# Spray Theory and Applications

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## Lecture - 35
## Multiphase flow modelling basics

Welcome back. We are going to continue our discussion of Multiphase Flows. Towards the end of last class we had derived the Williams spray equation, and we were in the process of understanding, how that can be applied to a general multiphase flow problem especially sprays.

What we are going to do today is switch (Refer Time: 00:38) slightly and see what are the different approaches available to us to study multiphase flows. And then see where the Williams spray equation defaults to which of the approaches would best be supported by the Williams spray equation approach, because there is an advantage to using the probability density function formulation that we saw earlier.

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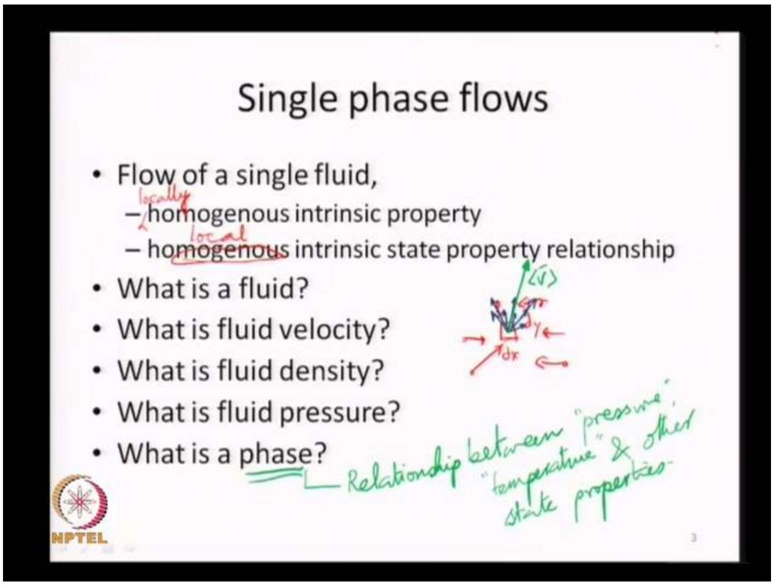

Single phase flows

- Flow of a single fluid,
  - locally homogenous intrinsic property
  - local ~~homogenous~~ intrinsic state property relationship
- What is a fluid?
- What is fluid velocity?
- What is fluid density?
- What is fluid pressure?
- What is a phase?

Relationship between "pressure", "temperature" & other state properties

So, let us look at some basics of Multiphase flow modeling today. Now will start with our understanding of what is a single phase flow? A single phase is quite commonly is known to us, it is a fluid that has a homogeneous intrinsic property at least locally homogeneous intrinsic property; say what you mean by intrinsic property is let us say temperature or specific volume or velocity is also an intrinsic property. And an intrinsic state property relationship, what we mean by that is that say for example, an ideal gas relationship is one that defines, is one that relates the pressure locally at a point to the temperature.

So, the key word here is to say that these are local relationships, and also locally homogeneous intrinsic property. Now based on this if we go out to define what is a fluid, this is again I am not going to well for a very long time on this, we all now know that a fluid is a collection of molecules say for example, water in a beaker is a collection of about 10 power 23 molecules would be in order of magnitude less or in order of magnitude more. But essentially each the molecules are in a state of random motion, when you consider water in a beaker, just because the water is at rest does not mean the molecules in the water are also at rest.

Now in that context, what do we mean by fluid velocity? Fluid velocity is essentially an average velocity over the range of over a period of time. So, if I was to locally observed molecules passing through a certain spatial volume, in (Refer Time: 03:39) spatial volume, the average velocity of all the molecules that passed through that point over that short period of time is what we would in fluid mechanics, term as the instantaneous fluid velocity.

So, what we do is typically we take a little spatial volume some dx dy and we have all these molecules that are passing through in different directions. We wait for a few to cross these boundaries, so let us say I have one crossing there one crossing here. If these velocity vectors were indicative of the real molecular motion, then we would find an average emerging out of this; as you can see I will draw the average, in a sort of an exaggerated sense. So, this average velocity over all the molecular motion is what we typically define as our fluid velocity.

Now the fluid itself we now know is a hypothesis; that is there are molecules, molecules are made of atoms, atoms are made of sub atomic particles, but after having learnt that we still like to restrict our attention to what we have traditionally or classically known as the fluid. So, the fluid having a velocity sort of intuitive it is observable by the naked eye and most instances, it is observable.

