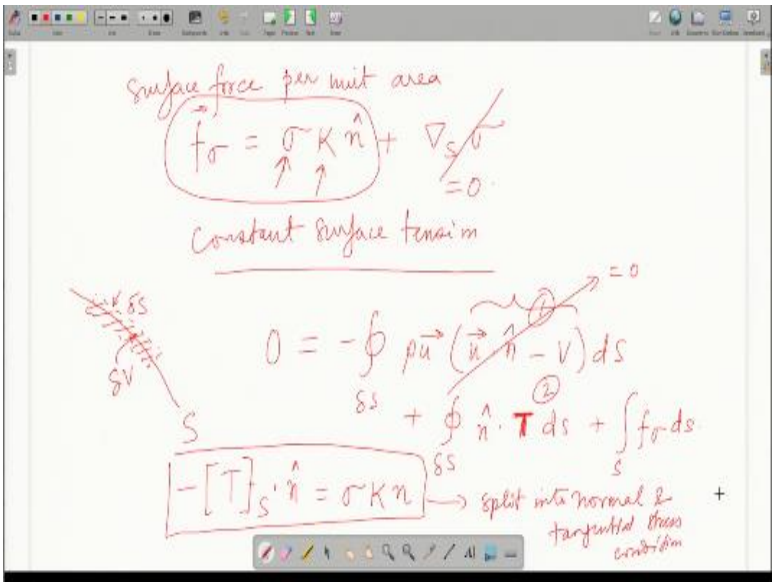

And using these concepts, we can further show that the surface force per unit area if you are expressing it as f sigma that will be indicated as sigma times Kappa times n plus sigma s times sigma. Remember that this is the surface tension coefficient. This is the curvature term. This is the unit normal, is of course, a vector and usually, when you have a constant surface

tension then that would lead to reduction of this expression or simplification of the expression in the sense that the second term will then go to 0.

Now, this again you may recall that the Nabla S which operates on sigma, it is essentially the surface gradient. We had talked about the surface gradient in the previous lecture. And as long as we have a constant surface tension we are reducing the expression to a much more simpler form f sigma equal to sigma k n. So, once you do that and you apply the conservation of momentum principle to the control volume that we drew earlier.

If you remember we had the interface drawn like this and we had an elemental control volume drawn across that portion of the interface. If you apply the conservation of momentum principle to this control volume on the interface, then you can write it as. So, you remember that this is the stress tensor. So, the integration is around the edges of the control volume, the control volume happens to be this say the delta V.

As far as these two terms are concerned the first two terms are done that way. And therefore, we have represented it as elemental surface area dS, which is comprised of the periphery whether whereas the volume is what is enclosed. And the first term for incompressible flows it can be easily shown that it this will go to 0 because, as you remember, we had shown in the previous lecture that this term is unique uniquely 0 for both the phases.

And in the absence of phase change, of course, it will give you a net m dot equal to 0. Right. Now, we can show that by rearranging the remaining terms, this can be written as the jump kind of nomenclature that we explained last time. And just to keep it simple, we are writing it by assuming constant surface tension. So, this is essentially the form and this equation now has to be split into normal and tangential stress condition.

And if you do that, then you will be able to understand how the jump conditions are being implemented here. So, these are the two jump conditions, one is coming from the normal port, the other is coming from the tangential part of that equation. So, the normal part is the first one while the tangential part is the second one and in this expression these D with superscript k are essentially the tangent vectors that we had defined in the context of the three dimensional elemental surface.

If you recall that we had considered two such orthonormal tangent vectors and we took a cross product in order to correlate that with the surface normal unit normal. So, that is how the whole set of equations connect with each other. So, now, we have a more complete definition of the jump conditions at the interface and then when you are looking at the conservation equations in general applicable for the bulk fluids in the two phases.

Let us say fluid 1 and fluid 2 then the bottom two equations will apply separately for the fluid 1 and fluid 2 regions and when it comes to the interface, you have to ensure that these equations are applicable at the interface. So, that the jump across that interface is suitably implemented.

