Two Phase Flow and Heat Transfer

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Lecture No: 14
Lattice Boltzmann Method

Hello welcome in the fourteenth lecture of Two Phase Flow and Heat Transfer. Today we will be discussing about mesoscopic Lattice Boltzmann methodology.

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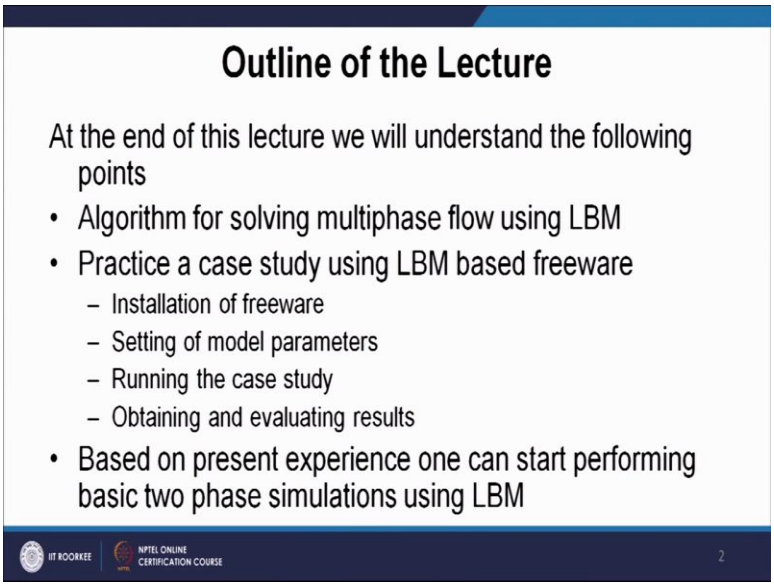

So at the end of this lecture we will understand the following points. First we will be explaining the algorithm for solving multiphase flow using Lattice Boltzmann methodology. We will be giving you a practice of LBM methodology using a freeware. There we will be showing you how to install the freeware, how to set up the model parameters. I will be showing you also how to run the case study and finally what results have been obtained and then how to analyze that result that also I will be showing you.

Based on the present experience you can start performing basic 2 phase flow simulations in Lattice Boltzmann methodology. So to give you 1 outline of Lattice Boltzmann methodology, first let us see that what are the macroscopic equations Lattice Boltzmann methodology is solving. Here I have given you 1 schematic which is Lattice Boltzmann equation LBE which takes information from Navier-Stokes Equation and boils down into physical Lattice Gas

Automata information. In between it does some mathematical analysis using Boltzmann equation.

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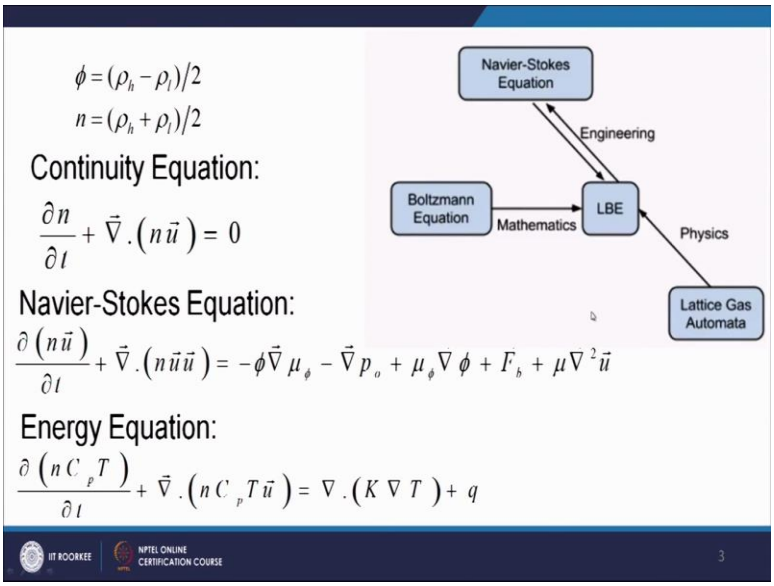

So it is a coupling between engineering problem, mathematical problem and physical insight. So let us see how 2 phase flow can be solved in this framework. For 2 phase flow you know that as we are having 2 different phases, So it involves with 2 densities. We consider the higher density of the phases Rho h and the lower density is Rho l.

So at the beginning we will be defining 2 parameters phi and n. So, phi will be nothing but (Rho h - Rho l) / 2 and n will be (Rho h+ Rho l) /2. For example let us say you are dealing with air and water. So air will be something around 1 kg per meter cube and water will be 1000 kg per meter cube.

So you will be finding out that this n will be becoming (1000 + 1) / 2. So that means something around 500.5 okay. And your phi will be becoming (1000 -1) / 2 that means 499.5 okay. Next let us see the governing equations which are required for solving this 2 phase flow examples involving let us say gas and liquid.

So first we will be having 2 different equations for both the phases that means the gaseous phase or liquid phase. It can be some other 2 phase flow problem also solid liquid or solid gas

situations. So if you have 2 continuity equations and if you see if you remember your continuity equation formats from your fluid mechanics analysis.

Then you will be knowing that if you add both the continuity equations for gaseous phase and liquid phase, 2 different phases; then we will be getting some equations like this delt n/ delt t (n) where n is nothing but (Rho h + Rho l) / 2 + delt (n *u) = 0.

So basically if you see the continuity equation for individual phases, n will be replaced by Rho h and Rho l respectively. So once you add those 2 equations you will be getting 1 equation with n. And if you are having any phase changing in this equation, obviously the phase change will be having same magnitude but opposite in sign.

So once you add those 2 the right hand side will always become 0 right. Similarly one can write down the Navier-Stokes Equation. So you know that in 2 Navier-Stokes Equation that means momentum equations we will be having for gas and liquid once we add those 2 equations so you will be once again getting a equation having n as parameter okay.

