Introduction to CFD
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Lecture - 37
Numerical Solution of One Dimensional Convection – Diffusion Equation (continued)

We continue our discussion on one dimensional convection diffusion equation and we continue discussing about the exponential scheme.

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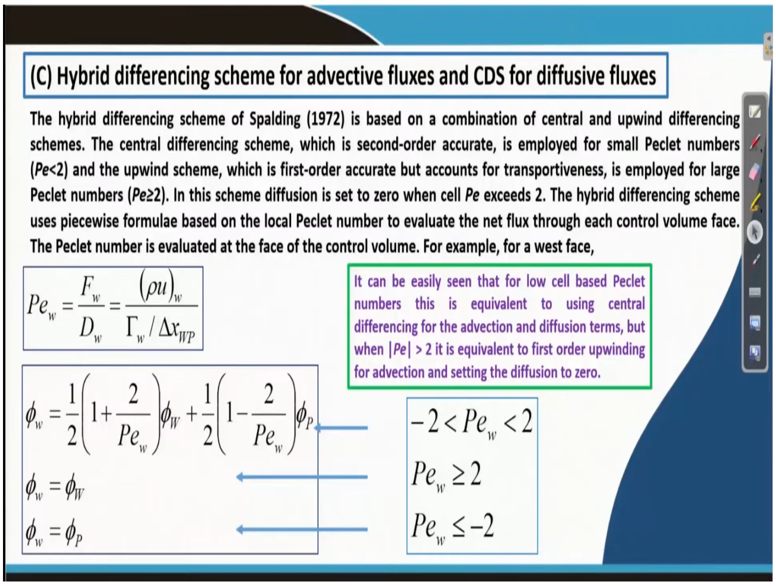

So, we will come to one form of the exponential scheme soon, which is called as the Hybrid scheme. And this slide talks about the Hybrid scheme in some detail. But before we do that we will do some calculations and come back to this slide.

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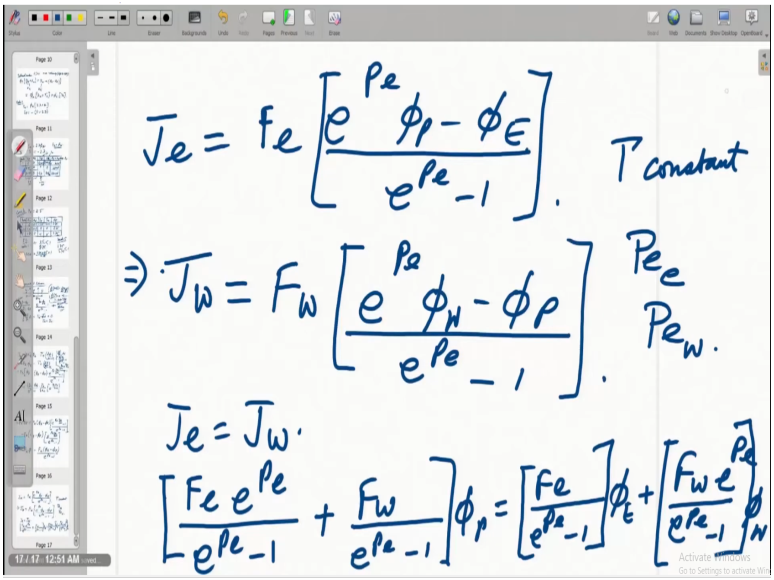

So, this is where we ended our last discussion. So, we were talking about exponents coming up in the coefficients of the different terms. And that is what makes it extremely expensive. So, we will find ways of reducing the expense. So, instead of having a perfect exponential profile fit. Let us see whether we can go for something like piecewise fits or less complicated profile fits. Alright.

However, they confirm closely to the exponential distribution as far as possible.

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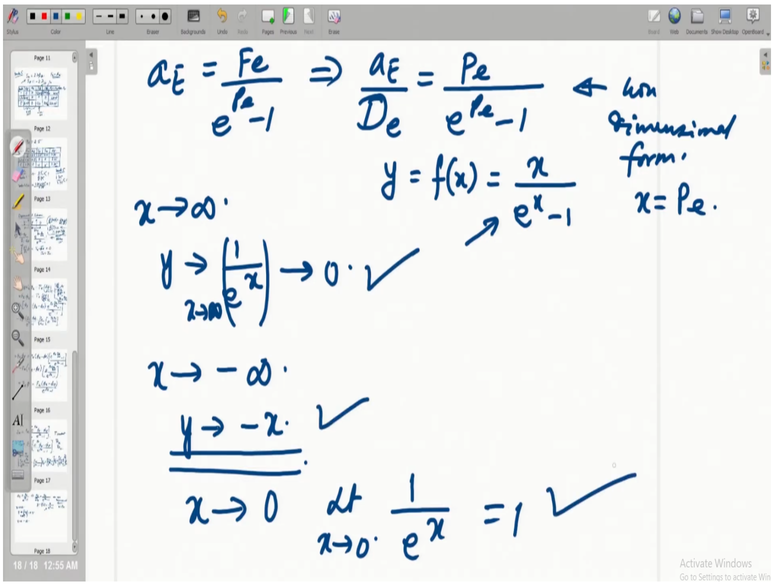

So, let us take one of the coefficients say the a E. So, from our previous discussion, you remember that it was written like this and we would prefer to write it in a non dimensional form where we put it as a E by D e. To compensate, it becomes P e over here in the numerator because P e is dif by d. And then this is essentially a non dimensional form. Right.