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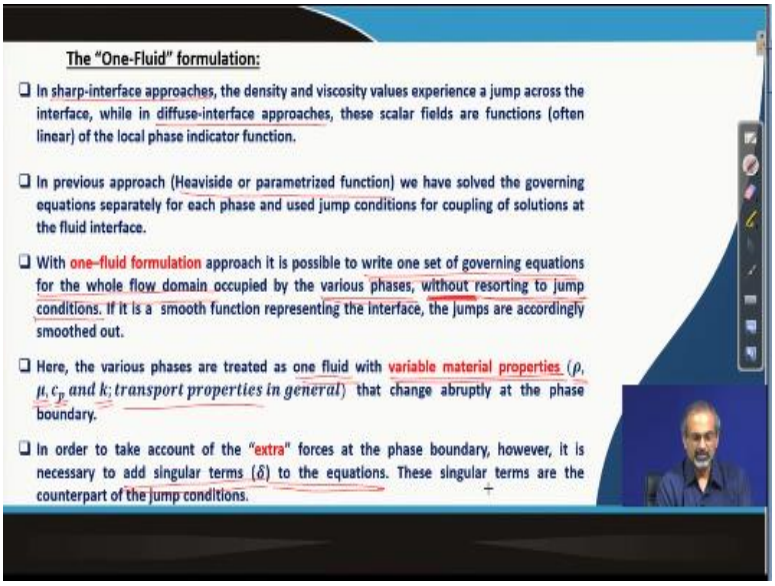

Now, we come up with a very popular kind of formulation, which is called as the one fluid formulation. So, we will quickly go through the points. So, we have discussed about capturing the interface using sharp interface approaches where the density viscosity values experience a jump across the interface while there could be diffuse interface approaches where the local face the property changes can be occurring in a more diffused manner across the interface.

So, these are the two possible ways. So, in the previous approach that is in the sharp interface approach, which is through say heaviside function or parametrize function, we solve the governing equations separately for each phase and use jump conditions for coupling the solutions at the fluid interface. We just finished discussing the jump conditions in the previous slide in fact.

Now, if we look beyond this approach, we can think about one fluid formulation approach which is possible when you write one set of governing equations for the whole flow domain. So, we are going to use one set of equations and we are going to apply to the whole flow domain where the various phases are embedded anyway, but we are not going to resort to jump conditions.

So, we are not resorting to jump conditions across the interface. So, it is a smooth representation of the interface and accordingly the jumps will be accordingly smoothed out in a certain manner. So, that we continue to use the single set of governing equations with a smoothed out version of jumps. And we do not enforce the jump conditions per se. So, of course, if you do not do that, you have to tackle the variation across the interface in some other alternative manner.

And that alternative manner in this case would be introduction of some kind of a source term, which gives you an analogous effect in the form of a car kind of forcing, which explains where the interface is. That means in spatial sense at a specific time instant, if in some regions of the flow, we are finding that the forcing terms are becoming active, then those are the regions which form a part of the interface.

So, in this approach the various phases are treated as one fluid, but with variable material property. So, we have to keep in mind that we do not have distinct definitions of two or more fluids separated by interfaces, but rather as if the same fluid is moving around with variable material properties in different regions and these different regions form different phases.

So, these material properties could be density, viscosity, specific heat, thermal conductivity and other transport properties in general, which can change abruptly and the phase boundary but for all practical purposes, the abrupt change here basically means a kind of smooth out change as far as the computational implementation is concerned.

Now, in order to account for extra forces at the phase boundary, it is necessary to add similar terms to the equations and these are the source terms we were talking about, which have to be introduced into the momentum equations, which are essentially the counterpart of the jump conditions for sharp interface approaches.

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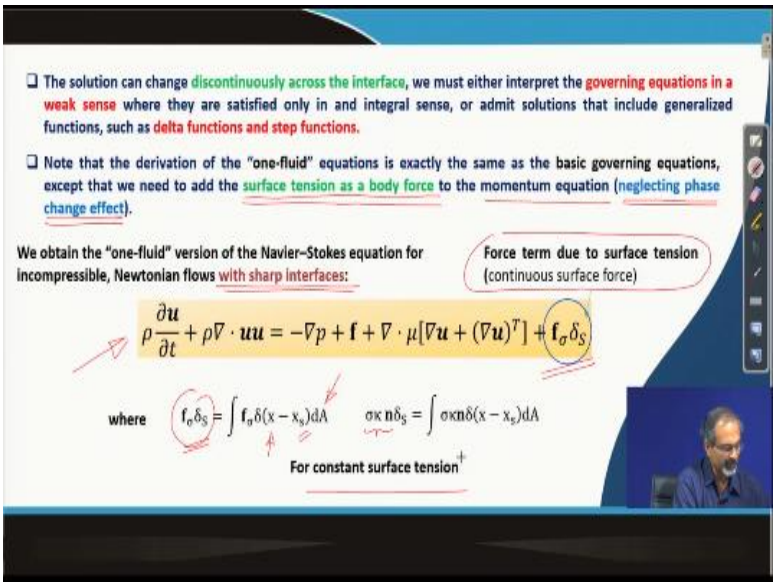

So, going a little further into it, the solution can change discontinuously across the interface, we must either interpret the governing equations in a weak sense, where they are satisfied only in an integral sense or admit solutions that include generalized functions such as delta functions and step functions that is heaviside functions. So, these are two possibilities. So, if it is discontinuous change, it is a sharp interface case.