So in the left hand side, we are having unsteady and inertia term and then in a right hand side you are having pressure gradient term over here, viscous term over here, buoyancy term over here. Apart from that we are introducing 2 new terms okay.

These are coming due to your chemical potential coming from your chemical thermodynamics. So if you write down, species based momentum equation then these chemical potential terms will be coming into picture okay. In a similar fashion if you are having energy involved, so you can find out the energy equations and for both the phases and add those.

You can write down energy equation in this way where in the left hand side you are having unsteady and convection term. In the right hand side you are having conduction and if you are having any heat generation right. So in LBM framework, first we LBM 2 phase framework, first we convert individual phase equations to some n equations like this okay.

So continuity equation involving n, Navier Stokes Equation involving n and finally if energy is there, energy equation involving n okay. So where n is nothing but (Rho h + Rho l) / 2. Next let us see for capturing of interface in Lattice Boltzmann methodology. We are having basically 2 approaches, first 1 is sharp interface.

Sharp interface means if you are having a sudden jump of the interfacial property that means let us say density or viscosity whatever you consider, if you consider that interface is very thin okay, so across the interface there will be sudden jump of the properties okay.

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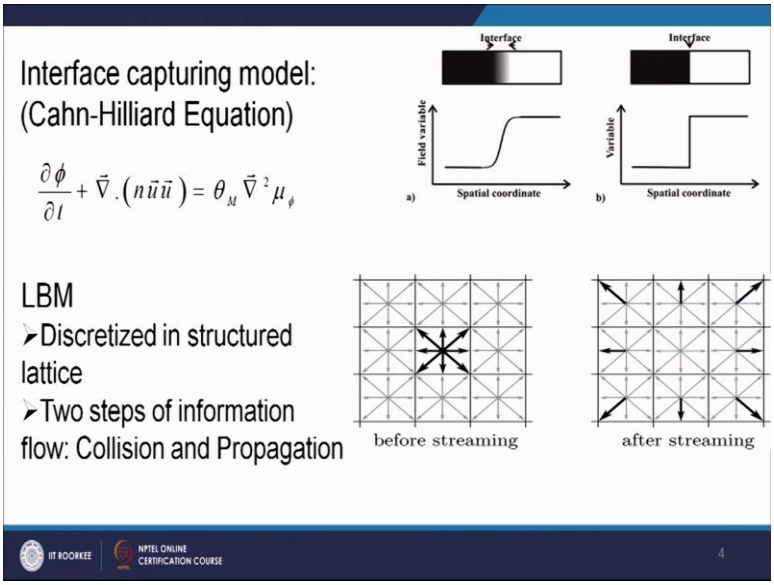

So let us consider this is density counter, variable is density so this side you are having gaseous and this side you are having liquid so there is a sudden jump across this interface okay. So that kind of thing we call as sharp interface concept. On the other hand another counter argument is there where people consider that the interface is not sharp that is diffused over a finite thickness.

So here you can see using color gradient you have shown the sharp change of color. Here it is gradually changing so the variable here also we have shown that it is gradually changing over as small thickness okay so that thickness is called interface thickness.

Now in this methodology this Lattice Boltzmann 2 phase methodology you always consider this diffused interface and for that you need to consider our Cahn Hilliard equation for interface

capturing okay. So, Cahn Hilliard equation, if you write down for gaseous phase and liquid phase separately and if you subtract, then you will be getting additional equation involving phi okay. So delt phi/ delt t is nothing but your unsteady term, here you are having convection term and on the right hand side you will be having a term involving the chemical potential.

Where, Mu phi is a chemical potential and theta m is actually mobility of the interface that means how easily you can change the interfacial configuration right. So altogether if you are having energy involved, you will be getting 4 equations are there okay.

So continuity equation, involving n momentum equation, energy equation and apart from that we are also having 1 equation called Cahn Hilliard equation involving phi right. Now let us see how the domain of our simulation can be discretezed in Lattice Boltzmann methodology. For example let us say this is our domain, a rectangular domain to start with.

So what we will be doing this domain will be discretizing in small volumes or small lattices rather in this case because in Lattice Boltzmann we consider that the domain is actually discretized with lattices. So here all these are actually individual lattices.

The discretization pattern will be more or less similar as we have seen in case of your finite volume of your finite difference methodology. Only difference over here is that in finite difference and volume you can go for non homogeneous discretization. But here in Lattice Boltzmann till now we are having provision for homogeneous discretization only.

So you see uniform size of lattices you will be giving inside the domain right. Now always Lattice Boltzmann is having certain mechanism to carry forward the information. So those information will be actually you know some information for your governing equation parameters that means your Rho phi and n in this equations.

So what we will be seeing let say some information is being generated over here on the center lattice. So this equation can flow depending on the lattice configuration in particular directions

only. Here I have shown you 1 typical example of D2Q9 structure which I will be explaining soon.

So you see the information which is being generated in this lattice can stay inside the lattice only so it is the first possibility. And you are having all other 8 possibilities also. So going horizontally left, going horizontally right, moving up and moving down and 4 corner directions. So all those 8 directions you are having apart from staying in the own cell.

So all these 9 directions are possible. So those actually information directions are actually first captured before streaming okay. So those are actually called collision stages. So after collision the information will be propagating depending on the streaming.

So what we do after deciding that which direction it will be going, the information is actually propagated due to propagation okay. So here you see we have shown after propagation what happens. So earlier this was our lattice of concern now you see left hand side, horizontal left hand side, horizontal direction has moved in the immediate left most lattice.

Similarly right hand side direction has moved to immediate right most lattices. And then top directional information has moved to the upper lattice, down directional information has moved to lower lattice, like that the corners are also taking the respective directions okay.

