Introduction to CFD

Prof. Arnab Roy
Department of Aerospace Engineering
Indian Institute of Technology - Kharagpur

Lecture - 35
Numerical Solution of One Dimensional Convection - Diffusion Equation (continued)

We continue our discussion on numerical solution of one dimensional convection diffusion equation.

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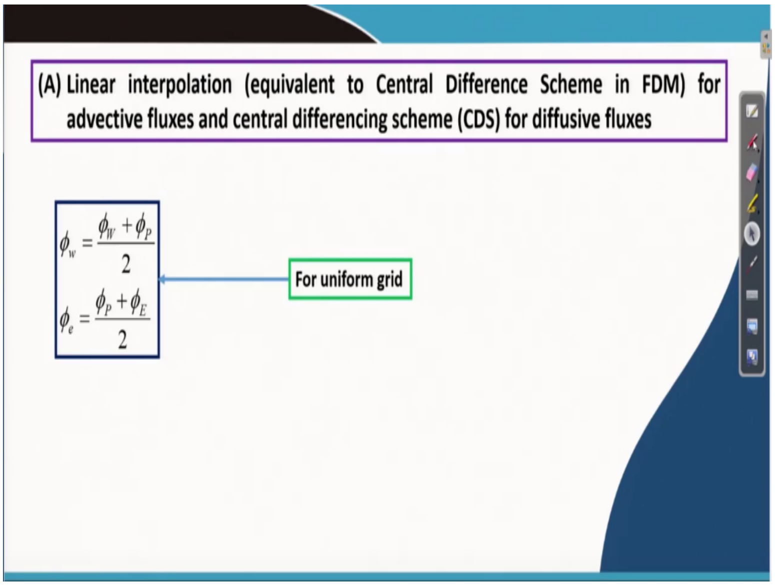

So, last time we started our discussion on linear interpolation. And we will continue the discussion on that. Now, so we recall that we looked at the scheme for different boundary nodes as well as internal nodes. So, we continue to look at the formulation for that.

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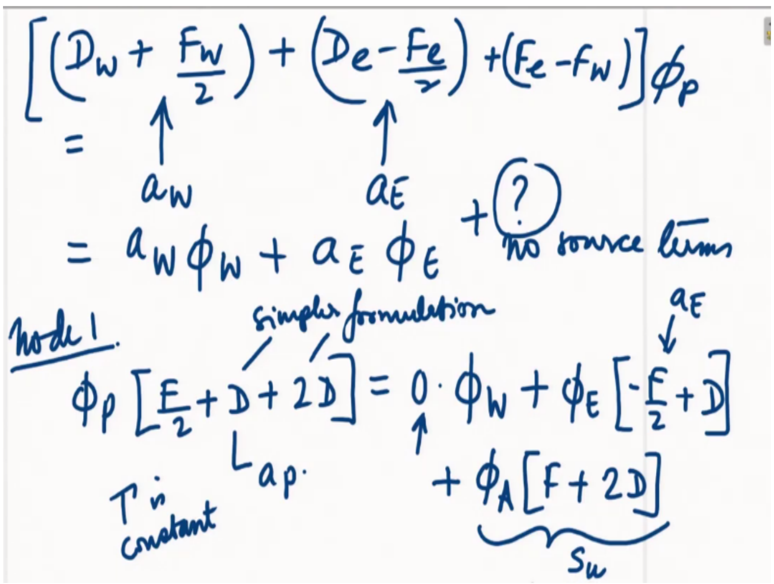

So, if you recall, the internal node, had a representation like this. And these coefficients are actually linked with the a W and a E. So, we recall that the D w + F w by 2 was a W and this was equal to a E. And when you go out to the right hand side, you find that it is equal to a W phi W + a E phi E. And notice that there are no source terms here. That means we have all the terms, represented in the form of the phi's corresponding to each node, and the coefficient associated with the respective phi.

So, there is no additional term here. So, there is no source term, as we said. However, if we go back to say the left boundary node which we call as a node 1, so, the node, next to the next left boundary. For that node, if you look at the equation, it will appear as. So, what I am doing over here essentially is I am not distinguishing between say D e and D w. And I am assuming that gamma is constant. So, in that case, all the D terms will be reduced.

It will not have any suffixes associated with it. Right. So, that makes the, you know, formulations simpler. So, this would help us in doing a simpler formulation. That is why we are making that simplification. So, that is the a P for the node 1. And then when you go to the right hand side, the coefficient associated with phi W will be 0 because you do not have a node on the west side, because the boundary comes up before that.

This is the coefficient for phi E. So, we call it a E. And then we are left with a term, which looks like this. So, this is essentially a source term. We will call this source term as S u. Alright, and now let us try to put these equations in a certain format. So, what is the format?