If it is through application of generalized functions that we introduce certain source terms in governing equations and try to simulate the interface then it is talking about the diffused interface. And moreover, if you have discontinuous changes, then you have to treat the equations in weak form. Note that the derivation of one fluid equations is identical to what we do for basic governing equations, except that we need to add the surface tension as a body force and this is a very important issue here.

Surface tension has to be added as a body force to the momentum equations. And then that is the only change by assuming that there are no phase change effects. So, if there are for the phase change effects, then you have to consider the mass exchanges at the interfaces. So, one phase may vanish to some extent converting itself to the other phase and so on. And there could also be implications in terms of the energy conservation.

Now, in the one fluid version of Navier Stokes equations, then we have the interfaces accommodated in the form of a forcing term due to surface tension and this has a form which we have discussed earlier and we are introducing the delta function and remember that as

long as this x falls somewhere on the interface, which is defined by this S, then the delta function becomes active.

And therefore, you have a spike font in that region. So, as long as you lie anywhere on the interface, then this term will become active and you are essentially integrating over an elemental area as you go along the interface that way and you are considering that you know the surface tension is essentially constant and that is what makes the representation of f sigma simpler in the form of only sigma k n which we have discussed earlier.

So, the constant surface tension is therefore, an assumption here further we may add a little bit on the continuous surface force, which we had indicated here or often abbreviated as CSF.

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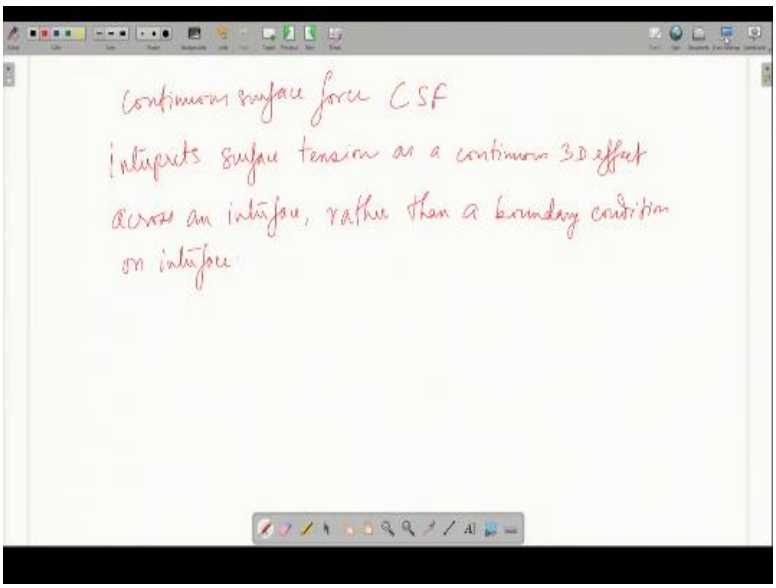

So, that is essentially an approach which interprets surface tension as a continuous 3D effect in general across an interface, rather than a boundary condition on interface and a volume force due to surface tension on the fluid elements lying within a finite thickness transition region which defines the interface replaces the discontinuities. So, this is essentially the concept and this aligns with the assumptions of the one fluid approach.

So, we had a basic look at how the governing Navier Stokes equations would then have to be modified when you try to look at it from one fluid perspective.

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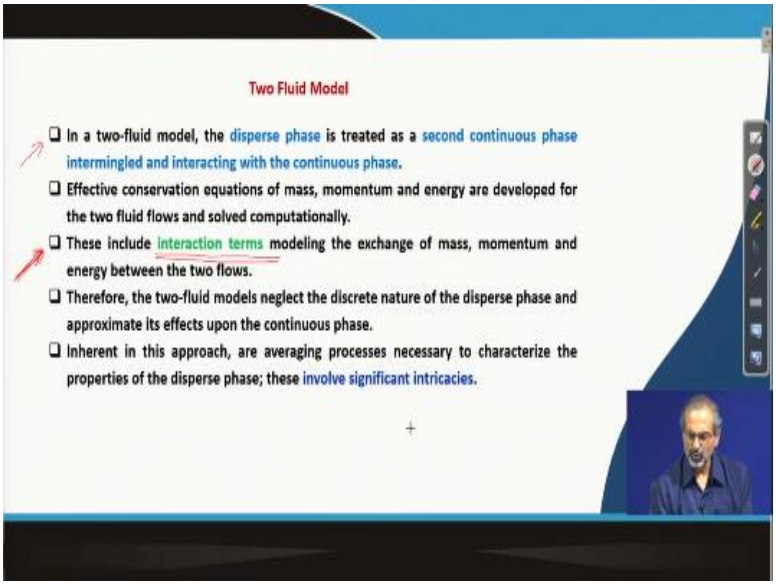