So if 1 information is being generated in the center cell it propagates in the neighboring cell in this fashion okay. Depending on only the lattice structure whatever we consider here we have considered a D2Q9 lattice structure. So these 2 steps are very, very important. First 1 is collision and second 1 is propagation of information depending on the specified directions okay.

Then let us see that what are the lattice directions possible, I will be showing you here only few but there are many more like this. So first 1 is over here D2Q9 which I have already showed you so this is a zeroth direction apart from that 1,2, 1, 2, 3, 4 and the corners are 5 6 7 and 8 okay.
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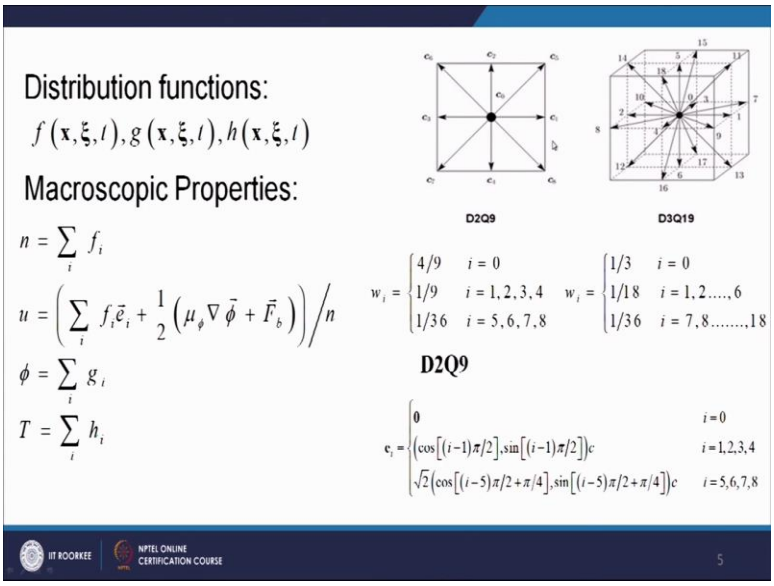

So 9 different directions are over there okay. In a similar fashion, in a 3 dimensional lattice if you consider that means if the problem is in 3 dimensional natures will be having D3Q9 in structure okay. Here I have shown the schematic nature of the lattice directions in a Q and different directions are marked as 0 to 18 okay.

So you can find out that what are the different lattice directions right. Now after discretizing this domain which 2D or 3D lattices next our task is to find out the how to discretize the governing equations which I have told you in the previous slides that how to discretize those in this lattices.

Now for discretization as I have told you that it is involve some sort of collision, so you need to find out what is the probability density function for the collisions okay. So we have to go for some distribution functions over here okay.

So for each equation, information propagates information how it will be propagating due to collision between the lattices that will be found out by this probability distribution functions. Now here as you are having 4 equations, we require 3 probability density functions okay. So those are f, g and h okay. One by one I will be telling you the essence of this f, g and h. First let us take what is f.

Okay so f is actually you want probability density function whose summation will be giving you 1 macroscopic variable n okay. n if you remember, I have told that one is (Rho l + Rho h) /2. So summation (f) of all different directions depending on the lattice structure whatever you have taken okay. I can write down that its equals to n. So that means in D2Q9 structure starting from f 0 to f 8 we are having if you add all those f's, you will be getting the macroscopic property n okay.

In a similar fashion, you know u can be obtained in this fashion where f, I already I have explained ei that is the lattice directional velocity. So for example let say over here for D2Q9 structure the zeroth direction is having 00 velocity 0, 0 velocity x and y direction. And for 1 it is having (+ 1, 0), for 2 it is having (0, + 1), for 3 it is (-1, 0) and for 4 it is(0, - 1). So ideally for the corners it is having (1, + 1), (+ 1, + 1) then it is (-1, + 1).

Similarly you can find out the c7 and c8 direction corresponding e's. So we know what is the e direction. So we can add this fi into ey. If you are interested in x directional velocity, always add that x directional velocity component, If you are interested in v that means y directional velocity component then you add the y directional velocity.

Okay I have already spoken that how x and y can be designated in D2Q9. On the other head here we are having some terms which were there in the macroscopic equations, this is coming from the chemical potential term and this is your body force. If your problem involves body force those things will be coming over here. So that means using f only by knowing the distribution f you can find out n and u okay.

In a similar fashion, this g will be giving you phi and h will be giving you t. So summation (g) of all directions will be giving phi and summation (h) in all directions will be giving you t. Now whenever we will be adding the informations one important parameter we need to take care of, that is what is the weight of different directions.

So weights are typically specified whenever you will define the lattices usually the weights we give as for D2Q9 4 /9 for the zeroth direction. 1/ 9 for the 1, 2, 3, 4 that means horizontal and

vertical components and 1/ 36 we will give for the corner components that means 5,6, 7,8 okay. Similarly for the 3 dimensional lattice structure D3Q19 weights are defined in this fashion okay. Already I have told you about ei okay, which is nothing but directional velocity.

So velocity can be written in this fashion in terms of cosine and sin okay. I have already told you the magnitude 0, 0, + 1, 0, 0, + 1 something like that. So if you replace this things okay. The i by the corresponding number starting from 1 to 8 you will be getting those values once again back okay. Next let us see the algorithm by which we can go for Lattice Boltzmann calculation. As I have already told you first we need to define what is phi and n. Apart from that we need to get all other physical properties also starting from the chemical potential because it is involved in Cahn Hilliard equation.