Say for example, when I have a river is flowing, the velocity that is observable on the surface of the river is let us say a tiny dried leaf or a speck of dart that is moving with the flow of water, and the speck of dart has a velocity that is identical to the water just underneath the speck of dart. In that sense we are used to idea of a fluid having a velocity and we do not have to go all the way down to molecular velocities and acquire an average over some molecular velocity to really understand fluid velocity. So, we are going to remain at the level where we know what fluids are, we know what fluid velocities are.

Now density is also apparent at this same level, that if I took a certain volume of the water it and I can weigh the mass of the water per unit volume is what we defined as density; the same density would apply to any fluid that is made up of discrete entities. So, for example, we said we went down to the molecular level defined what a fluid velocities and then we said we are going to discarded and we are only going to restrict ourselves to the fluid velocity, that we classically know from observations. We will do the same thing with density.

So, density is also in some sense the mass of all the molecules that are contain in a certain volume per volume occupied by all the molecules. So, essentially we take a set of discrete entities and then take the mass of all the discrete entities divided by the volume occupied by those discrete entities at any given state being temperature, pressure, and etcetera. Now the reason I am sought of dueling upon these definitions is because, we will use the same ideas to define the same properties in the context of a dispersed phase continue. We will see what that is a little later.

Pressure is another quantity that we understand. Pressure is the average force exerted by molecular collisions on a given wall per unit time. So, it is like the average force exerted on the wall per unit area, the force itself is coming from molecular collisions with the wall. And this average force is measurable in terms of let us say a piston moving upwards. And so we can now again do the same thing that we know the origins of the force, but we do not have to completely pay attention to the origins of the force in order to define pressure, which is a force it is coming from the gas. In fact, the very first ideas of pressure originated from Hook’s law from like elasticity and a gas was thought to be an elastic medium just like a piece of rubber or steel and it exerts a certain stress and it as a certain property just like a Hook’s law. But we know now it is not entirely correct, but it is a sufficient phenomena logical model for a few different applications.

So, if I now use these ideas to define what a phase is, we are going to come back and talk about this. The phase is typically one that we can quantify the relationship between pressure, temperature and others state properties. So, essentially if I look at what is a phase? I we may sort of know three phases of matters solid, liquid and gas, but what is it fundamentally that separates the three phases; one is there appearance, that is what we are sort of first start about phases; but more than that it is this relationship between the stress field in the medium and temperature or temperature and let say density.

So, these relationships are unique for the same material in different phases. So, the relationship is different in different phases, for the same material. And when this relationship changes is when you know that the material has undergone a phase change. So, we will build up on these ideas in the context of a multiphase; we will sort of generalize these ideas into arenas that seem a little bit stretched, but we will show how they work.

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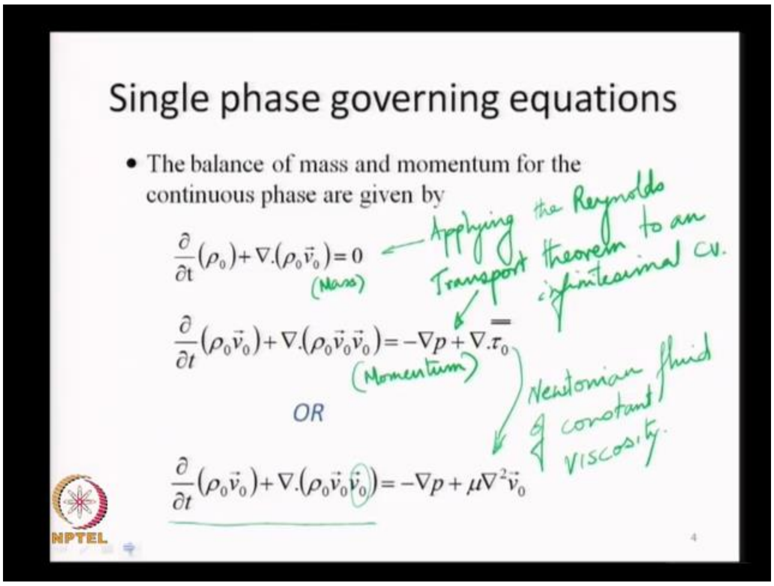