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$$a_P \phi_P = a_W \phi_W + a_E \phi_E + S_u$$

$$a_P = \underbrace{a_W + a_E + (F_e - F_w)} - S_p$$

$$a_P = \frac{F}{2} + 3D = 0 + \left(-\frac{F}{2} + D\right) - S_p$$

$$S_p = -(F + 2D).$$

$$\boxed{S = S_u + S_p \phi_P}$$

Let us try to write the boundary node equations in a format like this, say like this. And in this equation the a P would be a W + a E + F e - F w. So, if you recall this was the standard form of the a P for the internal nodes. But then you will find that this would not be sufficient, you would actually have to accommodate another source term here in order to balance. So, we will find out what that source term looks like.

So, look at this that the basic equation has one source term here. Again, the coefficient a P has a source term here. So, that is the distinction of boundary nodes from internal nodes. So, let us try to put the expression for a P and try to work out what this S P is. So, a P is F by 2 + 3D and that is equal to a W which is 0 + a E which is -F by 2 + D - S P. So, if you transpose the terms, you can figure out that the S P will turn out to be minus of F + 2D. Again, we already have identified S u.

So, if you look at the total source contribution for this boundary node, then it is actually coming from a contribution from the boundary value itself, which gets into S u. Because S u comes up in terms of phi a and then another part which is dependent on phi P. So, there is one part which is not dependent on phi P, but dependent on the boundary value, and other part, which is dependent on phi P. So, that makes the entire source term.

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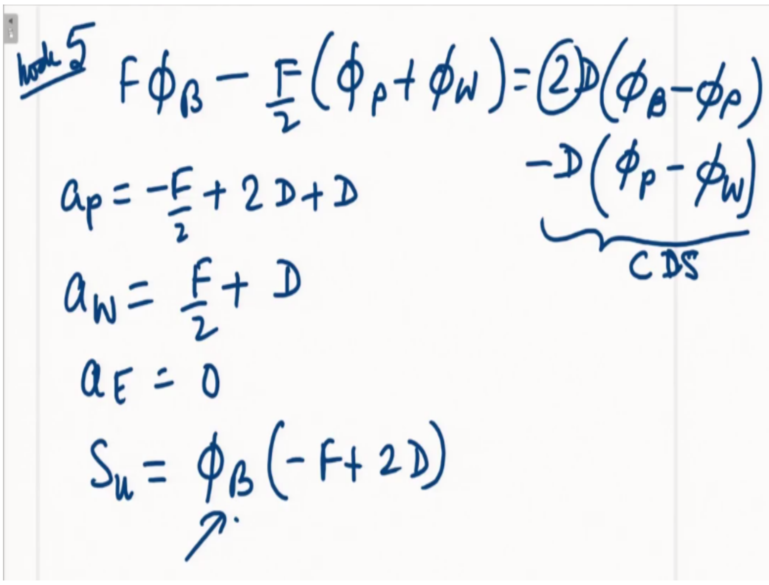

So, if you similarly do it for node 5, which is on the right boundary, you will find that one can show that. Okay, let us write down the expression. So, the equation looks like this for the right boundary. As you may recall, that on the right hand side we have a coefficient 2D, because the diffusion term works out as gamma by delta x by 2, because of the half grid spacing. That is why you have a coefficient 2 here.

And always remember that the right hand side, the diffusion term is always being discretized using central differencing. Even after we finish discussing this linear interpolation or central differencing scheme and go over to other schemes, even there we will continue with the central differencing for diffusion terms. Right now here.

If you rearrange these terms, you will find that a P will come out to be -F by 2 + 2D + D that makes it 3D, a w here will not be 0, because you have nodes on the west side, but a E will be = 0, because you do not have nodes on that side. And you can show that S u will come out to be phi B into -F + 2D. So, that is how the boundary value comes in the S u. So, once you are done with that you can look at S P.

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$\underline{S_P}$

$$a_P = -\frac{F}{2} + 3D = \frac{F}{2} + D + 0 - S_P.$$

$$S_P = -(2D - F)$$

$$S = S_u + S_P\phi_P$$

$$= (2D - F)\phi_B - (2D - F)\phi_P.$$

And as you can remember from the node 1 calculations. We first write down a P, which is -F by 2 + 3D. And then on the right hand side we write down F w + a E which is 0. And then -S P. From there, S P works out to be minus of 2D - F. So, we now have S u and S P, and then again the source, the total source contribution for the boundary node comes out to be. This is coming from S u and this coming from S P.

Now, we are kind of ready to make a table of coefficients which will help us understand how the scheme is functioning, what are the specifics of the scheme. So, let us make a small table.