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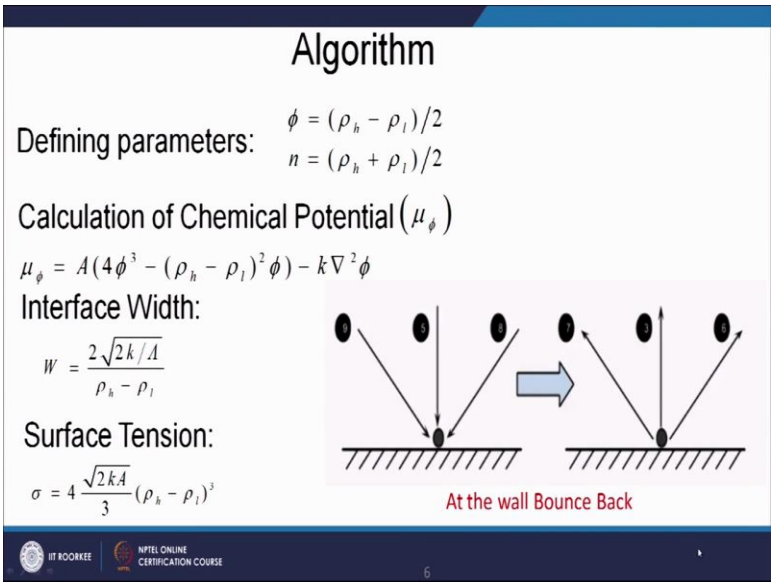

So you see Mu, phi which can be found out in terms of you know phi is (Rho h – rho l) and few other terms for example k, a those are constants okay. So those actually are found out based on some other physical properties of 2 phase flow. For example here k and a can be found out from the interface width. If you remember in case of diffuse interface I have talked about over here that if you are having diffuse interface concept, what is the thickness by, which the fluid property is changing from one phase to another phase that is the interface width w as well as we know that surface tension will be applicable in the interface.

So from the knowledge of w and sigma for your problem, you can find out what is k and a okay. Those k and a will be important for getting macroscopic parameters Mu, phi or chemical potential. So how to find out what are the relationship between k and a with w and sigma those are given over here. So once you know the macroscopic properties, you can easily find out k and a and hence you can find out the chemical potential, Mu, phi. Okay, next I will be showing over here what the discretized equation is.

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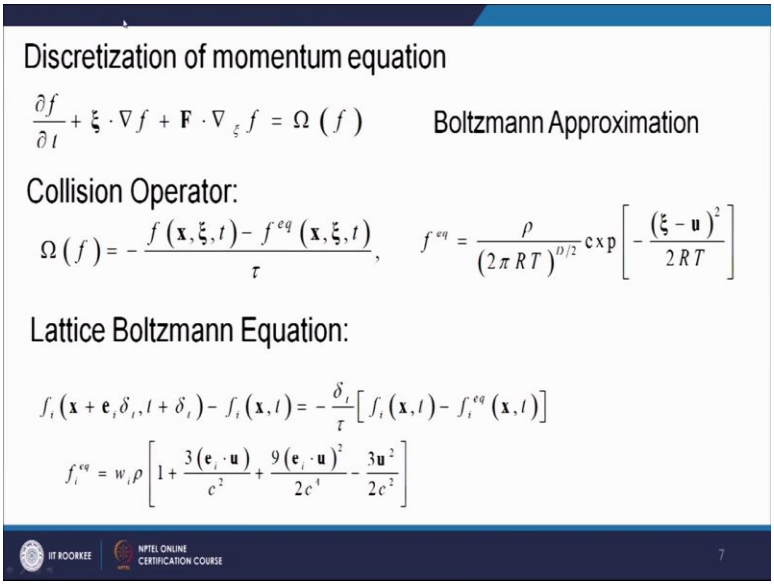

So this, we this discretization is actually following Lattice Boltzmann discretization that means your Lattice Gas Cellular Automata formulations. As you know that in finite volume method we go for Taylor series expansion. In case of Lattice Boltzmann equation, we go for Boltzmann approximation okay. So here, after doing this Boltzmann approximation what we find out the distribution function f is actually can be written in this fashion.

Where, you see this is the temporal part of change of f. Here we will be having the convecty part okay. Here we are having some sort of external force field part and finally here we are having the collision operator. This collision operator is very, very important because we are having always the collision between the lattices. So once we have the collision operator, here I have shown what is the nature of the collision operator.

So collision operator always depends on the present value of the distribution function and the equilibrium value. So equilibrium values means at whenever the system is almost in equilibrium. So in that condition what was that properties, what are the value of distribution function.

So that I write down here as f eq this is also very important factor, which is called relaxation factor Tau relaxation time Tau. So this will be also coming into picture in case of collision operator. Now here I have shown how to find out the equilibrium distribution function. You see equilibrium distribution function is dependent on the time; dependent on the temperature as well as it is dependent on the velocity and density.

So once you know the macroscopic property of the problem, easily you can find out what is the equilibrium function of the distribution parameter okay. And this Tau is actually dependent on the fluid property. For example for momentum equation, this Tau will be dependent on the viscosity, for energy equation Tau will be dependent on your thermal conductivity and so on. Okay, so once we put this collision operator over here, in this equation we get simplified equation of f okay.

That means at next time step so you see (t + delta t) that means next time step and (x + ei delta t) that means after propagation. So this is after propagation, propagation scheme I have already shown to you. You will be finding it is dependent on you know fi and then delta/Tau fi - fi equilibrium. fi equilibrium already I have shown you how you can calculate in case of your Navier-Stokes Equation.

It is dependent on your u, the velocity of the lattice macroscopic, velocity of the lattice, density of the lattice and then sound speed c okay. Apart from that wi the weight factor of different directions will be also coming into picture. Okay next let us see similarly type of equations for g and h. So I have already told you g will be important for finding out the interfacial location and it will be giving you summation of g will be giving you the value of phi.