## Single phase governing equations

- The balance of mass and momentum for the continuous phase are given by

$$\frac{\partial}{\partial t}(\rho_0)+\nabla.(\rho_0\vec{v}_0)=0$$

(Mass)

Applying the Reynolds Transport theorem to an infinitesimal CV.

$$\frac{\partial}{\partial t}(\rho_0\vec{v}_0)+\nabla.(\rho_0\vec{v}_0\vec{v}_0)=-\nabla p+\nabla.\overline{\overline{\tau}}_0$$

(Momentum)

OR

Newtonian fluid of constant viscosity.

$$\underline{\frac{\partial}{\partial t}(\rho_0\vec{v}_0)+\nabla.(\rho_0\vec{v}_0\vec{v}_0)}=-\nabla p+\mu\nabla^2\vec{v}_0$$

Now we defined what a single phase is. Now we are used to seeing Navier stokes equations in our advance classes in fluid mechanics, where we write down the balance of mass and momentum for a continuous phase. And the first equation essentially comes from applying mass balance in the form of the Reynolds transport theorem to an infinitesimal control volume. And the second part comes also from the same source except this is mass balance and this is momentum balance.

So, mass balance is some of all mass in and mass out should equal any mass accumulated. And momentum balance also says a same thing that some of momentum in and momentum out should equal any external force. So, this is essentially Newton second law applied to a fluid field on an infinite fluid entering a leaving an infinitesimal control volume. We are in more text books we will find the momentum balance equation sort of specialized to the case of a Newtonian fluid of constant viscosity and that Newtonian fluid of a constant viscosity gives us the relationship given here under.

Now if we think of, if we go back for moment to our William spray equation, the first two terms on the left hand side of the William spray equation look exactly like the first two terms in the momentum balance equation. Except instead of advecting the velocity field, we are advecting the probability density function. So, this material derivative you know is something that you will find commonly occurring in any field description of fluid motion.

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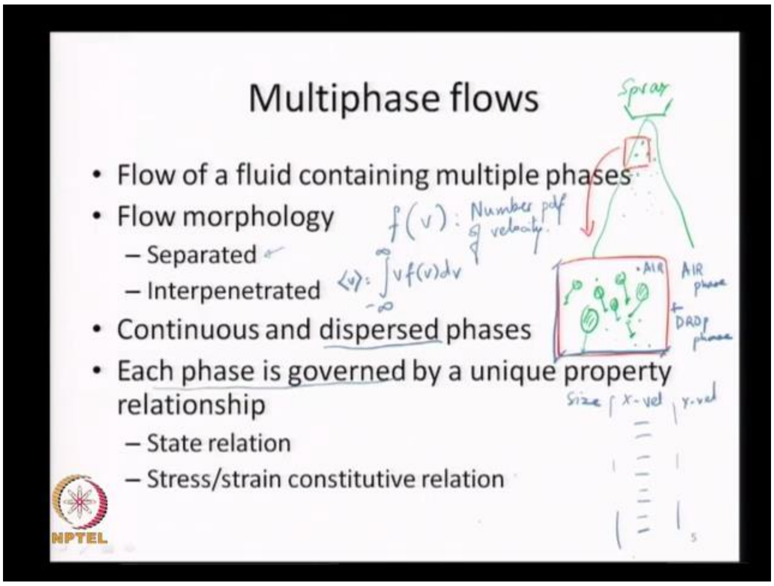

## Multiphase flows

- Flow of a fluid containing multiple phases
- Flow morphology
  - Separated
  - Interpenetrated
- Continuous and dispersed phases
- Each phase is governed by a unique property relationship
  - State relation
  - Stress/strain constitutive relation

So, with that as our foundation of what single phase flows are, if we look at what multiphase flows look like, essentially I can define the flow of a fluid containing multiple phases. So for example, I could have you know with the one multi phase flow we will looked at for all most two third of this semester is a spray. So, we will take a few examples to understand what this is. So, I have a lot of these drops in some very well defined spatial region called you know it is a reasonably well defined spatial region. And the flow itself if I zoom in to a part like that, it is composed of drops of different sizes and they are all moving with different velocities.

