Introduction to CFD
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Lecture - 50
Basics of Interface Capturing Methods for Applications in Multiphase Flow

In this lecture, we will begin our discussion on interface capturing methods for application in multiphase flow.

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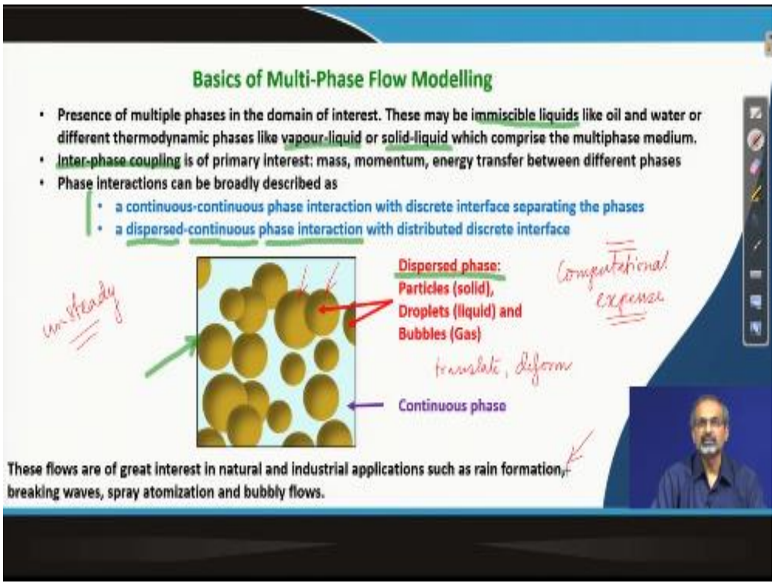

In this slide, let us look at the basics of multiphase flow modeling. So, in multiphase flows, we say that there is presence of multiple phases in the domain of interest and we would have different possibilities here. So, there could be immiscible liquids like oil and water or there could be different thermodynamic phases like vapor liquid or solid liquid and they would comprise the multiphase medium.

Now, whenever you have multiple phases available in the flow, there is the presence of phase boundary and across the phase boundary, there would be exchange of momentum and also possible exchange of mass and energy. So, there is the issue of interface coupling which has to be taken care of. So, that these exchanges of mass momentum energy can take place through the interfaces.

Now, how do the phases interact? There could be possibilities of continuous-continuous phase interaction in which case you will have discrete interface separating the phases and very often this could be a single surface without any kind of breaks or discontinuities. And if you have one of the phases in a dispersed manner, within another phase, which is essentially continuous.

Then you have the case of dispersed continuous phase interaction where if you look at this figure, you would get an idea of what we are trying to mean by dispersed continuous phase interaction because you can see that the bluish color region is indicated as continuous phase. Let us say it is liquid and in that liquid we have suspended particles which could be solid or they could be droplets of another liquids.

In that case, the two liquids are invisible or they may even be bubbles, which are essentially gas particles, if you call it that way. And in that case, you have the presence of a dispersed phase in a distributed manner in a continuous phase. And if you have that you can also understand that the interface in this case would be a collection of interfaces with one interface per entity of the dispersed phase.

That means if you consider any one of these particles, then there is an interface between that particle and the continuous phase. And then if you move on to another particle, then there would be a new interface between that particle and the continuous phase and so on. And these dispersed phase particles can vary widely in size. For example, if you have bubbles immersed in a liquid, you will have a wide range of sizes most often.

There could be much bigger bubbles, there could be much smaller bubbles and there could be again bubbles which are at an average size. So, the dispersed phase depending on what kind of phase it is, it can of course, translate and it can also deform and as we already said that there could be a wide range of sizes or distribution of sizes, which is possible.

So, when you look at it from CFD perspective, if you are trying to discretize your domain and trying to capture dispersed phase within a continuous phase, then it becomes a challenging problem because you have to have a discretization of the domain done in such a manner that you can capture the smallest phases by deploying a few grid points across the smallest particles.

And at the same time, you should ensure that in the process, you can also capture a large number of particles in the domain. So, that on an average you can solve the flow with enough number of entities of the dispersed phase immersed in the continuous phase. So, that you can bring out meaningful averages out of the simulation. So, if you have to deploy a reasonable number of grid points to capture the smallest particles, then you will find obviously that the grid numbers across each direction will become enormously large.