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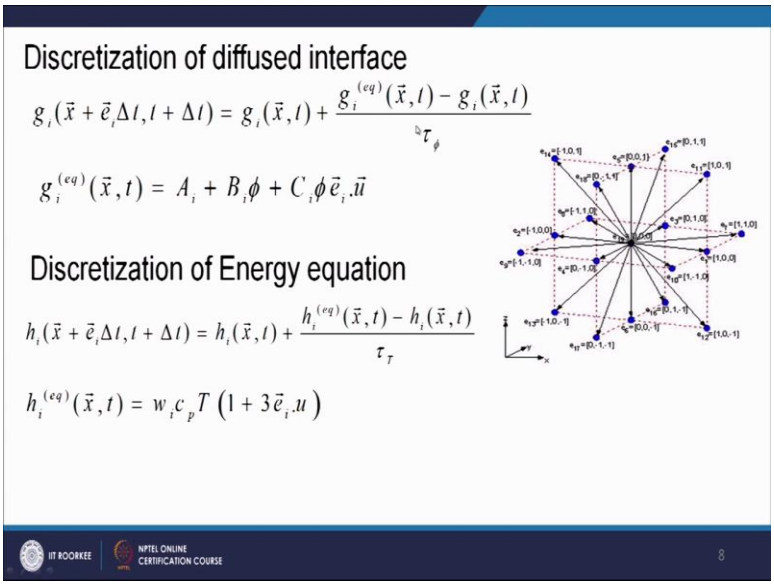

So here also you see gi after collision and propagation you can write down as gi x t + (x i - g i) equilibrium minus g i / Tau phi. Remember, this Tau phi and in the previous here Tau these are not equal . This Tau phi you will be depending on the fluid properties and Tau will be also depending on fluid properties but there functional natures will be different. So here also what is the value of g equilibrium, I have shown you over here.

So these are dependent on lots of empirical values ai, bi and ci and those can be found out, once you go for detailed description of the Lattice Boltzmann equation okay. Here I have not described all those issues. Similarly you can find out the discretized equation for h. Here you see this is h after propagation and collision can be found out. Once again from h equilibrium and Tau t and this Tau t is dependent on the thermal conductivity okay.

And equilibrium once again can be written in terms of the temperature of the lattice velocity okay. Obviously cp or specific heat at constant pressure will be coming into picture along with wi okay. So here once again I have shown you 3d nature of the D3Q19 structure along with the velocity vectors okay. So uv and wi have shown you over here.

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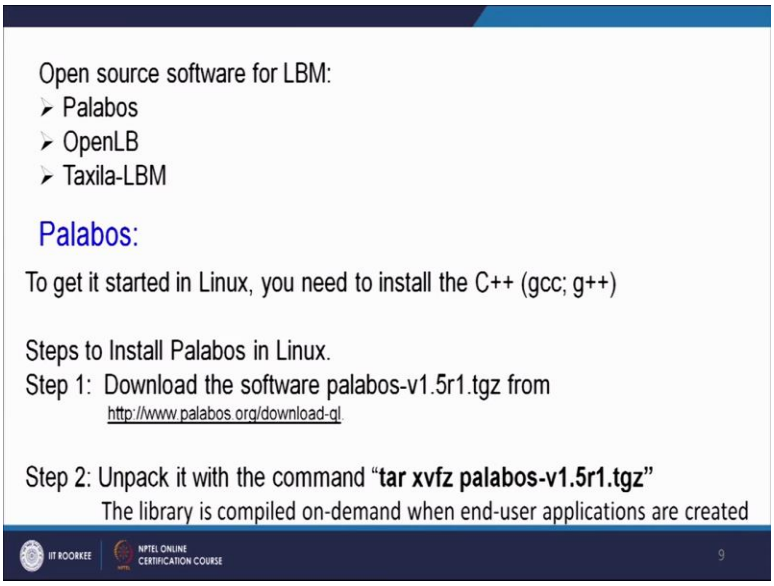

Okay, I will be showing you in detail that how Lattice Boltzmann equation can be solved using you know, some open source software or freeware. There are different freeware available you know in open source, which you can see, use. So some of the free wares are like this Palabos, Openlb, Taxila LBM. So all these are dealing with LBM's simulation of 2 phase flow .But today I will be giving you some example or using Palabos.

So this will actually give you some sort of chance to do some sort small simulation of 2 phase flow and practice this one. So let us see Palabos to get it started you need to know that it runs in Linux platform, Unix platform okay and you need to install C + + library that means g + + or gcc library which already I have shown you how to do okay.

Then let us see how to install the Palabos in Linux. First you need to download the software okay. So it will be downloading some Palabos version .tgz format okay. So it will be downloading so where from you need to download that also I have given you over here. Then you need to untar or unpack the software.

So, what is the comment for untaring and unpacking the software that also I have given over here. Now you may not to install the software because this library is compiled on demand okay. So installation is not there. So wherever require, whenever you will be trying the run the code it will be compiling the code on demand okay.

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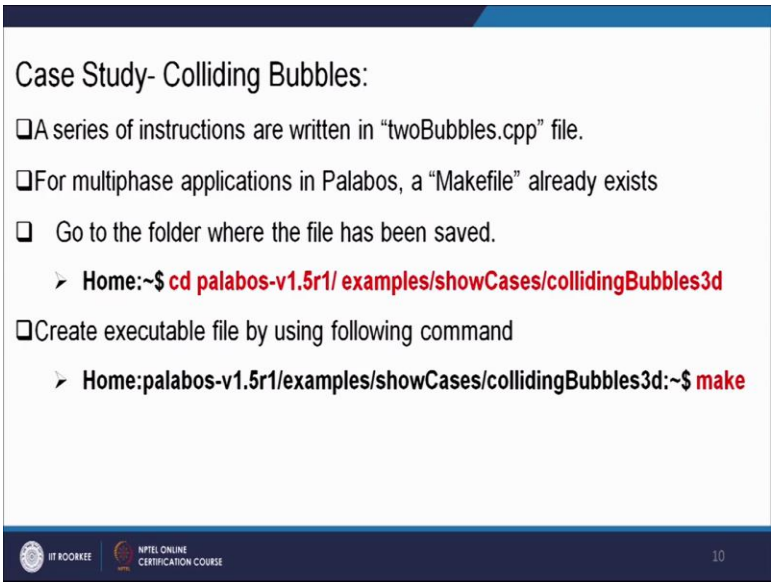

So whenever applications, user applications are there, it will be doing the compilation on demand. Next let us see a case study using the Palabos. So, what will be doing over here. First case study will be seeing over here for colliding bubbles let us say we are having 2 bubbles which are colliding among themselves okay.