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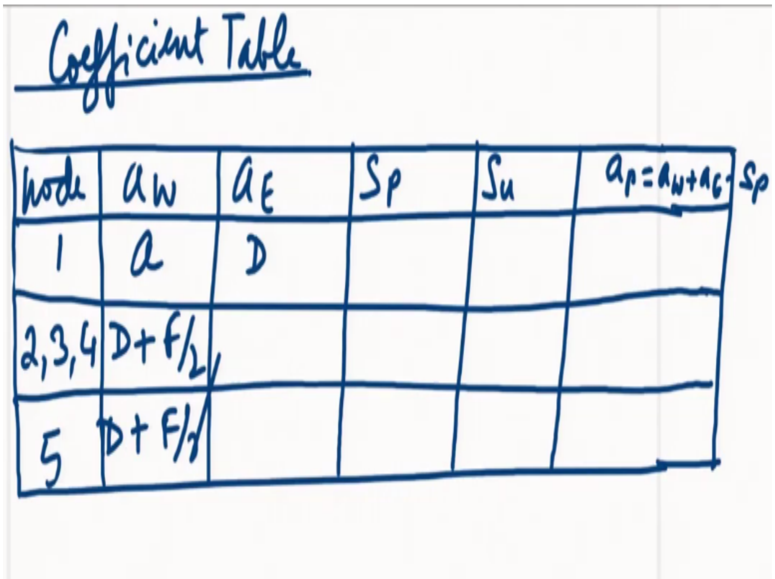

Coefficient Table

node	a_W	a_E	S_P	S_u	$a_P = a_W + a_E - S_P$
1	a	D			
2,3,4	D + F/2				
5	D + F/2				

So, we will call it say as a coefficient table. And let us see how we prepare it. So, on top on the first row what we do is we write node. And then we write down, a W a E S P S u. Then on the last column, you write down, a P, which happens to be a W + a E - S P, which we have already seen. Now, special conditions for node 1 and node 5. And we have same formulation for the internal nodes 2, 3, 4.

So, if you go back to your equations you will find these expressions coming up. Sorry, we will rewrite it here, once more.

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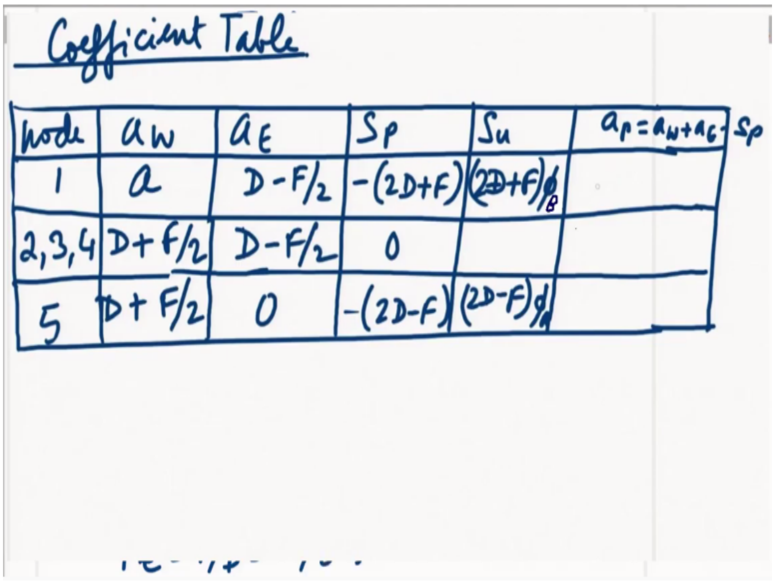

Coefficient Table

node	a_W	a_E	S_P	S_u	$a_P = a_W + a_E - S_P$
1	a	D - F/2	-(2D+F)	$(2D+F)\phi_B$	
2,3,4	D + F/2	D - F/2	0		
5	D + F/2	0	-(2D-F)	$(2D-F)\phi_A$	

So, this is F by 2. You have D - F by 2 here. And here we have a 0 here minus of 2D + F 0 minus of 2D - F here 2D + F into phi A and you have a 2D - F into phi A here for S u. And then a P, which is essentially a summation of a W a E and -S P comes out to be this, although different nodes. Now, we will try to figure out a small problem with numbers. We will do two cases. So, let us call it say as case one.

And for this, you are choosing some numbers. So, the density, the velocity, of course we have them in dimensional form. And we will have to figure out based on these values. What is the F. F is rho u. So, that comes out to be .1 kg per meter square second, and D comes out to be gamma by delta x which is .5 each per meter square second. And therefore, the important number, the Peclet number happens to be .1 by .5, which is .2.

It is a small Peclet number that we are talking about over here. So, with this small Peclet number, how does the coefficient table look like?