And therefore, it becomes computationally very expensive. So, from a CFD perspective, the computational expense is certainly linked with what kind of ranges of sizes you are trying to look at. And, of course, these interfaces are unsteady that means they are going to move with time, they could also deform this time. And we will talk more about governing equations, which address the distribution of these phases and how we can handle the conditions at the boundaries a little later in later slides.

Come to the bottom line of this slide, we find that these flows are of great interest in both natural and industrial applications, starting from rain formation to breaking waves, which you find in the ocean coast spray optimization, which could have a large number of applications including say combustion and bubblly flows through pipes and so on.

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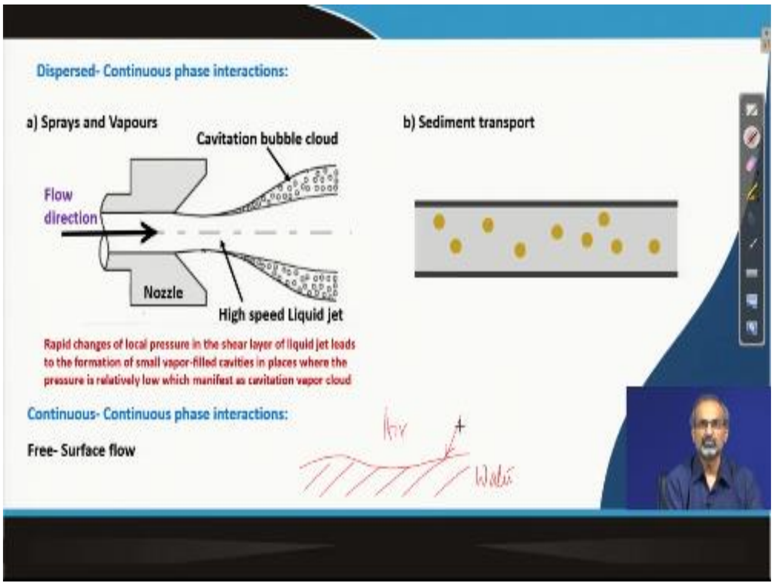

Let us look at a few instances of dispersed continuous phase interactions. So, in this figure (a) as you can see spray and you have a high speed liquid jet emerging out of a nozzle and then there could be rapid changes in the local pressure in the shear layer of the liquid jet and this would often lead to formation of small vapor filled cavities in the edge of the jet and the formation of cavitation bubbles.

So, you have continuous liquid phase in the form of the jet and you have the formation of bubbles which exist in a dispersed manner in the periphery of the jet. So, this is an instance of dispersed continuous phase interaction and other instance is given in the figure (b) where you find that there are particles moving through a pipeline, which are essentially carried by the bulk flow of the fluid, the particles are indicated by the yellow spots.

So, they are essentially the sediments which are transported through the bulk fluid motion. So, you have a dispersed particles in a continuous liquid and then you can have instances of continuous-continuous phase interaction, one instant is a free surface flow. So, if you imagine that you are looking at the waves formed in on a river surface, then they may often look like this.

So, you have air above and you have water at the bottom and very often, you have two continuous media interacting with each other. Other as long as the interface remains intact, it does not become discontinuous. And then, you can consider these two media as two different continuous phases.

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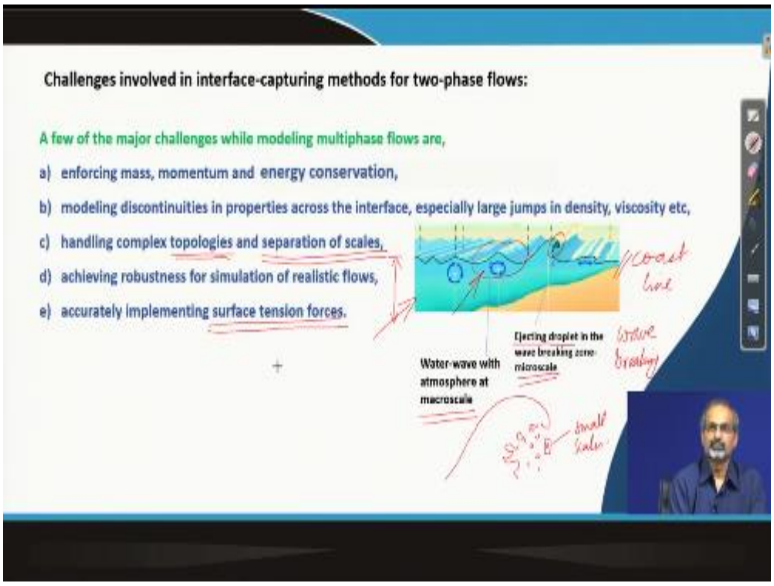