So a series of instructions will be writing in a .CPP file let us name that CPP file as twobubbles.cpp file okay and then we need to run that code okay using some makefile. So makefile you can find out in the same directory where you have actually stored Palabos. So you can go in the directory and find out that make file which, is already existing. Then what you need to do, you need to go to that folder okay where, this .

CPP file has been saved. So how to go to that folder using cd that I have shown you over here okay. Then how to run that executable file using makefile. So you have to just give the command make okay. Once you give the make command, it will be developing the executable files.

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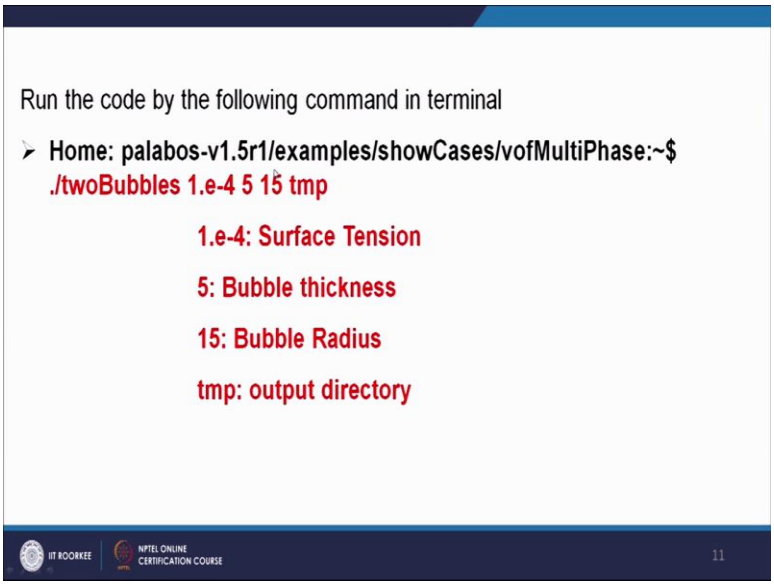

To run that executable file what you need to do, you need to give a command like this ./twobubbles that is the name of the CPP file and then few parameters. So first parameter is 1*10 to the power of - 4 which is nothing but the value of surface tension. Then phi, which is nothing but the thickness of the interface okay around the bubble. And then we are having 15 which is nothing but the radius of the bubbles okay, which are colliding and then tmp is the output directory, where it will be writing the results okay.

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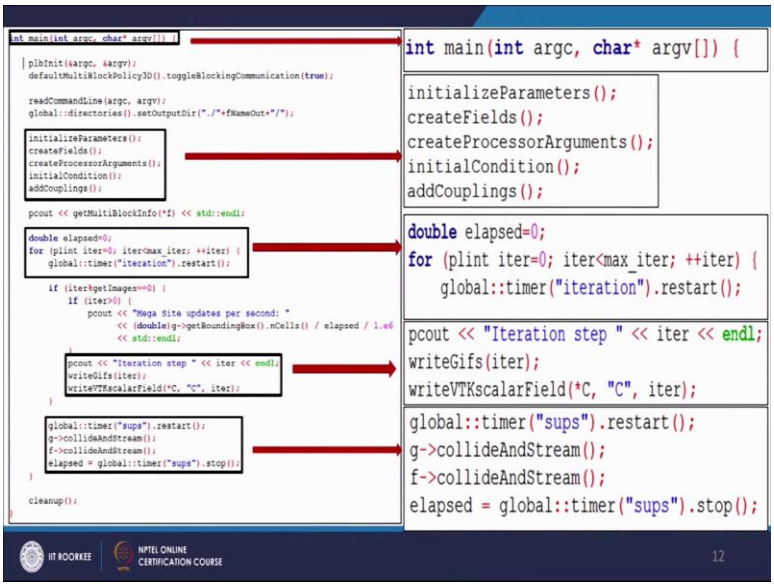

Next let us see little bit of code. So here I have first shown you the main code, main points I have highlighted over here. You see this is the line written in the C++ version. What is the main code into means that mean this is the main code. Next I have shown you some enlarge portion over

here. You see this here we are doing some functions that means initialize parameters. Here we have initialize the bubbles I will be showing you. Then create field.

So I have to create the fields which are important for here. Here it is f and g and then create processor arguments. So which processor if it is parallel simulation, which processor will be doing, which component that will create over here. Initial conditions that means where the bubble will be staying initially, what are the velocity and temperature conditions those will be giving over here in initial conditions.

Add couplings so here we can add coupling between different equations. Let us say we are having f equation, g equation. So you can add couplings between f and g. Then you see here, we have run the time loop that means we have to advance forward in time. So that the bubbles can come closer to each other and collide. So we have started from iteration 0 that means time = 0 to some maximum value max iter okay in the steps of 1.

So it will be doing the time limit okay. And then you see, here in the loop we have written the external file, all the informations in different time steps we have written in some external file. So that we can visualized the result. So here you see the writing writegifs at every iteration and writevtkscalarfield. So vtkscalarfield is important for seeing the result contour in some external software like you know paraview or something like that.

So we are writing the external files okay. All the results then here what we have done these are very important g equation. We are collide and stream. So we will not be going in detail of this function collideAndStream but here we are adding the equations and for f equations will be going for collideAndStream okay. Each time step this f and g equations will be collideAndStream okay. Next let us see little bit part of the initialization. Otherwise things will not be clear.