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node	a_W	a_E	S_p	S_u	a_p
1	0	0.45	−1.1	1.1	1.5
2,3,4	0.55	0.45	0	0	1.0
5	0.55	0	−0.9	0	1.45

+ve. −ve.

Boundedness of the solution

Scarborough Criterion

$$\frac{\sum |a_{nb}|}{a_p} \begin{cases} \leq 1 & \text{for all nodes} \\ < 1 & \text{for at least one node} \end{cases}$$

Let us try to have a look at it. So, if you quickly redraw the table. Without putting on the calculation details, we will just try to put the numbers here. So, that we can understand how the scheme is functional. So, these are the coefficients on top, more numbers here on the first column and then if you do the calculations, you will get these numbers for the different coefficients. So, this is .45 - 1.1 0 - .9 1.1 here, 0 elsewhere.

And then a P of course is essentially a collection of those coefficients a W, a E and minus S P. So, there are certain important things we need to look at. We find that these coefficients are all positive. We also find that the S P is negative. And based on these values, we actually have to do certain checks for the boundedness of the solution for which we are going to invoke a criterion, which is called as the Scarborough criterion.

And that says that if you have all the nodes in your grid and the values, put into a table like this, then do the calculation in this form, and try to find out what this comes out to be for each node. Now what does that mean each node would have a value of a P. Now for boundary nodes a P would also include effect of source term. But internal nodes do not have sources effect of sources. So, a P is the net coefficient for the corresponding grid point. While a n b are the coefficients of all the neighbors.

And on top in the numerator we are taking the modulus of the values. So, they could be positive or negative but we just take the modulus of the values, and then try to figure out what this ratio comes out to be. Now, by the Scarborough criterion, you should have the value of this coming to be less than equal to 1, for all nodes and for at least 1 node. It should be <1.

So, if this is satisfied, then the boundedness criterion of the solution would also be satisfied. So, let us try to figure out whether for this particular problem statement, we have gone about satisfying the crowd Scarborough criterion or not.

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node 1 $\longrightarrow \dfrac{0.45}{1.55} < 1$

nodes 2, 3, 4 $\longrightarrow \dfrac{0.55 + 0.45}{1.0} = 1$

node 5 $\longrightarrow \dfrac{0.55}{1.55} < 1$

S_P remains negative

So, if you do the calculation for node 1 for example, you will find that the numerator comes out to be .45. The denominator comes out to be 1.55, which is of course <1. So, nodes 2, 3, 4, if you do the calculation, so you will find that on the numerator, you are left with .55 and .45 which are coming from a neighboring nodes and what you have for the particular node is 1 in the denominator, and that is equal to 1.

And then from node 5 comes out to be .55 by 1.55, which is also <1. And clearly we have satisfied Scarborough's boundedness criterion. Another criterion, which is important for boundedness to be satisfied, is that S P remains negative. In fact, this would ensure that we end up satisfying Scarborough's criterion. Additionally, we have to keep in mind that is there a possibility that Scarborough's criterion may be violated?

No Scarborough's criterion would also mean that if you are doing the calculations with all the coefficients remaining positive, then that would ensure boundedness. So, if the coefficients become negative under certain circumstances, will that create a problem for the linear interpolation or CDS scheme.

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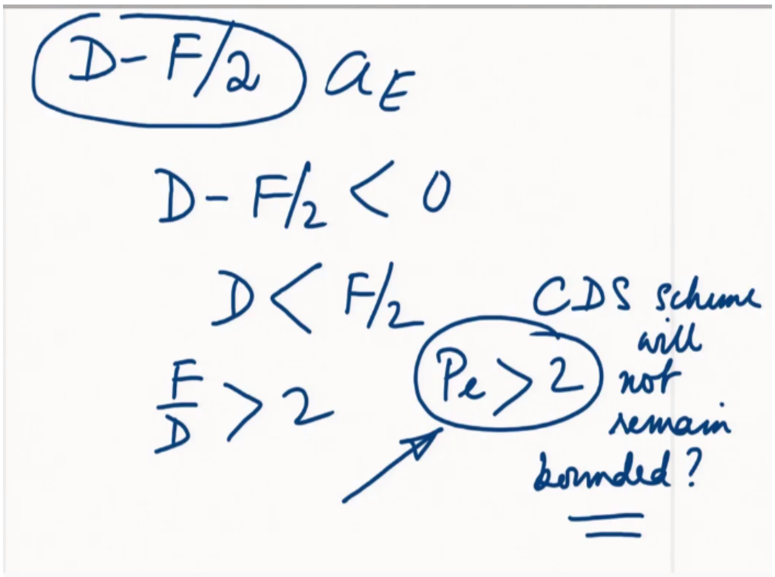

Is there a possibility? Yes, if you look at the table of coefficients, there is a possibility of this coefficient which actually comes from a E to become negative under certain circumstances. What is the circumstance? If you have a situation that this becomes <0, then you will have a negative coefficient. So, if that happens, what is the condition we get out of it? We get F by D > 2, which means for Peclet number > 2 the CDS scheme will not remain bounded.