In constructing our pdf we already done this to some extent, how do I construct the velocity pdf or more relevantly size velocity joint pdf in a situation like this. We stated one point, let us say I define a part here and a part here and wait for particles to cross those to blue lines. And every time a particle crosses one of the two blue lines, I take account of it size and velocity and over time I would have accrued enough statics to generate a probability density function in this 2 variable size and velocity. Really speaking it is size and in this particular example 2 components of velocity. So, it would be a 3 scalar, 3 component 3 dimensional pdf.

Now what would I then define as the average velocity of all the bubbles or of all the drops in this instance; it would be the number average, let us just take the simplest of instances and then we will see what other kinds of average is there may be. So, the simplest would be I have a long list of averages of all the different drops that I was able to sample; there x component of the velocity and y component of the velocity, so I have size x velocity and y velocity, we have seen this in real data as well. I have all this data, if I do the average over all the velocities the x velocities I get the average x component of the velocity purely averaged by the number of drops that I sampled, and likewise I can get the average y velocity component.

If all the drops were of the same size, then whether I average weighted by number or I average weighted by mass I would essentially get the same result. So, if we go back for a moment to our water in the beaker example, if I want to find the fluid velocity starting with the molecular description, I take an infinitesimal control volume and average the velocity vectors of all the molecules that I can sample at a given point. And this averaged velocity is essentially the number averaged velocity because the mass of each molecule is same.

So, if we extrapolate that understanding of fluid velocity to sprays. We now looking at drops which are let us say 0.1 mirco meters in sized to 100 micro meters in size, but the basic idea that I can sample over a period of time, acquired data on individual drops velocities and from that construct an average velocity or a number averaged velocity of all the vectors, from all the individual drop velocity vectors; could now become a fluid velocity for that drop phase. So, just as I went from individual molecules velocity vectors average to give me the fluid velocity, we can go from individual drops velocity vector to give me a fluid velocity for the drops; now because the drops are not all of the same size, you can now define a second kind of average called mass average velocity.

So, if for example, f of v, I will only define in the pdf in the velocity vector v and even one component just to simplify our math on is slide here. If f of v is a number pdf of velocity, then I can do an integral v f v minus infinity to infinity dv and this gives me an average velocity. Or I can also define x cubed f v f x comma v, if I want to define mass average velocity; I need to have the diameter as another independent variable. So, I can define like an x cubed f of x comma v dv, going minus infinity to infinity divided by the total mass.

So, this is we saw this kind of a definition and we are defining size velocity correlation, that I can define a mass averaged velocity, where I take the velocity oh sorry this is the v here sorry of course, we are trying to define the average velocity weighted by the mass of a given particle. So, I can now write down 2 different kinds of velocities for the same fluid at a given point, whether it is based on a mass average velocity or a number averaged velocity. We will come back to revisit this proposition in a in a lecture or 2, yes two what are the consequences of having this size as another variable when I am now trying to define a fluid an equivalent fluid.

So, let us come back to this idea that there is a possibility of an equivalent fluid. So, about to erase this I can make some space here for the slide. Now what is this equivalent fluid? Just as we said that once I understand sought of the origins of fluid velocity from molecular motion, we do not need to go back to the molecular origins of fluidic velocity to write balance laws and to do other things with it. Like I said if I want to understand the flow of a river, I just drop a little dried leaf and watch the dried leaf move, I do not need complete understanding of the fact that the water in the river is made out of molecules and etcetera.

So, we will do the same thing here and say once I have defined this drop field or drop phase velocity, I do not need to go back to the level where I see individual drops. Say for example, if I have a spray, the spray itself is composed of drops, but in a typical observation let us say with your naked eye or with a reasonable speed camera, with a low speed camera, you may not see individual drops, if you look like a white fluid that is emanating from the tip of a nozzle, where I can see this white fluid is where I know I can make the approximation that the drops themselves make up a fluid called drop phase. This individual drops now are no longer important the idea of this smeared fluid is what I want to focus on.

The drops just like the way we discarded our idea that water is made of molecules, we going to discard this idea that spray is actually composed of discrete drops that we can now throw away and keep just the idea of this white fluid will call that drop phase. Drops make up the drop phase, but I do not need to know that drops make up the drop phase; I can define a phasic velocity field for that drop phase in a region where I can make this observation that I do not see the individual drops.