We move on to look at the different challenges which are involved in interface capturing methods in CFD for two phase or in general multiphase flows. And if you look at the challenges, they are as follows. So, you have to enforce mass momentum and energy conservation. And as we said that very often we have to enforce these exchanges at the interfaces or through the interfaces.

We have to model discontinuities in properties across the interface because you are handling different phases and therefore, you can very well understand that there would be jumps in the properties of the respective fluids in terms of say density, viscosity, could be thermal conductivity, specific heat and so on. So, we have to model the discontinuities in the properties of the fluids across the interface.

And then, as you saw earlier that you may often have to handle complex topologies in the sense that if you have especially a dispersed phase immersed in a continuous phase, then you have large number of entities of the dispersed phase. And therefore topologically the problem becomes more difficult. You have to handle each of the entities and its boundaries often in a three dimensional sense and that is certainly a complicated issue.

And then there could be wide separation of scales, which can be better explained through the diagram that we have here. So, this is a diagram indicating the ocean waves in close proximity to the coast line. So, the coast line is somewhere here and the ocean gets deeper in this region. So, as the waves approach the coast line, you can find that waves in this region are more on a macro scale in the sense that you know there are larger lens scales associated with these waves.

The wavelengths are larger. Amplitudes could be larger, but, even then, you know, it is a continuous-continuous two phases which are interacting with each other. So, we have existence of macro scales here, while the moment the waves come closer to the coast line, there is a tendency of the waves to break. So, due to wave breaking, we have formation of or ejection of droplets in the wave braking zone and that can lead to micro scale formation.

So, if you zoom close into that region, what it looks like is you know structures of this kind and there are droplets emerging in that region and therefore, you have very, very small length scales to cover. So, these are small scales, which you have to cover and they are much smaller than the scales we talked about in this region, which are the essentially the macro scales.

Now, computationally this problem will become very difficult to tackle because of the so called separation of scales, there is a wide difference in terms of the lens which are concerned. So, on one hand you have to probe deep into the smallest structures. So, that you can capture the droplet breakup and things like that. On the other hand, you have to cater to the much larger length scales over which the bigger waves are operating, without which you will not be able to capture their effects.

And of course, the entire picture has to be captured simultaneously. So, that we can capture the physics in general. So, that makes the problem computationally enormously complicated. And additionally, as you can understand that in regions where you have formation of smaller structures, the mesh, the grid, in whatever way you deploy it also has to be reasonably fine with a coarse grid.

You will not be able to capture these structures, because they will automatically get filtered out, because the grid scales are much larger than the actual length scale which the physics dictates. So, that way the computation becomes very difficult both topologically as well as because of the wide separation of scales. And very often these governing equations or boundary conditions, which you have to enforce at the interfaces can give rise to stiff system of partial differential equation.

And therefore, the numerical solver which has to be used in that case has to be robust enough to simulate realistic flows involving such phase interactions. And then you also have to take care that the surface tension forces which are existing at the interfaces are also represented or modeled accurately enough. So, that the physics is well captured.