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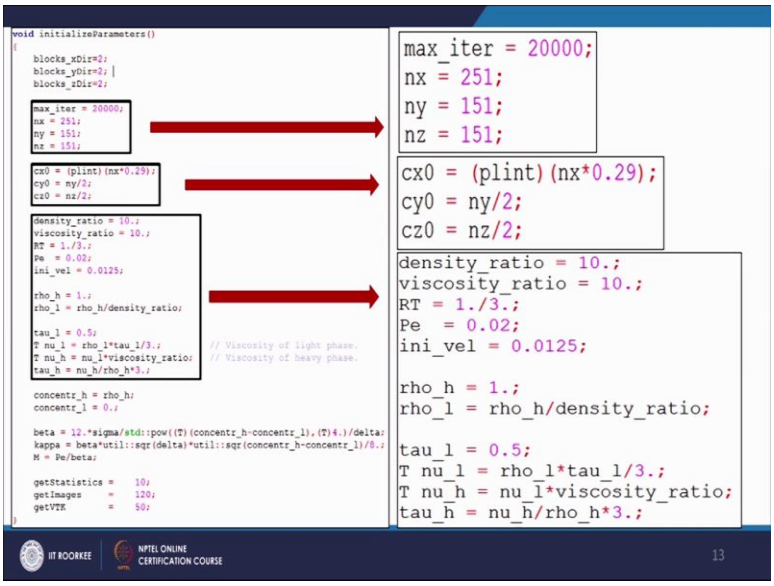

So here you see in this part I have shown you that you can give what is the max iteration that means maximum how much time in the code will be running. Here I have given to 20000 nx, ny, nz these are the actually domain size okay. So you are having 251 as length 151 as width and 151 as height okay. So it is actually 2:1: 1 ratio, the domain okay. Then here we have given you see cx0, cy0 and cz0 these are actually the center of the bubbles okay.

So cx0 is x coordinate, cy0 is y coordinate and cz0 z coordinate. So we have given all the cx0, cy0 and cz0 in terms of nx, ny and nz. Then here you see in this loop we have given the density and viscosity values okay. So density ratio we have taken as 10 viscosity, ratio between the fluids we have taken as 10 and here we have given some other parameters also like initial velocity (()) 28:10 number okay.

And we have also given what is the density of the highest density fluid and what is the density of the lowest density fluid depending on the density ratio of 10. So this is Rho h /density ratio. Similarly, the viscosity Tau 1 we have considered as .5 and similarly Tau h can be calculated by nu h / Rho h *3 okay. So nu and tau those are kinematic and dynamic viscosities okay. So for higher fluid and lower fluid we have shown you over here.

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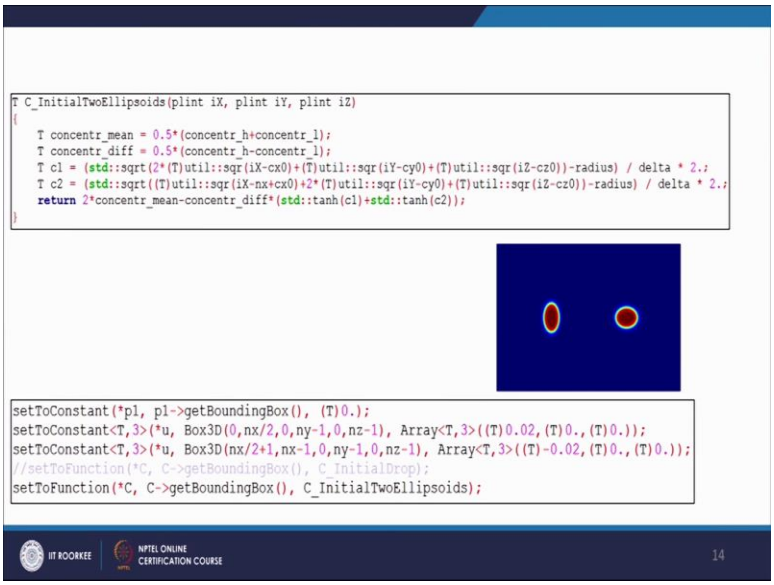

Next let us see the initial position of the bubbles. Actually we are solving this kind of simulations. So here you see we are having elliptic bubble over here, another elliptic bubble over here in this side. We have given some velocity towards right, here we have given some velocity towards left and we have shown how they can collide. To show that you see over here we have given that what is the concentration.

So this is actually definition of your phi and your n okay. This is n and this is phi and here you see we have given the bubble contour. So first equation if you see this is actually 2 *x square. So 2 into you see x square so that means this bubble we have given this ellipsoid we have given. And second one tc2 you see, we have given 2* y square. So that means ellipsoid in the y direction we have given okay. And then here we have given the initial condition you see, here we have given for the first bubble.

So bounding box we have created in the left hand side. So you see over here we have given the velocity as 0.02 okay. And for another bubble we have given -0.02. So first bubble is moving the left hand side, bubble is moving towards right hand and right hand side bubble is moving towards left hand okay.

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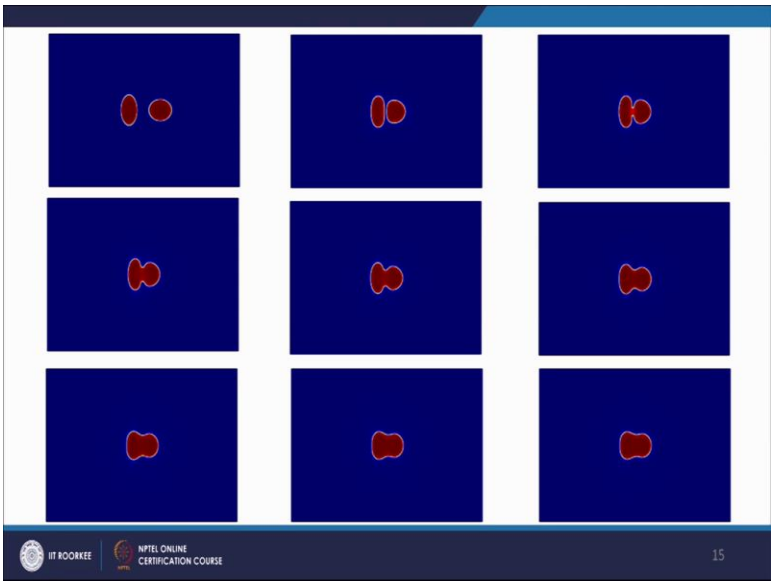