Now, if we consider this equation to be of the form y = f x. So, let us say x is nothing but Peclet number, then this becomes x by e to the power of x - 1.

So, this is a function and we need to understand how this function behaves over a wide range of x. How y behaves? So, that is the idea. Now, let us say that when Peclet number becomes very strongly positive, so extends to infinity. In that case, what would happen to y? y would tend to 1 by e to the power of x where x tends to infinity. So, we could not get to this form straight away.

Actually, if you substitute extends to infinity in this expression; then you have an infinity y by infinity form. So, you have to go for the L'Petals rule. And then you take a derivative of the numerator and the denominator separately. So, d dx of the numerator then divided by ddx of the denominator with the same limit applied and that should give you the identical limit as the original rule as per the L'Petals rule.

So, by L'Petals, it will come to this expression and you work out this limit and that tends to 0. That means, for very large Peclet number, the a E by d will tend to 0. So, we were talking about very large, positive Peclet number. Remember, not it could also be very large, negative Peclet number when the flow changes direction and becomes opposite. Right? So, in that situation, what is it that we will have? We will have y tending to – x.

Why is it? Because in the numerator, you will have in the numerator, you will have x which is very large, it is tending to negative infinity and in the denominator, it is e tending to minus infinity which is very small. So, it is x by -1 which is left and therefore y will tend to - x. So, we are done with the extremely large positive and negative values of x. Now, what about x in the range of very small Peclet number. So, x tending to 0.

Again, you will see if you directly substitute, it will become a 0 by 0 form indeterminate. So, use law petals rule and then put limit x tends to 0. Take the derivative, so, you will be left with 1 by e to the power of x which gives you a 1. So, now you have 3 limiting values for different ranges of Peclet numbers. If you try to put these values, what do you get finally out of it?

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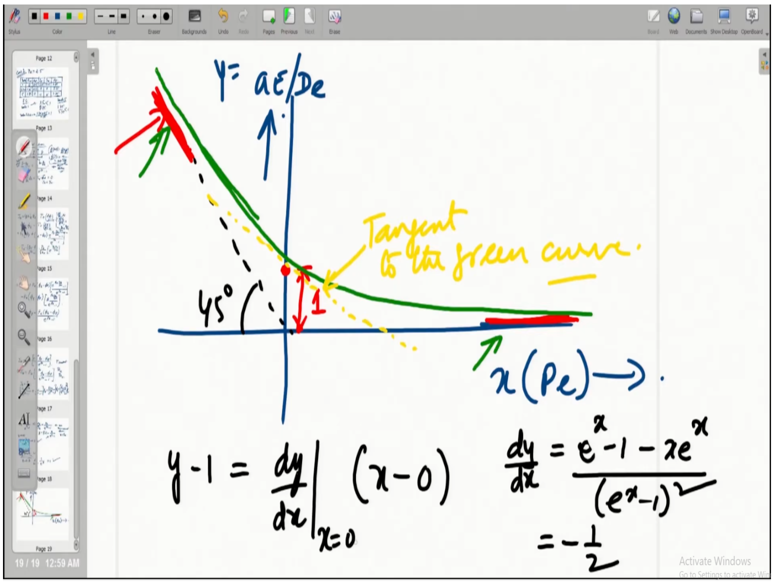

Let us try to make a plot. So, y which is essentially P e. No, sorry. y is not p e rather y along the y axis what we are plotting is a E by D e. Alright. P e is x, so, x or P e is along this direction. Of course, this is y certainly and what we have got is that at large Peclet numbers, we have got a distribution like this positive here and what happens in a negative sign, you have to have a 45 degree line here.

And then you have again for very large negative values. You need to have a line here. Right? So, this is what you have got, because y = - x will give you a line of this kind. Right? And what do you have at extending to 0, you have a y = 1. So, let us mark this as 1. So, that is the intercept here. How about the exponential plot itself? The exponential plot may be actually like this, somewhat like this.

That means, it asymptotically matches to these solutions and Peclet numbers become either very much positive or very much negative. But in the intermediate values, you know the curve remains highly non linear. And it would be costly for us to go for exactly satisfying it. So, what do we do? One way of handling this problem is using the odd of linearization.

That means, what we will do is we will try to compute a tangent here. So, the yellow line is a tangent to the green curve. That is what we have done here. Okay. If you do a tangent to the green curve, then what condition should it satisfy? It should satisfy the condition y - 1 = dy dx at x = 0 times x – 0. This would be the equation of the straight line. Okay. So, of course, it comes from the here straight line equation forms; different forms of straight line.

This is y - y 1 by x - x 1 kind of form equal to dy dx or M, the slope of the straight line. Right. So, how do I find out dy dx, I know y = f x. So, dy dx which is the slope is given by e to the power of x – 1, so, -1 come in the index. So, it is e to the power of x – 1 - x e to the power of x and then e to the power of x - 1 square here. And this then if you try to substitute x = 0 there, again it will be a 0 by 0 indeterminate form.

So, L'Petals rule again from where you will be able to show that this is equal to minus half. So, you take the derivatives of numerator, denominator separately and put the limit it gives you minus half.