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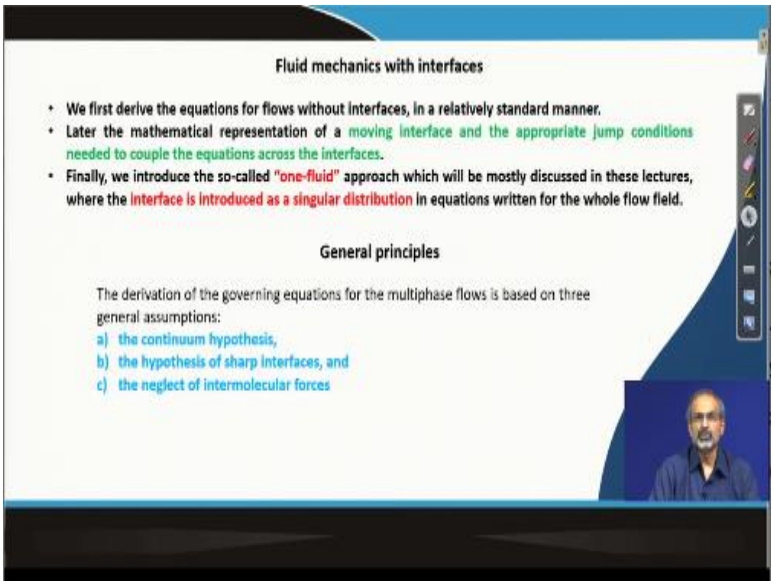

If we look briefly at the fluid mechanics with interfaces, in this slide we would like to outline the basic strategy that we first derive the equations for flows without interfaces, which are the general governing equations which we are familiar with and they can be derived in a relatively standard manner making all the basic assumptions and approximations. And also in forms which are applicable either in differential or integral form.

And then, later, the mathematical representation of a moving or evolving interface and the appropriate jump conditions need to be coupled with the equations across the interfaces. So, once you appropriately accounted for these conditions at the interface then the same sort of governing equations can be made usable for a multiphase problem.

And then we would talk later more about a so called one fluid approach, which will be mostly discussed in the upcoming lectures in this course, where the interface is introduced as a singular distribution in equations are written for the whole flow field. So, wherever these singular distributions become active, then automatically the interface is accordingly simulated when the computations occur.

So, it is essentially a single fluid, but with different fluid properties in different regions incorporated across the interface and the interface definition or location is introduced through a similar distribution, which is going to be discussed later and it is forced through a certain source term in the momentum equations. The general principles involved in fluid mechanics with interfaces are as follows.

So, the derivation of the governing equations for multiphase flows are based on 3 general assumptions, one is the usual continuum hypothesis, which is applicable for the Navier Stokes equations and Euler equations, then we incorporate the hypothesis of sharp interfaces and then we neglect intramolecular forces. So, these are the basic issues which we take care of when we derive the governing equations and we apply to multiphase flows.

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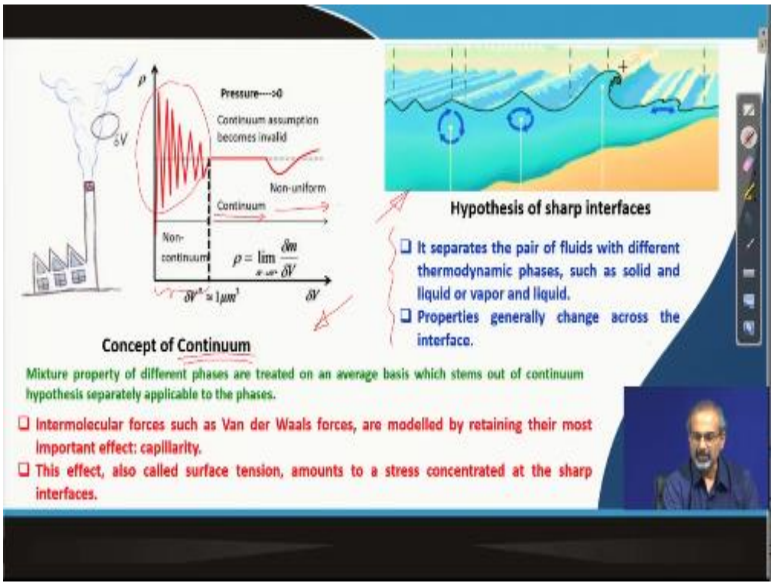

We are looking back once again at the picture that we use to talk about separation of scales earlier. So, we have discussed that to some extent already, so, let us look at the other issues that we indicated in the last slide beginning with the concept of continuum. So, we all recall that macroscopic properties that we see when we are talking about a fluid dynamics problema, could be velocity, could be density, could be temperature.

So, though we in general handle the **(()) (17:30)** all in a macroscopic sense, but their root cause lies in moments at an atomic or molecular level. However, the continuous nature of the medium gets lost when we probe so, deep into small length scales. So, that we can see the atomic or molecular movements and therefore, using the average properties becomes difficult.