So, what would this lead to? We can speculate that this would lead to some numerical instabilities. Right, we will see them later through some simulation results, but this is clearly going to create trouble for us. Let us do a quick problem, where we actually get to see that. So, we earlier did a case with a few numbers chosen for the different parameters.

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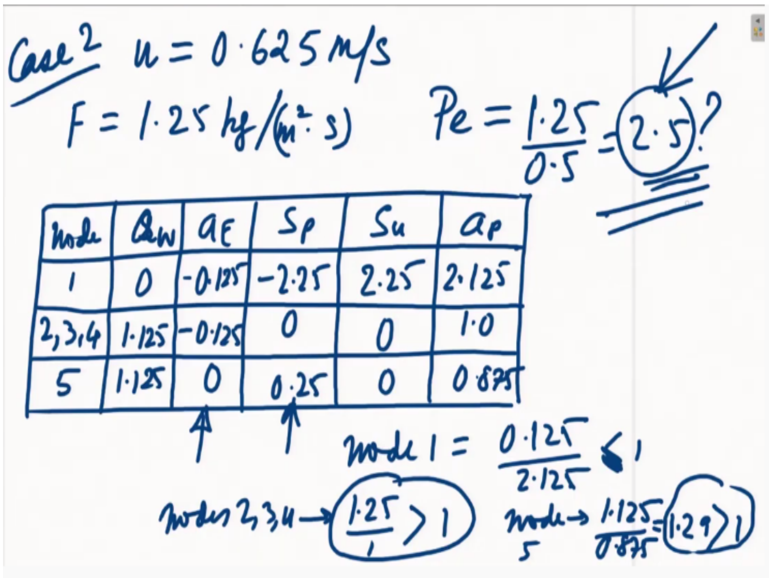

So, let this be the second case. And what we do is we keep all the remaining values same, we just change the value of u, which is the velocity of the field 2.625. What would this do to F? F would change to 1.25 kg per meter square second D remains the same as before. What would do, what would it do to the Peclet number? The Peclet number will become 2.5 and what we saw through the coefficient calculation. This is likely to create trouble.

But does it come up from the table of coefficients itself, let us try to see of course it should. So, again nodes here, so this is a W a E S P S u and a P. So, we just put the numbers together in this table, and we find that a W will attain values are like this. We do not see a problem here with sign. They are all positive. However, we see negative signs coming up in a E, and that is clearly going to create problems.

S P takes up a value of -2.25 which is okay, but we come up with a positive value here, which may create problems. Again, S u will look like this and a P will look like this. Now, if you do the Scarborough criterion check for node 1 will turn out to be, which is <1. Sorry. And then for nodes 2, 3, 4, it will be 1.25 by 1 which is clearly >1, and this will create trouble. Node 5, it is 1.125 by .875, which is 1.29.

Again, this will create trouble. So, this case is likely to create problems which of course we anticipated right in the beginning because it was having a Peclet number beyond 2. So, this could be a good time for us to have a look at some numerical results, which will make things still more clearer. But before we do that we will just try to write down the Case 1 situation in matrix form.

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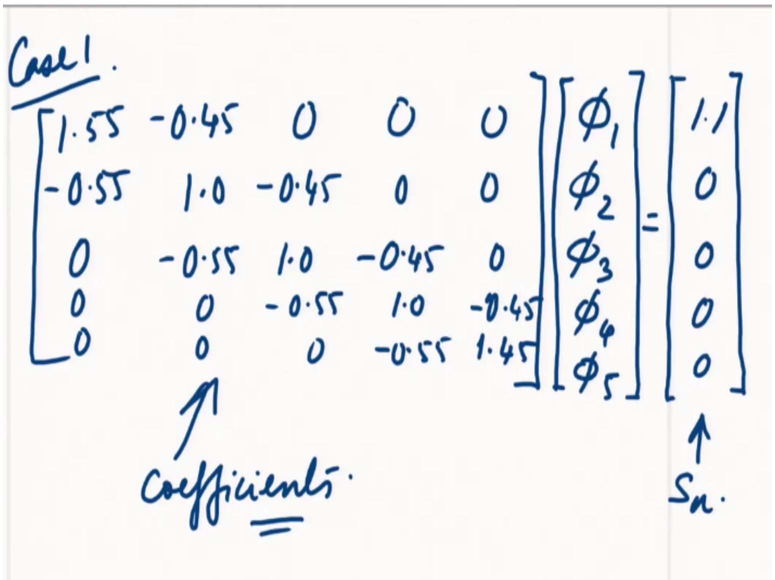

So, that we just have a glimpse of how the system appears when we try to translate it to a matrix form and where all the coefficients figure in the matrix. Of course you can figure out that **(()) (22:06)** structure is coming up, which is expected. So, let us call the values of the 5 different nodes as 5 1 to 5 5. And what comes on to the right hand side, you can clearly understand that the right hand side essentially is contributed from S u.