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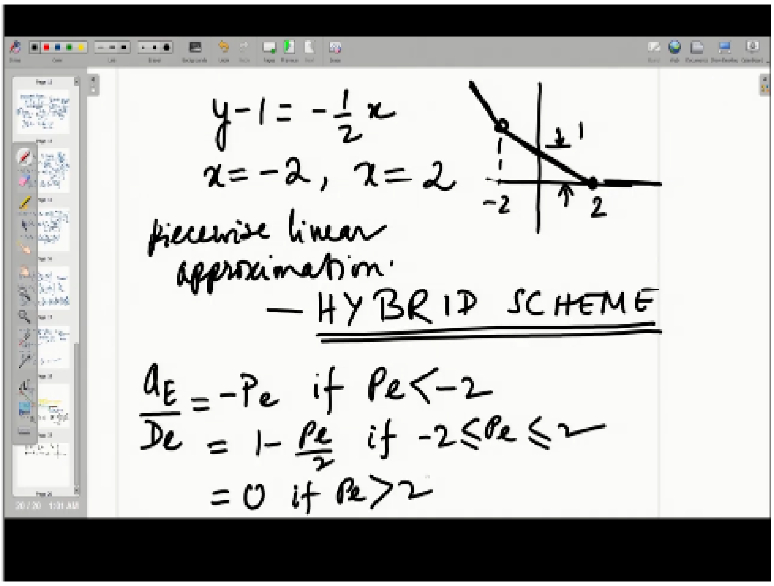

Which means the equation of the tangent is equal to this y – 1 = - half x. Now, where does this tangent meet the two straight lines; the one straight line is y = 0; the other straight line is y = - x. So, just solve for the points and you will find the points of intersection will be found as x = - 2 and x is equal to + 2.

So, the x = -2 confirms to very large negative Peclet numbers; x = +2 confirms to very large positive Peclet numbers. So, these are the limits. So, which means, now you have essentially 3 straight lines. Is it not? So, you have a piece of straight line here, a piece of straight line here and another one which you have matched up over here in between with an intercept of 1 on the y axis.

That is how the straight lines are coming. And you know exactly that this is -2 and this is +2. This is precisely how piecewise linear approximation of the exponential variation is achieved.

Right. What does that give rise to? it gives rise to what is called as a hybrid scheme? That means a scheme which would mix mix and match that means blend central differencing without upwinding.

That is why it is called as hybrid. And how does it coefficients look like? It looks like - P e, if P e is less than -2; is equal to 1- P e by 2, if it lies within this range and it is equal to 0, if P e goes beyond 2. And this kind of scheme essentially switches of the diffusion term beyond modules of Peclet number > 2. That is what it essentially does. Alright.

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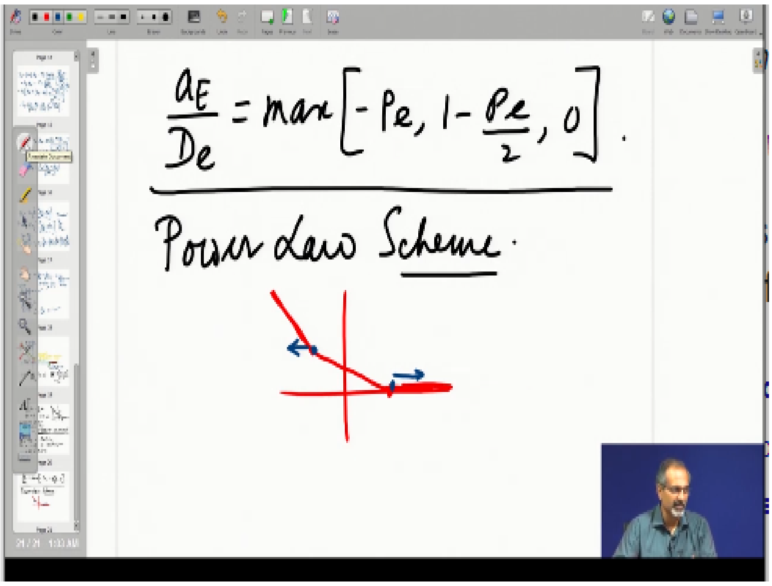

Now, this distribution can be written in a more convenient form, a more compact form which is very convenient for computer coding in this way. So, max of these arguments and you can check very easily that each one of these arguments when applied to the different 3 segments of the piecewise linear distribution, will give you the appropriate value for each portion. Alright.

So, this is essentially the hybrid scheme. Now, the cutoff of the diffusion term at modulus of Peclet number equal to 2 or beyond 2 rather gives rise to hybrid scheme. Now, there was a more sophisticated scheme which was devised later and that is called as the Power Law scheme which set the cutoff not at 2, but beyond 2 a little futher beyond 2. So, what does it achieve for you?

It achieves something like this that if your hybrid has achieved something like this. Hybrid has essentially achieved something like this for you. While, Power Law shifts the cutoff further, a little further. Alright. Shifts the cut off a little further, which means in go a little closer to the exponential variation the analytical formulators. Okay. So, that gives you superior you know calculations or superior accuracy then hybrid scheme, but at an additional expense.

But not as significant as the pure exponential scheme. So, that is the trade off.