We have to track individual particles or atoms and apply the necessary physics at that level. And we usually take that approach in say molecular dynamic simulations, but, when we try to deal with average properties, we deal with the medium as a continuous medium, and then essentially we go to much larger lens scales, then say the mean free paths which are involved for the medium.

So, if you are operating at atomic scales, then typically you are going to be at a very, very small control volume, which is indicated by the delta V region. And then you will find that the properties very widely vary and are a function of both space and time, because, if you are putting some kind of a probe into such a small region, then the probe will randomly encounter moleculer collisions and therefore, there would be spikes in whatever property it is recording.

And therefore, you will have a nature of this kind, but as you move to larger length scales, then mean free paths, the medium tends to behave like a continuous medium, and then you are starting to operate over continuum and then over a certain moderate range of scales, you can see that the properties essentially remain constant. But if you move to still larger land scapes, then there could be non uniformities which can show up further.

So, this is essentially the purview of continuum hypothesis. And then, as far as multiphase is concerned, so, when we talk about the mixture properties of different phases, they are treated on an average basis which stems out of the continuum hypothesis. And this concept would be applicable to all the phases that we tackle. As far as intramolecular forces are concerned.

So, forces such as Van der Waals forces are modeled by retaining them most important effect that is capillarity. And this effect, which is also called a surface tension amounts to a concentration of stress at these sharp interfaces and there are different means by which they could be implemented, either they could be implemented in the form of jumps in the stresses or they can be approximated as a continuous variation over a small length scale.

And that would define how you change your work from the stress distribution of one phase to the other. And then just a recapitulation of the hypothesis of sharp interfaces which we discussed already in a previous slide, it is the separation of the pair of fluids with different thermodynamic phases such as say solid and liquid or vapor and liquid and properties generally change across the interface and the interface can involve wide separation of scales. And the example that we gave was very small droplets here, very large waves here and so on.

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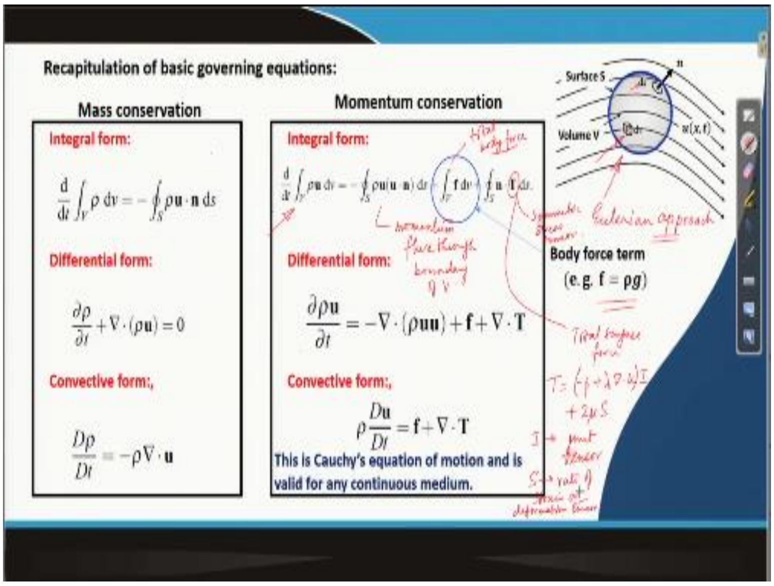

Now, we come to the recapitulation of the basic governing equations of fluid flow involved in multiphase problems. So, in the corner we have a small diagram, where we are talking about a small control volume as you can see the control volume has a surface and there could be a small elemental region of that surface indicated by ds and there is an outward pointing normal from that a elemental surface area.

And the volume that is enclosed by that surface is given by v. And, in general, we would assume that there is a velocity field which is a function of both space and time, which is moving through this region and we would assume that this region is fixed in space. So, that is typically what we do in Eulerian approach. And we try to monitor the flux of different quantities across the boundary of such a control volumen.

So, that we can develop the respective conservation equations which involve mass momentum and energy. So, if you look at mass conservation for instance, you will find that if you integrate the effect of mass flux and possible existence of mass sources and things in the control volume, then you will be able to come up with the first form which you have over here.