So, take a regular perfume spray, we have seen this video many times in the region near the nozzle, if my frame rate is let us say tens of hertz, that is I am capturing the video of this spray process at a frequency about 10 to 20 hertz, at that time scale I do not see individual drops I am not freezing individual drops and all I see is a smeared motion of drops and I can at that time scale and the spatial resolution replace all the drops with a fluid.

If I was framing if I was taking a video and a very very high frame rate, I would not be able to do this. The analogy also applies to molecular motion that if I want to understand what the fluid is doing at let say 10 power minus 9 seconds, 10 power minus 12 seconds, on that time scale I cannot use the idea that there is a fluid velocity. Because the random motion of the individual molecules plays a role in the transport process. Whereas, if I want to understand what the river is doing at a time scale that I observed with my naked eye, which is a tenth of a second or one second, all of that random motion is averaged out.

So, I only observe the averaged motion, this is exactly the same idea that will use to apply to smear out the features that a spray is intrinsically composed of which are these discrete drops and only focus on the drop phase. Now what sort of drop phase is this? Really speaking the spray itself is composed of these drops as I drawn with this green circles and the interstitial space is all air. So that means in this red rectangle, I have essentially two phases at the very least, I have the air phase plus drop phase; not drops drop phase. So, some fraction of this red rectangle is composed of drop phase, the other part of that fraction is composed of air phase.

So, if I now focus on this phasic level description of the movement of the motion of these entities and I can look at this as being composed of one of two ways, either the two phases are completely separated. Say for example, if I take water in a beaker and I want to understand what the water is doing and how the air is affecting the waters motion. The water and air are essentially separated. So, in the region where there is the water phase, there is no air phase and in the spatial region where there is no air phase, but there is air phase there is no water phase. So, this is what we will come to understand as being a separated description of phases.

The other option is like as shown in the red rectangle, that every infinitesimal volume will see what this word infinitesimal means, every infinitesimal volume in the spray has some fraction occupied by the air phase and the remaining fraction occupied by this drop phase, this is what we will term as interpenetrated phasic description. So, this is where every spatial region could potentially be composed of both the phases in some varying fractions and amounts. Now the likely we said we really have this drops has being the dispersed phase that is they are not continuously attached to each other, whereas the air is one continuous medium. So, even though we have discarded the idea that the drop phase is composed of discrete drops for some modeling purpose later on we will need to invoke this back again.

So, we will come back and see. So, we will just to refer to the two phases, even though we are now looking at both has being continua we are going to refer to one as the continuous phase and the other as the dispersed phase. The mean the whole our intention in calling this a phase is that we have elevated it to the level of a continuum, it is no longer we are not going to be as concerned when writing our balance laws with the fact that this is made of discrete drops.

Now we will see later on that the same idea that we started to define for a phase still holds and that each phase is composed is define by and governed by a unique phase property relationship which we will call the state relationship. And we will also be governed by a unique stress strain constitutive relationship. What do we mean by the stress strain constitutive of relationship or stress strain rate constitutive relationship? Say for example, the Newton’s law of viscosity which we refer to earlier on, is one that defines a relationship between the strain rates in the fluid to the stress field shear stress field in the fluid. That relationship governs how the motion of the fluid influences the stress level in the fluid. And in fact, just as a side it was discovered well before molecular structure of matter was ascendant discovered.

So, one does not need to understand the drop level detail in a phase to postulate a stress strain rate relationship for that phase at the continuum level. The whole stress field is essentially a continuum level property that we will use a little later on.

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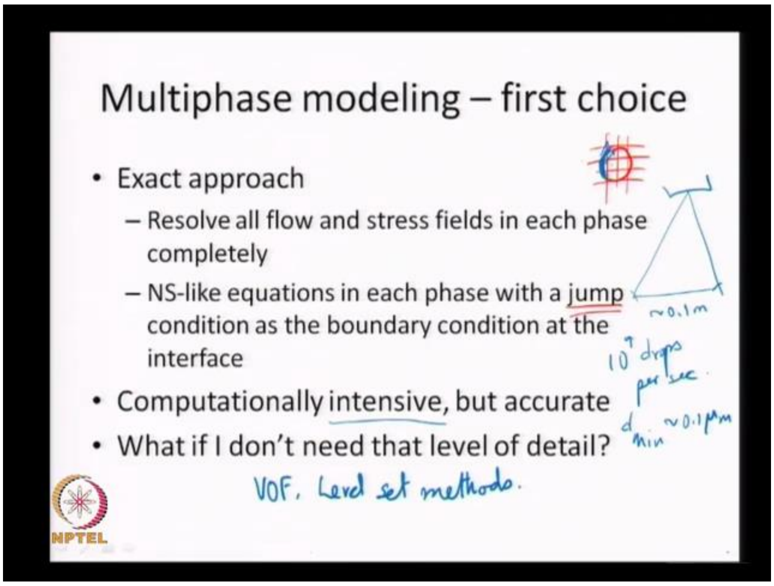