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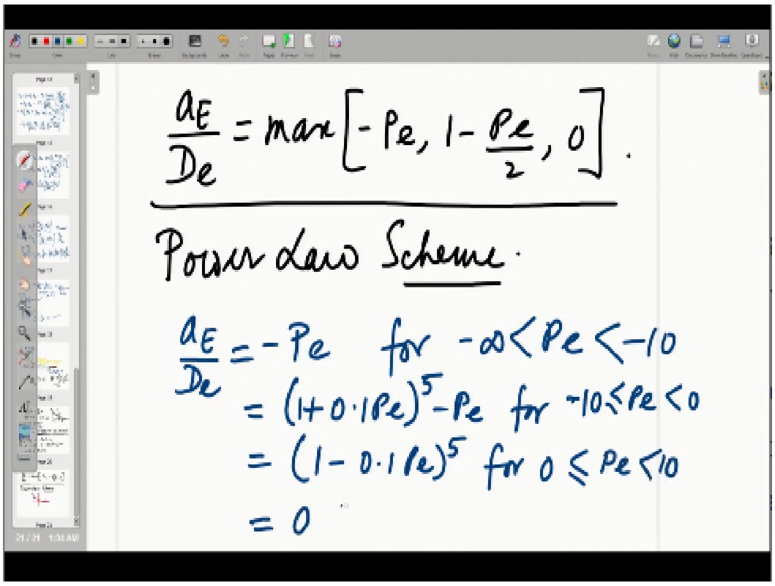

Now, if you do that what does it come to? What does the scheme come to? Let us try to define the scheme straightaway. So, for the Power Law scheme, the cutoff Peclet number happens to be 10. That means, on each side + or - 10 and the intermediate portion is patched not by a straight line, but rather a Power Law distribution which you can clearly see from this functional form which I am currently writing.

So, unlike hybrid scheme where we have used all piecewise linear regions. Here, we use Power Law in the intermediate region, in the modulus Peclet number grid is less than 10 region. So, this is how power law functions. And that means the Peclet number is certainly considered as the switching of parameter and switches of the deficient term at mod Peclet number greater than 10.

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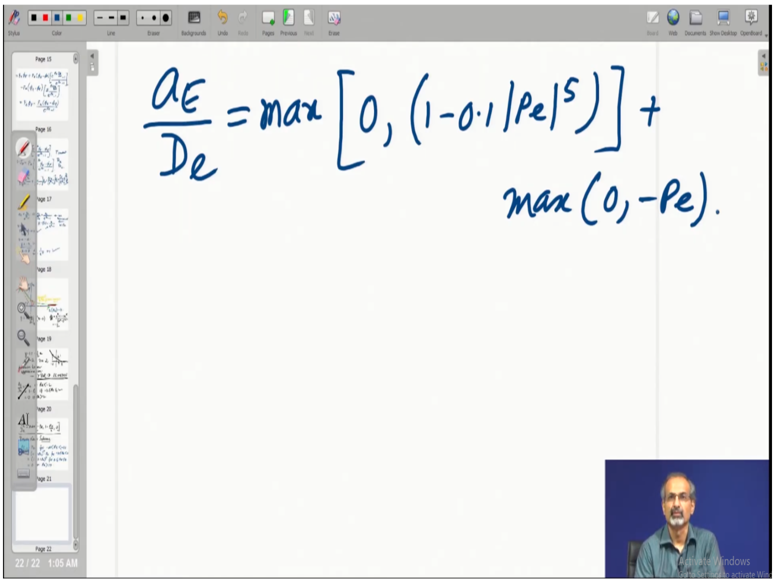

And if you use the max function for Power Law, then it comes to something like this which is a little more complicated than the hybrid scheme. But nevertheless very easy to code computer programs. So, this is how the Power Law functions. And now let us have a quick look at the slides where we sum of these aspects.

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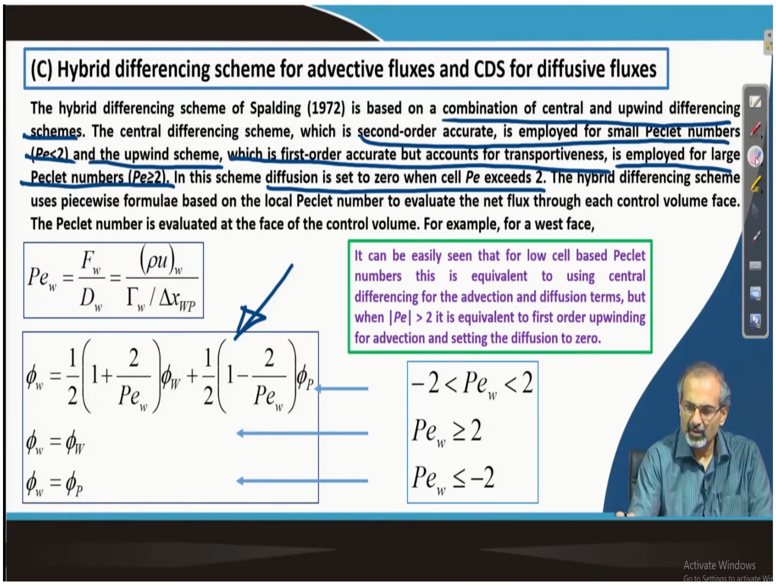

So, hybrid scheme as we said earlier that it is a combination of central and upwind differencing schemes and it is one in which diffusion is set to 0 when Peclet when cell Peclet number exceeds 2 and you can actually calculate the fluxes at the faces using distributions of this form. In the derivations, we have talked about how the coefficient a E by D e functions for a hybrid scheme.

From there, you can derive the flux calculations et cetera, which is shown straight away over here. And of course, it is a blend between the second order central differencing and the first order upwind. And second order is applied for small Peclet number and the upwind is applied at higher Peclet numbers. So, that you have the transportiveness property and the solution remains bounded at larger Peclet numbers.