This could be a good time to also look at another alternative approach which is called as two fluid model, which is more intricate than the one fluid model, but is also widely used in multiphase simulations. So, if we look at the points in a two fluid model, the dispersed phase is treated as a second continuous intermingle phase, which is interacting with the continuous phase.

And the effective conservation equations of mass momentum energy are developed for the two fluids and solved computationally and they would include interaction terms, which model the exchange of mass momentum energy between the two flows. Therefore, the two fluid models neglect discrete nature of disperse phase and approximate its effect upon the continuous phase itself.

Now, you have to keep in mind that this effect is primarily coming in through the interaction terms as we have mentioned in the third point. And in this approach, there are certain averaging processes which are necessary to characterize the properties of the dispersed phase and they could also add on to the intricacies of the computations. There are more modeling issues also, which can add on intricacies of the competitions. So, to keep things simple, we are confining ourselves to the one fluid model.

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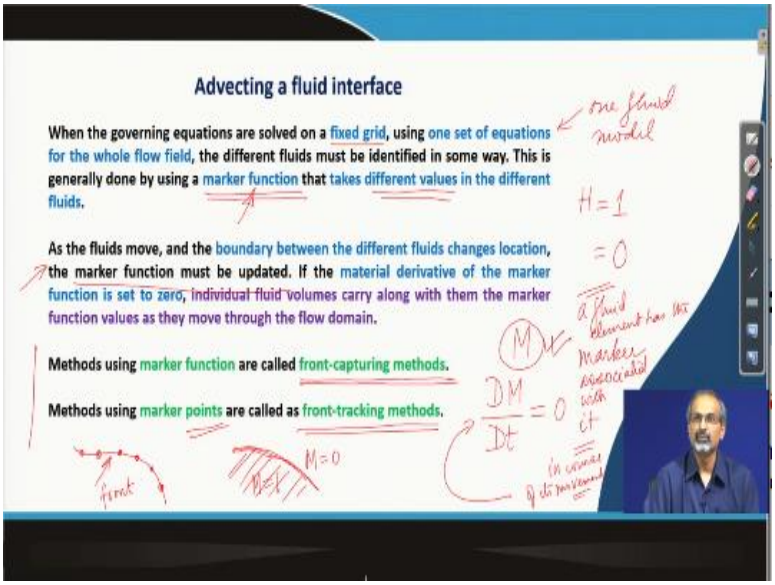

Now, we learn quite a bit about how jump conditions may occur across an interface and if you are solving the problem as a sharp interface problems, how these jump conditions have to be implemented through boundary conditions. And if you treat the interface or boundary as diffuse boundary, then there is also an issue of how you try to advect the fluid interface.

So, now, we will briefly discuss about advection of the fluid interface. Now, if we consider that the governing equations are being solved on a fixed grid with using one set of equations for the whole flow field, which is true for the one fluid model which we are going to further expand in the subsequent lectures of this module. The different fluids must be identified in some way.

So, you have to keep track of where the respective fluid regions are located at. Now, in order to do that, we make use of a very important concept Marker functions, which we had briefly discussed in the context of level set. Here, we will expand further on this concept and we notice that this Marker function will take up different values in the different fluids. And this is a very very important concept for example, we had earlier shown that in one fluid.

When we treat it as a sharp interface region, the heaviside function can take up a value of 1, in another fluid, it can take up a value of 0. So, that was a sharp interface definition. Even in the sense of diffuse interface, you can distinguish by assigning certain Marker functions. And we will try to discuss on what these Marker functions are all about. So, as the fluids move the boundary between the different fluids they would change location.

And therefore, the Marker function has to be accordingly updated. If the material derivative of the Marker function is set to 0, individual fluid volumes carry along with them the Marker function values as they move through the flow domain. So, if I say that a Marker function is given by M, then what it means is that the substantial derivative of M is going to be 0. Each fluid element carries along with it a certain information about M, a certain value of M.

So, whenever this fluid element is moving around to different regions of the flow, it is always carrying along with it the particular M value that it is carrying. So it has the Marker associated with it always. So a fluid element has the Marker associated with it. In course of its movement that is something we have to always keep in mind and mathematically it is represented through the material derivative equal to zero condition.