Multiphase modeling – first choice

- Exact approach
  - Resolve all flow and stress fields in each phase completely
  - NS-like equations in each phase with a jump condition as the boundary condition at the interface
- Computationally intensive, but accurate
- What if I don’t need that level of detail?

VOF, Level set methods.

~0.1m

$10^7$ drops per sec.

$d_{min}$ ~0.1μm

So, what are the choices for the multiphase modeling? So, I need to know that I have understood the fact that, I have every spatial region is composed of drops and air; some part occupied by drops some part occupied by air, what are the different ways by which I can model this.

First one is what we will call the exact approach, that is we know that Navier stokes equations are what we will call an exact model of the continuum description of the fluid at every point. So, if I take the idea that even though drops and air are sort of interpenetrated that is in the rectangle I drew in the red rectangle I drew, I have drops and air, but if I keep shrinking that size of that red rectangle; that is if I keep shrinking my observation length scale to the point where I can now look at a red rectangle about this size and on that scale this is just like the water in the beaker. The air and the water because I no longer have a drop, at that scale I have water and air completely separated out.

So, this idea of whether a phase is interpenetrated or separated is very much link to the observation length scales. In an experiment this is the resolution of your camera, in a computation this is your grid size there one to one analogues. So, if I am modeling this and if I clays my grid on the scale where the smallest of all the drops in the spray is completely observed and the way what we mean by observed is either computationally resolved or photographically resolved if I am making imaging observations. If the smallest of all the drops is completely observed; that means, I am looking at a separated flow in which the two phases are pure water and pure air or pure liquid and pure gas. And Navier stokes equations completely described each of the tool separately. So, in the exact approach this is what we will try to do, we will resolve all the flow and stress fields in every phase completely.

So, essentially you develop what look like the Navier stokes equations in each phase with a jump condition at the boundaries of the interface. So, quickly what do we mean by that? If this is my interface, the pressure field inside and the pressure field outside are related by the curvature or I say related by surface tension driven pressure jump across the interface. I could have other kinds of jumps across an interface or lack of jumps. So, I could develop other continuity requirements cross the interface say for example, the local water velocity just inside the interface and local air velocity just outside have to be kinematically similar as for as at least the normal motion is concerned.

So, the component of the water velocity normal to the interface has exactly equal the component to the velocity nor of the air velocity normal to the interface. So, this is like material replacement conditions. So, these kinds of conditions can be written at the interface and these are just like any other boundary conditions you would write for your single phase description. This kind of an exact approach is essentially only valid if I am completely resolving all the scales in every drop. So, if my computational grid is able to completely resolve every length scale at the continuum level. So, water as a continuum is completely understood, that is when this is this observable.

Clearly this is computationally very intensive, but accurate, but it is exact as for as the exactness as much as Navier stokes equations can guaranty exactness, this is exact. And in many instances I may not need this level of detail, now we did this calculation before, let us say we showed that in a reasonable spray, we are producing about 10 power 9 drops per second and there are all spatially concentrated in some region; let us say on the order of 0.1 meters, cone about 0.1 meter in diameter. So, if I want to completely resolve this 0.1 meter diameter spray, where the smallest drop has enough grid cells in it to notice what is happening at that scale. So, if the smallest drop is like I said on the order of 0.1 micro meters; that means, my grid as to be at least that size if not fraction of that size with the grid being fraction of that size, if I want to look at domain that is 10 power minus 1 meters. So, with the grid that is about 10 power minus 7 to 10 power minus 8 meters, I want to look at a three dimensional spatial region, that is about 10 power minus 1 meters. So, we are looking at approximately 10 power 8 to 10 power 7 to 10 power 8 cells in a every dimension that is about 10 power 21 cells.