So that they can collide. Okay, then I have shown you some result over here. You see we have started from this configuration okay. As time progress they are coming towards each other. Here they have started merging of here they have merged and you know taking the final shape slowly progressing like this and finally you see due to surface tension it is becoming union bubble okay. So starting from 2 bubble situation how bubbles are colliding and they are merging. That we have shown over here. So the steps of the code also I have explain. So if you want, you can have look at this one and practice this LBM simulation okay.

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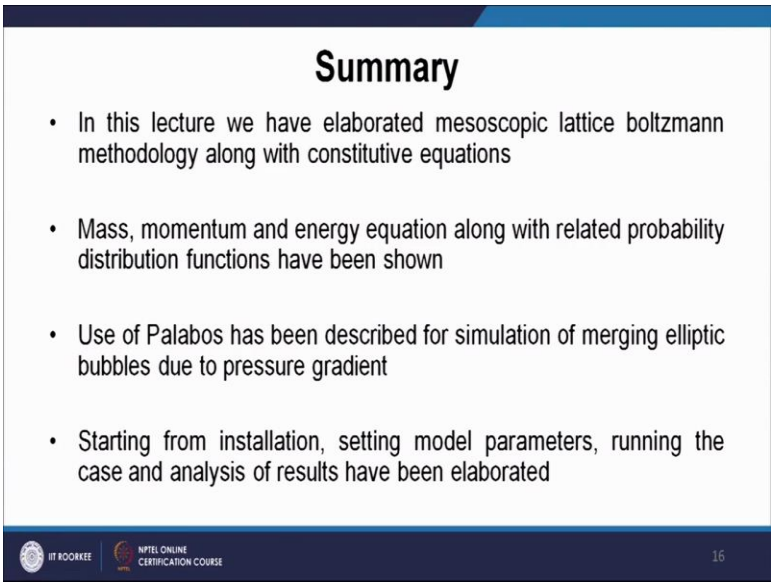

So let us summarize this lecture, in this lecture we have elaborated mesoscopic Lattice Boltzmann methodology along with constitutive equations, mass momentum and energy

equation related to probability density functions we have described. We have also shown you 1 freeware call Palabos and the use of Palabos for this Lattice Boltzmann equation we have showed you okay. And then in this Palabos freeware we have shown from installation setting, the model parameter, how to run and how to analysis the results those things we have shown you over here. So apart from Palabos you can try any other freeware or some software you can use for practicing this Lattice Boltzmann methodology okay.

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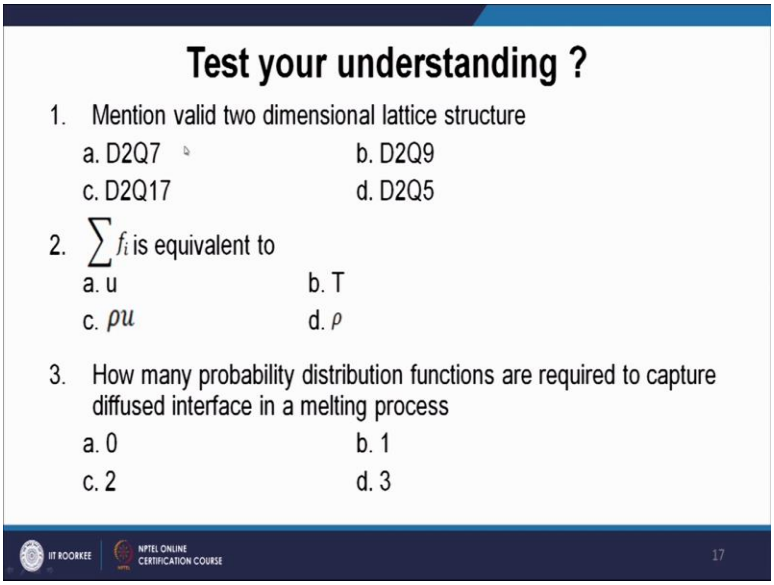

So let us test your understanding at the end of this lecture, as usual we are having three questions over here. First one, mention valid two-dimensional lattice structure. We are having 4 options over here to remember 2-dimensional lattice structure. So we are having D2Q7 you know that 2 symbol is the 2 dimensional nature. So D2Q7, D2Q9, D2Q17 and D2Q5.

So already we have shown you D2Q9 is probably the correct one but you will be finding out that if you reduce the corner directions then D2Q5 lattice structure is also possible, which I have not shown you in this lecture. But you remove the corner directions and only keep the horizontal and vertical positions these will be D2Q5 position. So the correct answer will be b and d both D2Q9 and D2Q5 other 2 cannot be accommodated in 2 dimensional structures.

Next summation of fi is equivalent to, this is very simple. I have already told you the summation of fi is equivalent to, we are having 4 answers. u, T, Rho u and Rho. All of we know that

summation of fi will be equivalent to Rho. So d is the correct answer. How many probability distribution functions are required to capture diffused interface in a melting process. So melting process means it will be involving heat transfers as well as you know interface.

So it will be diffused interface concept okay. As well as we are having definitely the continuity momentum equation so we are having your continuity momentum equation, energy equation and diffuse d equation. So we are having options as 0, 1, 2 and 3. So definitely correct answer will be f g and h. So correct answer is 3 okay. So with this I will be ending this lecture, thank you.