So, S u is the one which contributes to the right hand side. Okay. The rest of the terms here in the coefficient matrix, of course, come from the coefficients we have already calculated and which figure in the table that we have used. So, of course through a matrix in motion you can solve for 5 1 to 5 5 to give you the distribution. Now let us take a few minutes now to have a look at some numerical results.

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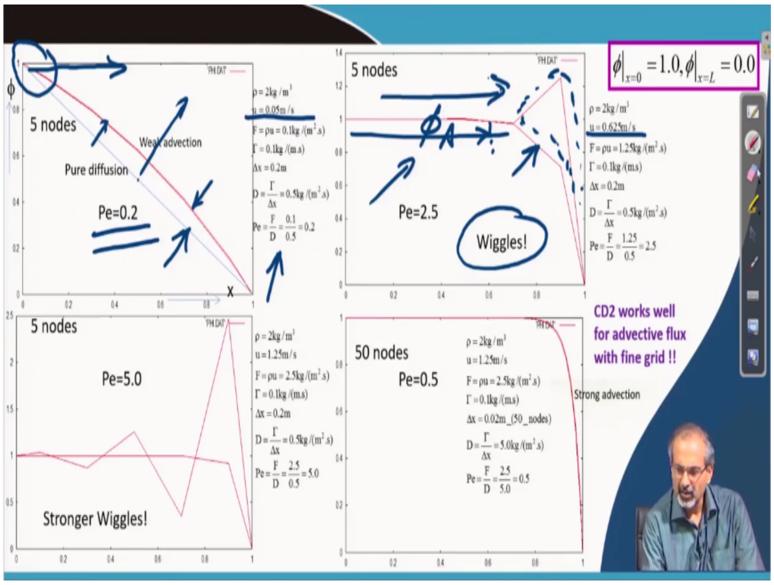

So, here is a result, where we have a domain of unit length, which is indicated along the x direction, and you have 2 boundary values of the domain. So, on the left of the domain you have a phi value of 1 on the right of the domain the phi value is 0. The phi values are indicated, along the y direction. And what you see over here is all the values that we have discussed about they figure over here that is the Case 1 that we talked about. Alright.

So, this is the Case 1 result when you have a low Peclet number 0.2. Alright. So, as a reference, we have also indicated the pure diffusion plot over here that means if there was no convert advection no effect of advection, then the distribution of phi would have looked like that. However, we have advection to a weaker extent. And that would mean that the curve deviates off. And how does it deviate off? It deviates upwards.

Why is it that it deviates upwards? Only then we can go closer to phi = 1, as we approach the left boundary regions, of course, at that left boundary precisely phi will always be equal to 1. But as advection becomes stronger, what happens is, it has a stronger sweeping effect of the left boundary value towards the right. Now since the advection is weak. It cannot sweep the value of phi = 1 further downstream in a very strong way.

And therefore, you remain close to the pure diffusion case only with a slight deviation towards the upper side. So, this is the physics behind the car, going on to the upper side. Alright. So, if that is the issue, we should see a stronger movement towards the upper side, if we make the flow, move with a larger velocity. And that is precisely what happens when you go to the Peclet number 2.5, because now the u has become stronger.

So, if you remember that u value over here is .625, while here it was .05 meters per second. So, what does it do? It sweeps the value of phi A much further downstream much closer to the right boundary. So, what does it do? It advects phi from the left boundary far into the domain. And therefore, the phi A value is retained as far as nearly set this region. Right, so, that is primarily the difference between the left figure and the right figure on top.

However, we have a big problem here. We have Wiggles. We have a strong. You know oscillation in the solution on top. And what you see at the bottom is the exact solution. Where was the exact solution in Peclet number 2. It was almost merging with this curve. So, what we understand is that in Peclet number .2 the central differencing scheme did a good job in capturing the physics, because we could not distinguish between the numerical result, and the analytical result.

But here, up to a good extent, it did follow the analytical curve, but towards the end it deviated off because it started oscillating.