So, this is how the two are blended together giving you a hybrid formulation.

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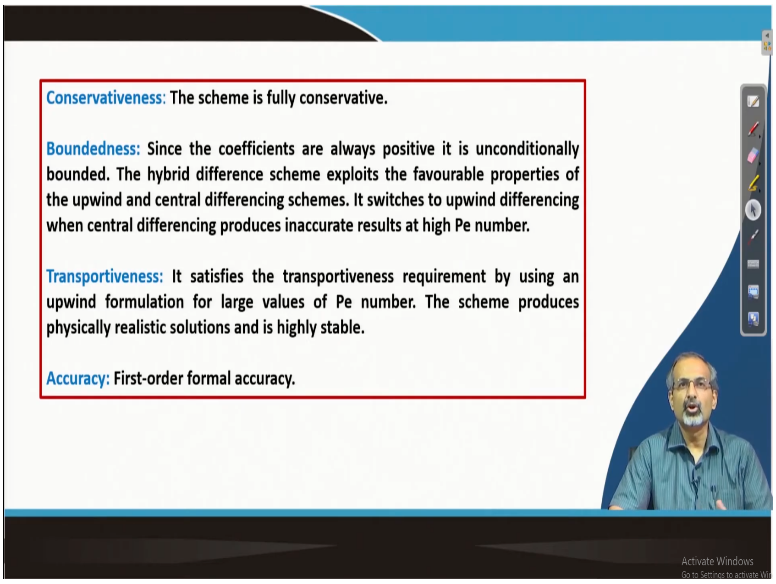

So, because the Power Law scheme is also a very related scheme, let us go to a slide where we discuss briefly about Power Law. And before we do that these are the properties very quickly on the hybrid scheme that it gives you a conservative formulation. It gives you boundedness because it accounts for the hybridization between central and upwind. So, upwind actually helps you to bring in the boundedness and the transportiveness again, is assured at large values of Peclet number this way.

And therefore, solutions will remain stable even when the advective effects are very strong. And first order formal accuracy strictly for larger Peclet numbers, but at low Peclet numbers, it would actually give you as good as second order accuracy. So, this is how it functions.

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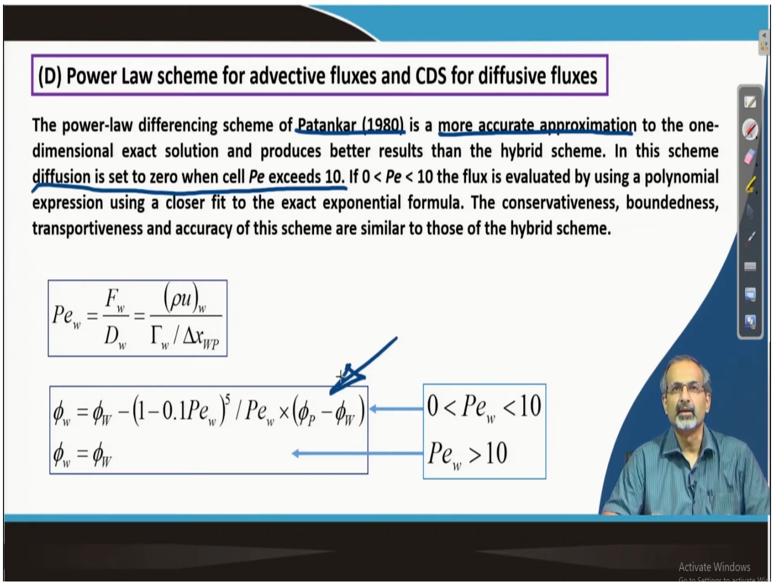

For Power Law again, which is a little more advanced version, and in actually came a little later, in 1980. It is more accurate and approximation as we discussed earlier, because of approximating nearly the exponential distribution in the intermediate Peclet number range instead of using a piecewise linear approximation for the coefficients. And therefore, you are expected to have more accurate approximations as a consequence.

And in this scheme, the diffusion is set to 0 when Peclet number or the cell Peclet number exceeds 10. And it is conservativeness, boundedness, transportiveness and accuracy are of similar order, but accuracy is strictly speaking of a higher order then Power Law, because of the superior approximation that we apply here in the intermediate Peclet number ranges.

So, we have discussed about a number of schemes already now, which are either first order accurate or second order accurate or a blending between the two. So, now, we will finish our discussion with another scheme where little superior accuracy is possible, little more superior accuracy is possible.

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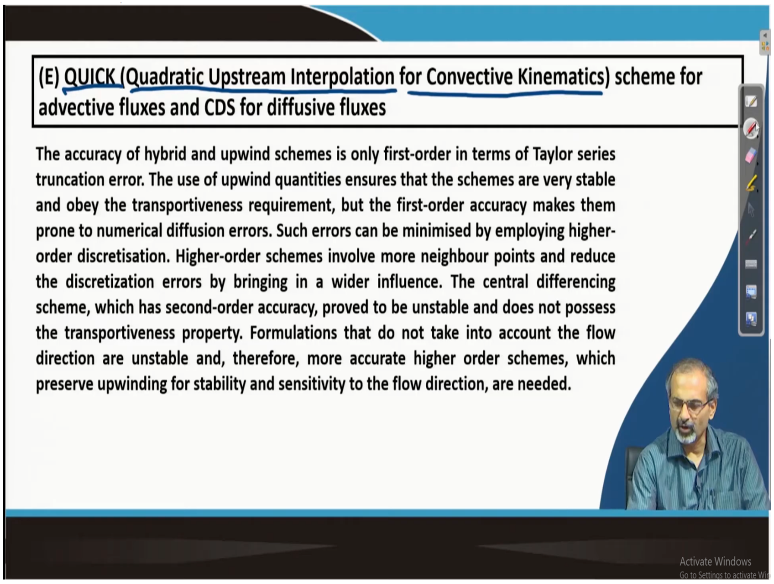