So, this is just to show the futility of this effort and also the futility of this effort for a real spray. I could look at a smaller region and do this kind of a calculation, get some information from this kind of a simulation to be used later on in a slightly course grind simulation, but for now if I was to focus on just the exactness, it is clearly computationally intensive and this level of what does this simulation give me this tells me what is happening inside every drop and tells me where every drop is headed and tells me what would happen if 2 drops approached each other exactly.

So, if I model these jump conditions, somehow also accounted for 2 drops coming close to each other and then allowing the fluid mechanic process is to proceed further, either in terms of a bounce of or either in terms of a coalesce like a event. So, if I allow my jump conditions to also include these different possibilities, then I will know a lot about what every drop is doing over time. Now we only talked of spatial resolution here, but the same kind of logic also applies to temporal resolution. So, if I want to understand what the drops in a box are doing, I need to know the time scale over which let us say two drops may approach each other and coalesce.

So, the time scale of my simulation should be so short that I am able to capture this entire dynamics, which like my high speed video. So, exactly analogues to the speeds required in my video, if this is the level of detail I want to capture. So, if this is the level of detail I want to capture that fixes the speed of the video as well as the spatial resolution that I need to capture of the video and clearly the size of the video, I have would generate would be humongous that is like our level of detail.

So, if I do not need this level of detail for a real spray, what as what are my other choices? We look at those choices and essentially the way this will focus will come back to the to the other choices in the next class, I want to say few more things about the first choice the sort of the exact approached modeling, this is what is referred to some times as either volume of fluid or level set methods. When you say you are using volume of fluid modeling or level set methods, this is essentially the level of detail that we are trying to capture. So, where is this useful? This is useful where the idea of a drop itself is not clear yet.

So, if I have a bunch of drops and I just want to model what the drops are doing, this is too much detail, but if I do not know if there are drops, if there are if there are no drops, this I mean I cannot do this drop phase replacement because our next idea is to smear out the details that a phase is composed of discrete drops. So, if I do not know that there are discrete drops, I would falling to a pet, where I may take pure water in a beaker and think that that is made out of drops. So, specifically this kind of an approach is almost required, if I want to completely capture primary atomization in a spray. So, what is happening in the primary atomization zone, I have bulk liquid coming out of the nozzle exit, this bulk liquid is in a purely separated state.

So, because I still have the notion of water, the notion of whatever fluid I am trying to spray as being separated from air. So, I cannot make the assumption that I can take every spatial region near that in that zone and that infinitesimal region would be composed of some fraction of drops and some fraction of air. I cannot say that for sure in the primary region very close to the spray nozzle, where I have this continuous phase and this continuous phase is breaking up into drops. This part is best modeled by this exact approach and they some very nice work emerging in this area in the last 10 years, where as some very detailed simulations of this kind of modeling approach apply to the primary atomization region, that is being yielding results that would tell us what the drops are going to be doing later on down streams.

So, the result of this model would form the initial condition for later drop propagation models. So, what does this tell us? This tells us how what does this when I apply this exact approach to the primary atomization region, what we will find is the process by which, the bulk liquid is elongated stretched or whatever are the fluid mechanic process is that that cause this bulk liquid to breakup into a drop and from this process, we also allow the drop to acquire the velocity that the bulk liquid imparts to it. So, all of this is completely contain within the food print of this simulation.

So, you just define the properties and the constitutive relationships, governing stress and strain rate in each of the two fluid separately, which you would do any way if you were doing single phase simulations of these fluids, you define a state property relationship for each of the two phases separately and then go on to define these jump conditions. Once the jump conditions are known the single phase solution procedures apply to each of two phases separately, with these appropriate jump conditions are completely sufficient to cause to completely model the breakup of this bulk liquid into drops.

It is like we said computationally very intensive, but gives us a very high level of detail, which may be required in that region, if I do not want this computational detail, but still want to capture the phenomenology of what could be expected from the primary atomization region, the only modeling approach that is available below this level of detail is our linear instability or in some sense a perturbation or non-linear instability analysis.

So, it shows one more time the real utility of linear instability calculations, in that you can capture a lot of the detail at least qualitatively that you would see in this kind of an exact modeling approach from simple algebraic equations.

We will stop here and will continue our discussion in our next class, where we will look at other modeling approaches that may be more computationally attractable.