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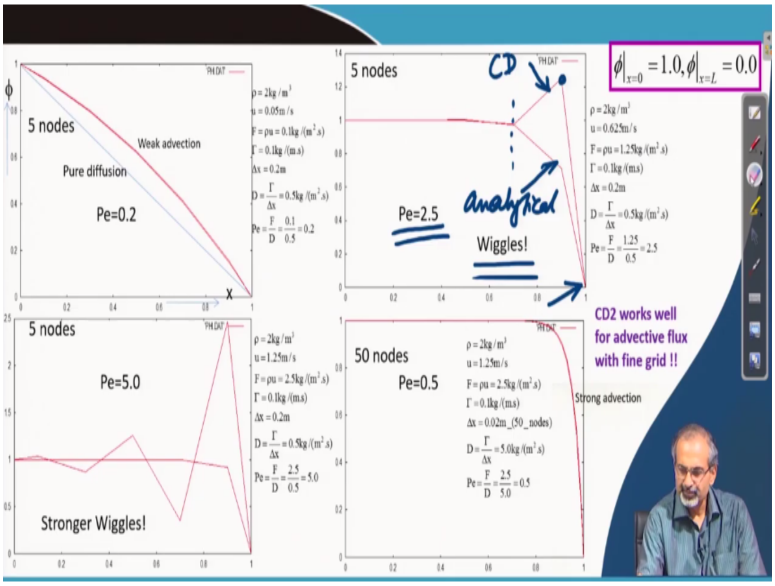

So, if you say that up to a region like this. There was a close match, because we were seeing the same curves. But then the central differencing went up, so you have a point out here. While the analytical result went down which is expected of course because you have to match up with the phi B value on the right side of the domain.

So, where was the problem? Problem was with numerical instability caused by a fairly large Peclet number in terms of the central differencing scheme because central differencing cannot work beyond Peclet number 2. So, that was the difficulty. Now, let us see that is there any way by which we can solve this problem. So, there could be a remedy. But before we look at a remedy we look at a situation which is even more adverse.

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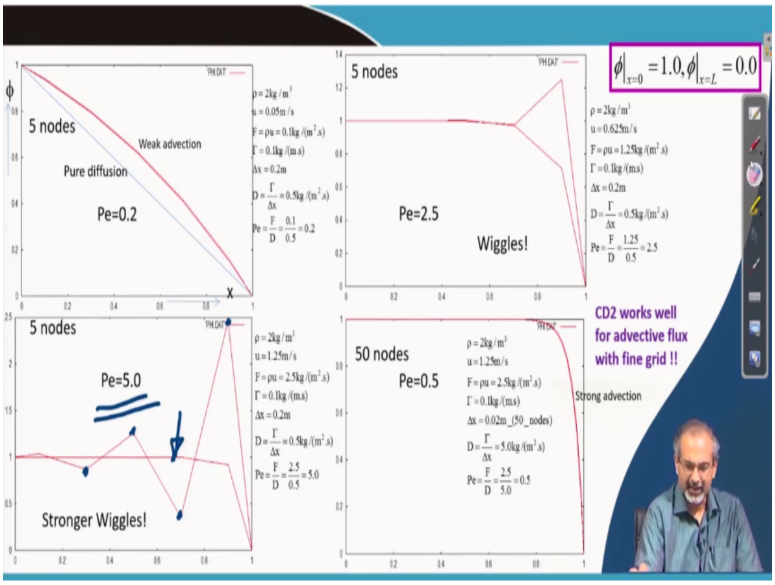

If we push it to Peclet number 5, you see that the solution oscillates further. So, there are more points which are oscillating off. You know from the analytical solution. So, you can expect more and more of those oscillations coming up. If you push it to Peclet number, larger and larger and beyond a certain point, of course you will probably end up with, **(()) (28:57)** number kind of situation in your numerical calculations.

That means, the computer will not give you any solution at all, it will crash. So, there is a way of course, to solve the problem.

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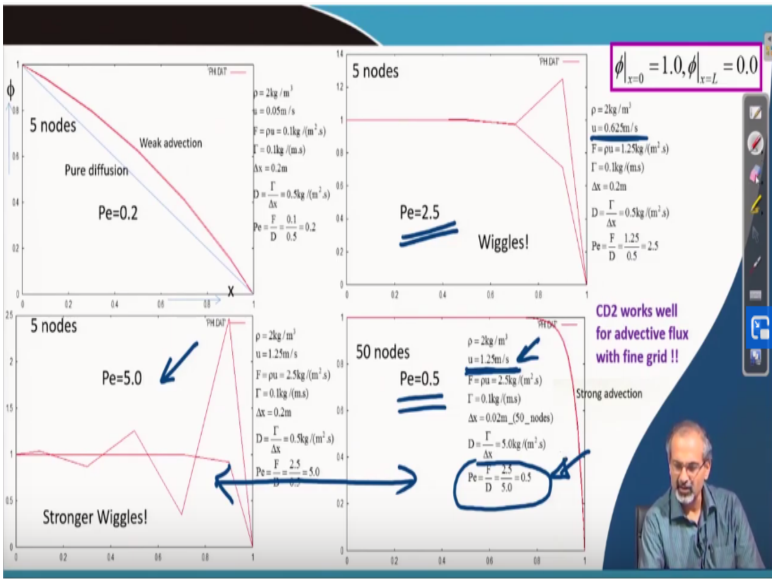