But at the expense of more computing effort. That scheme is called as the QUICK scheme, Quadratic Upstream Interpolation for Convective Kinematics, which uses quadratic fit involving 3 nodal points to calculate the values of phi at a particular cell face. So, let us do calculation on how QUICK scheme works. Before we do that will just put a small grid together.

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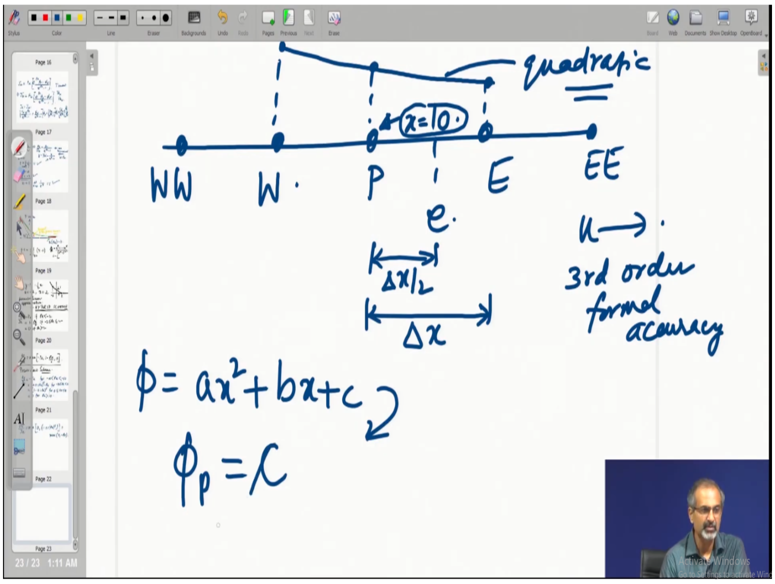

And show the different points which are of importance to us. So, let us say, we want to compute the value of phi at the point e and the velocity is moving from left to right. In the case of QUICK, what we do is, we take 3 nodes and make a quadratic fit; making sure that we have taken two upstream nodes and one downstream node in the process.

So, as far as the phase e is concerned, because the flow is moving from left to right, the two upstream nodes are P and W, while one downstream node is E. Alright. So, that is how the quadratic fit is made. Remember that because it is a quadratic fit on a uniform grid, it gives us third order formal accuracy. With 2 points, it gives second order accuracy like we have seen in central differencing.

With one point value, it gives first order accuracy like we have seen first order upwind scheme. So its 3 points on the uniform grid, we will get third order accuracy. So, that is how QUICK is certainly more superior then all the numerical schemes we have discussed till now for advection diffusion equation. So, say this is half grid spacing delta x by 2, while this is 1, and so on. And this is uniform grid, as we mentioned already.

So, let us try to fit a quadratic in this manner where we set the x = 0, well, not here, but rather at this point at P equ at P we set x = 0. Alright. So, if that is the case, from this equation itself, we can say phi P is equal to C, because there x is equal to 0, Right. Now, we substitute for the other nodel values.

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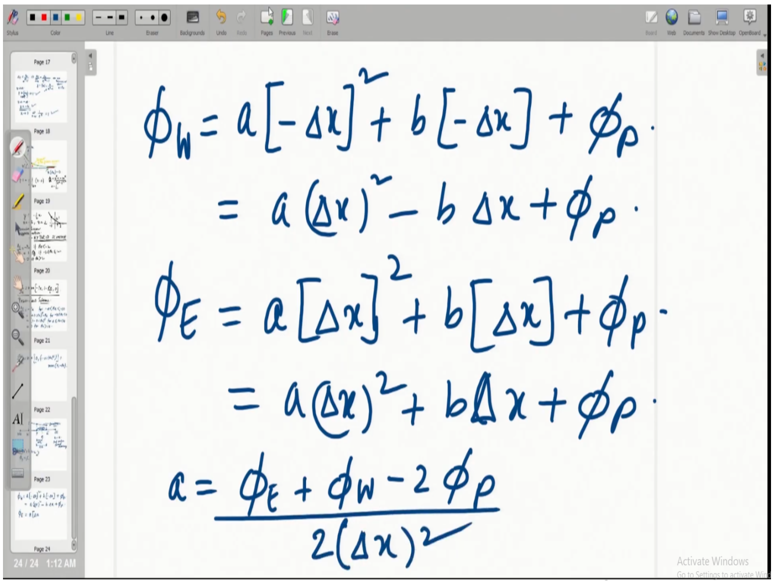

So, you will find that phi w is equal to a times - delta x square + b times - delta x + C which is phi p already. Now, this becomes a delta x square - b delta x + phi p. And then if we add the equations for. Okay. Before we add we write down the equation for phi E. So, for phi E, it will be this. So, we have, we do not have any negative signs here. So, that will help us to eliminate some of the unknowns and solve.