So, that talks about the time rate of change of mass which is within that control volume and then the right hand side of the equation talks about the mass flux across the surface. So, when the sum of the two effects is equal to 0, you have the in-flux of mass balanced exactly by the out-flux of mass. That means there is no mass stored within the control volume as such.

And mast in general, this should be true for elemental mast control volume like the one we have tried showing inside this finite control volume, which is infinite similar in extent, and then out of this integral form of the equation emerges the differential form which is true for the smallest of elements. And therefore, it involves the derivative based expression. Again, by applying the concept of material or substantial derivative, we can also show that the same equation can be represented in terms of the material or substantial derivative of density.

So, that is broadly the idea of the mass conservation equation which we have of course, learned in a basic fluid mechanics courses, but we are just recapitulating the ideas once more. And then comes the concept of momentum conservation, where we find again applicable for that small elemental control volume we have found the indication on the left hand side is the rate of change of momentum in the fixed volume v.

And then on the right hand side, we have different terms, we can indicate the first right hand side term as so, this is the momentum flux to the boundary of the volume and then the second term is the total body force. Very often if we have gravitational force applicable for heavier fluids, we would indicate it through the body force term. And then comes the total surface force term.

And that of course, involves the symmetrix stress tensor and that dot product essentially indicates the force on the surface element ds. So, we have that small elemental surface on that element what is the surface force acting and we can show that the stress tensor for Newtonian fluids will be indicated as minus p plus lambda times divergence of u times and unit stress tensor I plus 2 Mu S where S is the rate of strain or deformation tensor.

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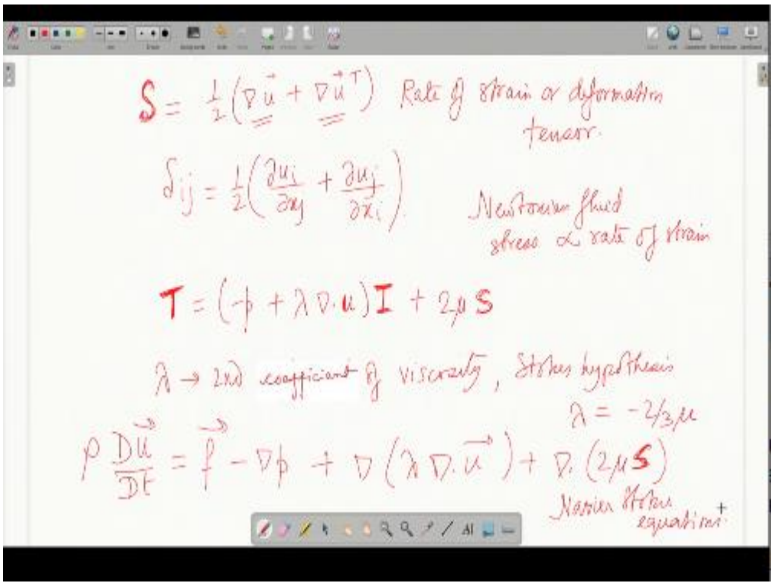

So, I is unit tensor and S is rate of stream or deformation tensor and into it you can show that this stress tensor S is given by this and of course, as you can understand these are all tensors because Nabla operates on the u vector and if you look at the elements of the stress tensor, you will find that they work out to be and if you recall in the stressed. So, this is our rate of strain or deformations tensor which was part of the stress tensor T.

And remember that because we are handling a Newtonian fluid, we have stress is proportional to rate of strain and based on that the strain tensor T has this expression and here lambda is second coefficient of viscosity and from Stokes hypothesis, we know that lambda is equal to - 2/3 Mu. So, we have made a number of approximations or assumptions rather to finally, express the momentum equation in a form like this.

And this is the well known Navier Stokes equations. So, these are the details essentially which we need to keep in mind. So, that we can fill in the gaps. And so, remember that starting from the Cauchy is equation of motion, which is applicable for continuous médium. You can very easily show how it translates to the Navier stokes equations through the assumptions that we imposed.

And we showed the form of the Navier stokes equations. We will proceed with the remaining issues of interface tracking techniques for multiphase flow in the next lecture. Thank you.