Can we bring down the Peclet number to below 2? Yes, one way of doing it is to refine the mesh to put in a lot more nodes. So, that Peclet number for the same velocity. In fact, over here the velocity is larger than the Case 2. It is twice as that of Case 2, which was here. So, here it was .625, but in this case we are using 1.25 was also used here. But you can now see that there are no wiggles anymore, because the Peclet number has been brought down to .5.

And now you have a smooth solution, and not only that you have a fairly good match with the analytical solution they almost merge with each other. You cannot probably distinguish the two curves. So, of course Peclet number 5 is it was not a trivial case, which we saw over here.

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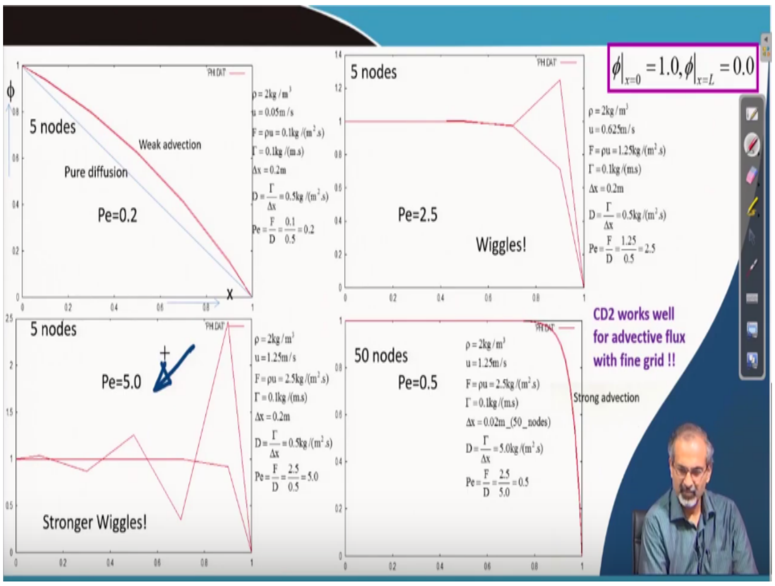

And for the central differencing scheme we found a way to solve the problem by putting in lot many number of nodes. So, earlier we were using 5 nodes we multiplied it by 10 made it 50 nodes, and then it sustained the strong advection. And now you can see that for Peclet number .5, how far the phi A value from the left end has made its way into the domain. That means there is a strong advection of phi from the left to the right end of the domain.

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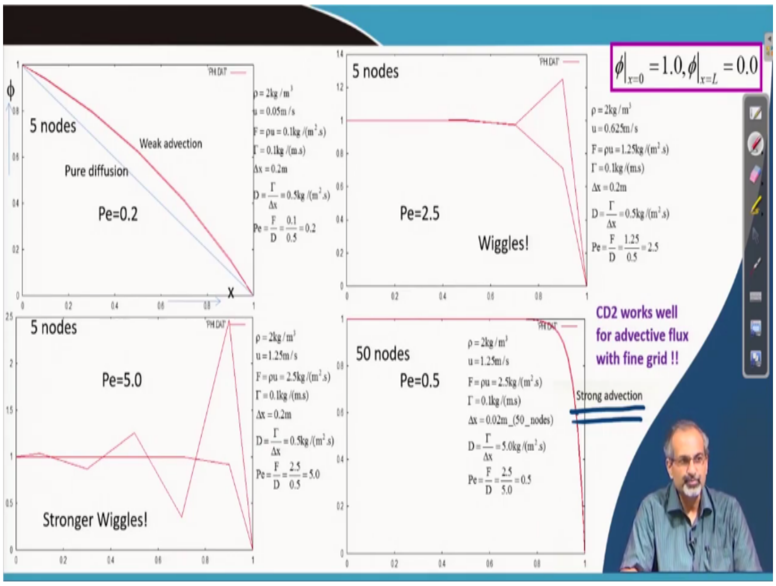

So, that is what makes it a strong advection case. So, we find that the CD2 scheme works well for advective flux with fine grid. And when advection becomes strong CD2 would work as long as we can keep the Peclet number below 2. And that can be achieved by using a fine mesh. So, we will continue our discussion on other numerical schemes in the next lecture. Thank you.