So, if you add the two equations, you can actually solve for a, because b gets eliminated. So, a comes out to be like this. Right.

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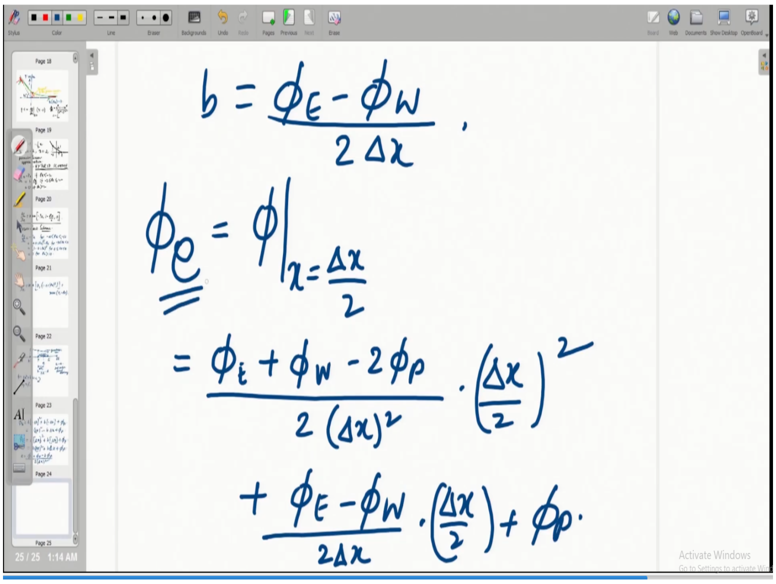

And then you can subtract the two equations and you can show b is equal to this. Right. And then what you need to do is substitute these a's and b's into the original equation and then rearrange the terms. After you do that what do you come up with, you come up with an expression like this. Okay.

What we will do is we will straight away write an expression for phi e by substituting the value of x is equal to delta x by 2 in the quadratic, because you have already solved for a, b, and c. So, you now have the quadratic. In that quadratic, you just substitute x is equal to delta x by 2. If you do that you will get phi e. So, what will phi e come out to be?

It will be phi E + phi W – 2 phi p by 2 delta x square into this, plus phi E - phi W by 2 delta x into delta x by 2, plus phi p. So, this will be the value add the east face.

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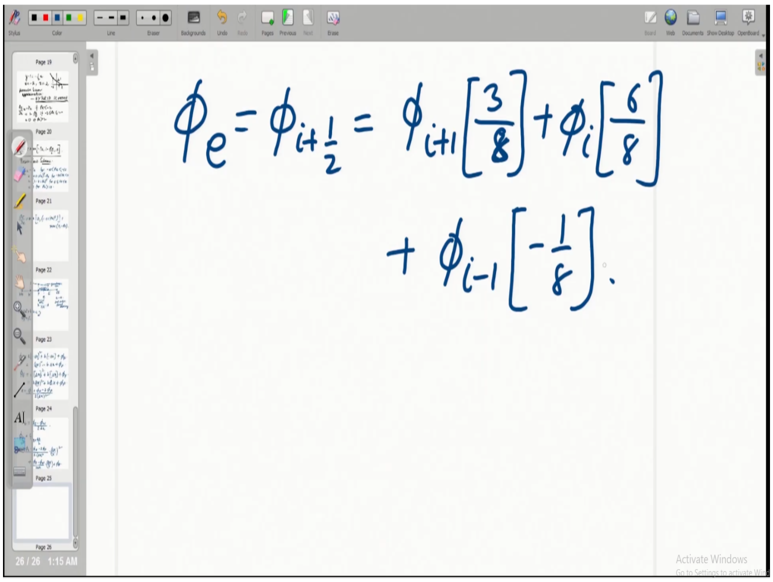

If you just rearrange the terms, this can be written in an index form. If I consider the nodal point p s I then this gives me the indices phi i + 1, phi i, phi i - 1 and so on. Right. So, this is the form of QUICK. Alright. For the East face value of phi. Okay. You can similarly calculate for the west face of phi and you can calculate for flow moving from right to left also. If you go back to the slide, you can actually have a look at that format here.

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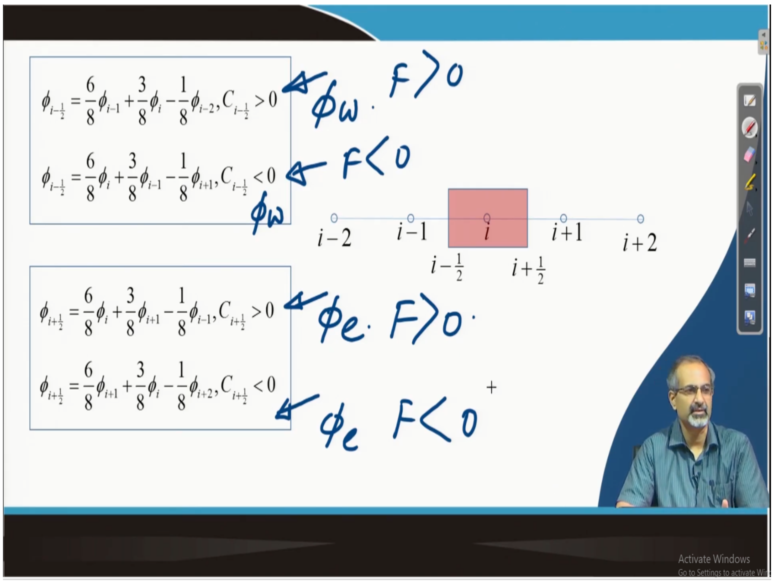

So, in this slide, you can easily see that for flow moving from left to right, this is how phi w can be worked out. From flow moving from left to right, this is how phi e can be worked out. So, this is F > 0, this is F > 0, and these are for F < 0. So, this is the phi w expression for F < 0. Again, phi e expression for F < 0. So, from that one equation that we have worked out now. We can actually derive all these equations just by shifting it by half cell width. Right.