Now, when methods are used, where Marker functions are deployed, we say that we are using so called front capturing methods and when we use Marker points, then we have front tracking methods. That means as though there is a region which is carrying certain Marker function of a certain value M = 1. This is another reason, M = 0. And this front is advancing in some manners, then we are using Marker functions to demarcate the two phases.

While there could be approaches by which we have a collection of points which are moving through the domain and the collection of points define the front. So, if we have such Marker points, and we are tracking those Marker points, we have so called front tracking methods and if we have Marker functions and we are tracking them. We have the front capturing methods.

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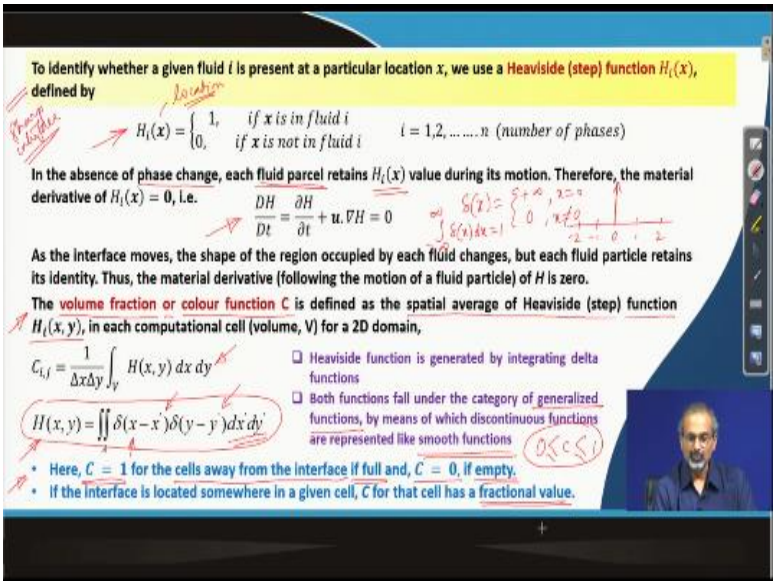

To identify whether a given fluid i is present at a particular location x, we use the heaviside or step function H i x and that is defined through this function that H i x =1 if the vector x lies in fluid i; r is equal to 0 if the vector x is not in fluid i. Of course, the vector x is essentially carrying locational information. Now, in the absence of phase change, each fluid particle retains the H i x value during its motion.

Of course, remember that whenever I am talking about heaviside function, we are talking about sharp interface. Now, since we are discussing one fluid model, where we are actually going to take the route of diffuse interface, we are not going to perpetually carry through the concept of heaviside function, but when it comes to implementation, we will change the word mainly to Marker functions.

But those Marker functions will depend on how we connect them with the heaviside function description which is nothing but the sharp interface description of the problem. So, that dependence always has to be kept in mind. Now, as long as it is the sharp interface and there is no phase change, a fluid parcel or a fluid element will satisfy the material derivative of H = 0 condition like what we described in the previous slide.

So, as the interface moves, the shape of the region would change and the fluid particles would retain their identity as the shape of the region changes. Now, we introduce one of the Marker functions which is called the as the volume fraction or color function C, which is defined as the spatial average of the heaviside step function. Now, before we do that, we have a quick look at the heaviside function itself.

So, in a two dimensional plane, it is comprised of product of delta functions integrated over an elemental area. So, when x lies in the region or rather when x lies in the region covered by x dash and y dash and y lies in the region covered by x dash, y dash, then these respective delta functions will give a spike in their values. Because if you recall from our earlier courses in mathematics, the direct delta functions have a spike like behavior.

So, we say that the delta function could be defined as delta x equal to positive infinity, if x = 0 and is equal to zero, when x is not equal to 0. And additionally, when you integrate it from negative to positive infinity, this gives you a 1. So, the function looks like this. We have a very large spike here. So, you are using such delta functions here and integrating and that gives you the heaviside function in 2D.

And that you are spatially averaging in order to give you the so called volume fraction or color function C. And remember that heaviside function or delta functions, they are, they fall under the category of generalized functions and these functions are used for discontinuous represent, I mean with these functions, discontinuities can be represented in a smooth manner.

So, from there we are able to get a tool, which will act as a Marker function which we are naming as volume fraction or color function. And that C can take a value of one for cells, which are away from the interface and cells which are full and C = 0 if they are empty. So, if the interface is located somewhere in a given cell, C for that cell has a fractional value. So, that basically means that C can live within this region. So, we will discuss more on this in the subsequent lecture. Thank you.