Introduction to CFD
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Lecture - 38
Numerical Solution of One Dimensional Convection - Diffusion Equation (continued)

In this lecture, we will complete our discussion on the one dimensional convection diffusion equation.

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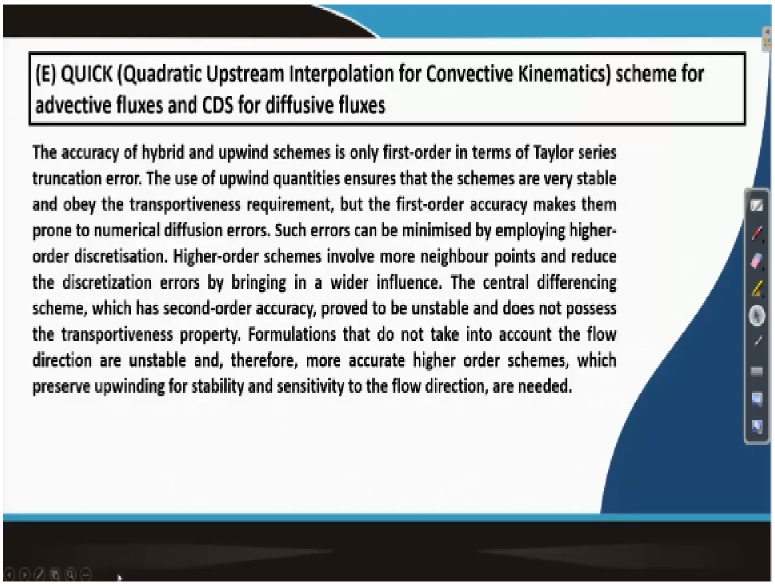

The last lecture concluded with discussion on the QUICK scheme where we saw that we use a quadratic fit using three nodal points in order to reconstruct the value of phi at an interface. We also saw by analyzing the coefficients of QUICK that there could be numerical instability problems. So, if we were to extend this problem to do a two dimensional problem. How would numerical schemes like QUICK are first order upwind scheme which we have already discussed work.

So, if you recall that we have already learned a number of techniques now. So, we began with central differencing technique, then we went on to first order upwind then we looked at the exponential scheme and from there the simplified versions the hybrid and the power law scheme and finally, we had looked at QUICK. So, now for looking at the two dimensional convection diffusion or advection diffusion problem.

Here just looking at how QUICK and the first order upwind scheme would work. So, let us make a small diagram to understand the behavior.

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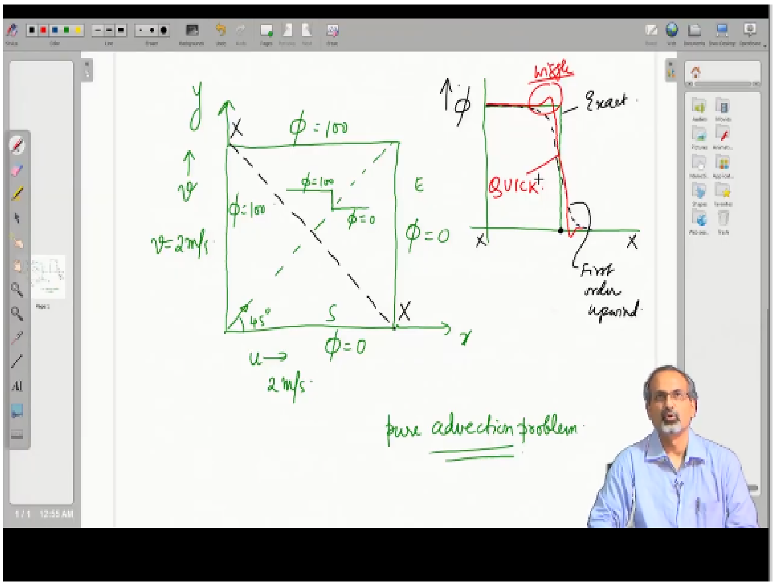

In a two dimensional problem, let us see how we would pose the problem to begin with. So, this is a two dimensional domain in the x y plane and we have the u component of velocity defined in this direction. Let us say, this two meters per second. v component defined as two meters per second. The more important thing is that both of the velocities are identical, which would mean that the resultant velocity will moves along this 45 degree line.