Or other one cell width. That means, if I have worked out this, the phi at i plus half. In that expression, if I substitute i e = i - 1, then I get a i minus half. And therefore, I can generate the expressions for east and west faces both for F > 0 and F < 0. That is how it all works. Right.

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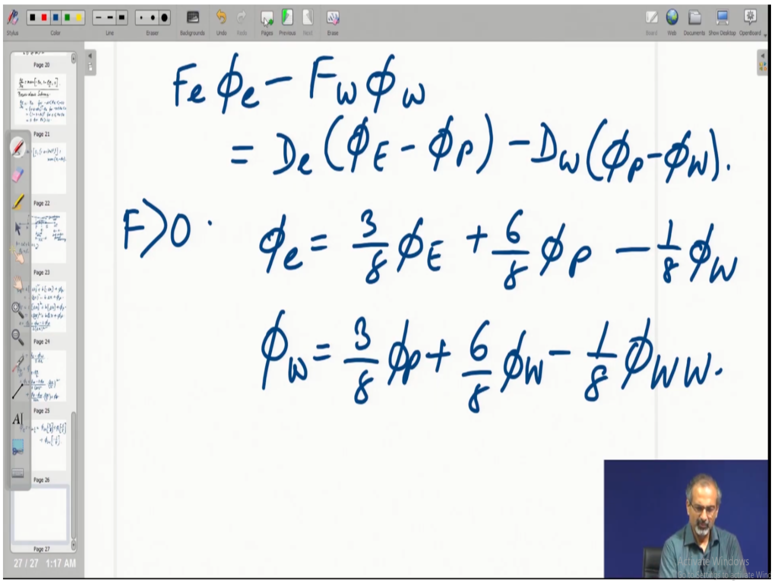

So, if that is the thing, then we have now understood how we can even apply QUICK to our transport equation. So, let us go to our transport equation and try to apply QUICK to it and see what happens. Again, as I mentioned many times earlier, that the right hand side the diffusive part, we continue to do a CDS, the central differencing second order. Right. And we are considering F > 0, so, phi e is 3 by 8 by phi E + 6 by 8 phi P - 1by 8 phi W.

So, that is phi e and the phi w can be similarly written as 3 by 8 phi P + 6 by 8 phi W – 1 8 phi W W that means the node to the west of the W node. Alright. So, now, you have to collect all the terms and get the coefficients. So, for phi P, what do I get as coefficients. I get these terms, put together gives me the a P.

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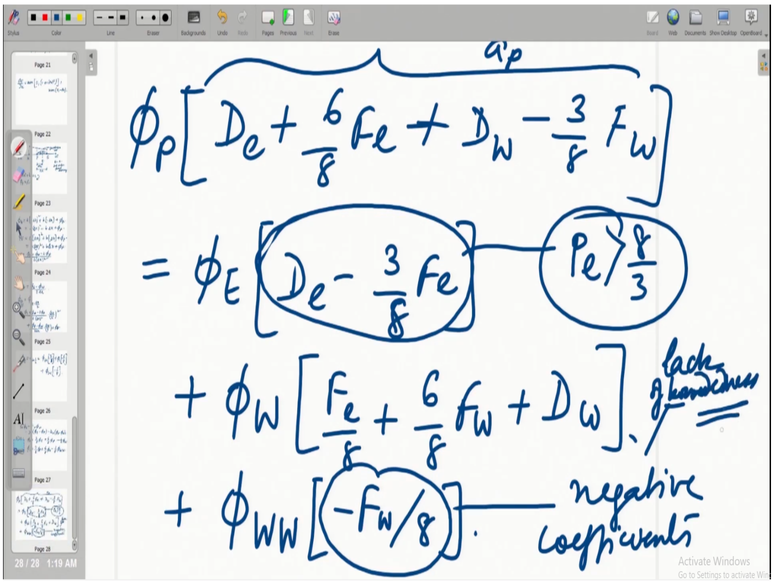

So, this whole expression gives me a P obviously. It is getting more complicated, because I have a quadratic interpolation. That gives me phi E times D e – 3, 8th 3 8th F e + phi W times F e by 8 + 6 by 8 F W plus D W + phi W W times - F W by 8. So, this is what you get. Alright. So, what is the outcome of this? It gives us some very, very important clues out here.

We have a situation similar to what we found in the central differencing that there is a case where this coefficient can become negative. Actually, we can easily show that as Peclet number, the cell Peclet number exceeds 8 by 3, this coefficient will become negative, which is a recipe for problem, numerical instability, lack of boundedness and this inevitably will live in negative, all the time. Right.

As long as u is from left to right that means F is positive. So, then what is the difficulty with this situation? The situation leads to negative coefficients and therefore, this will lead to lack of boundedness. And therefore, though it has higher formal order of accuracy, QUICK scheme would develop certain numerical instabilities if we are not very careful about the cell Peclet number limit. Thank you very much.