So, if you have a squared domain like the one we have sketched over here, the phi variations would depend on the boundary conditions that you are specifying. The phi if you are specifying as 0 on the east and the south faces. So, let us say this is the east; this is south face and on the north face and the west face. We are specifying phi is equal to 100 then because, we are solving a pure advection problem.

That means, we are not going to take the diffusion term, we just take the advection term that means, the phi would be transported in such a manner that there would be a step change of phi about this line. That means, this would be the phi = 100 value; this would be the phi = 0 value existing across the dotted line. That is how phi would be transported because you have equal velocities along the two directions.

Now, this is a very challenging problem for any numerical scheme where the flow direction is skewed. It is not aligned well along the coordinate directions. Now, how does the numerical schemes face this challenge? If you try to solve this problem with two dimensional implementation of QUICK on one hand and first order upwind on the other, then let us see how they behave. As far as first order upwind is concerned.

We already know from our past experience that it has a diffusive behavior, so, it would probably behave like this. This does not come as a surprise really! Now, this plot is actually representation of how phi changes along this line, which we marked as say, XX alright. So, this is something like that XX right. And this may be just around the mid-point of that XX line where the jump change would actually occurs.

So, this is the exact variation of phi while the dotted line is the first order upwind response. How would QUICK respond? QUICK may respond with little bit wiggle here. It would actually capture the sharp change better than the first order upwind scheme in a way that its response is sharper. However, it is having or developing the problem of wiggle. So, the red line is the response of weak.

So, the question to ask now is that we find that as we improve the formal accuracy of the scheme by means of which we are capturing such sharp changes, we are able to capture the change in a sharper manner that the sharp change does not get diffused because of artificial viscosity. But, on the other hand, we see these numerical oscillations coming up on the wiggles coming up.

So, is there a possibility by means of which we still have a good enough shot capture and we avoid wiggles? So, can there be a solution from both ends? So, that is the question to pose now, and we will try to answer that question in a simplified manner by doing short discussion on the possible strategy. So, in order to place this strategy, let us try to revisit some of the formulations we are already familiar with.

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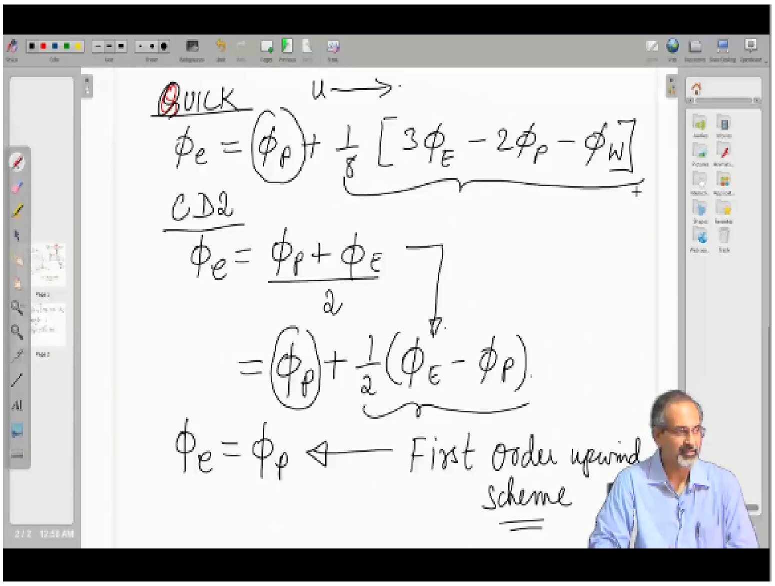

So, in the QUICK scheme for example. Okay let us change the color. In QUICK scheme, when the flow is from the left to the right that means, u is moving from left to right, we say that phi e would be reconstructed by using the formula phi p + 1 by 8 3 phi e - 2 phi p - phi w. This is already known to us. We have done it in the previous lecture. So, this is how phi e is being discretized while if you look at the central difference scheme, say the CD2 scheme.

How did we do phi e? We did it by phi p + phi e by 2. Right. Now, in the CD to scheme if you try to take the phi p out then you would have to make an adjustment in order to retain the expression. So, this expression would reduce to a form like this, if you try to keep the phi p aside. Why are we keeping the phi p aside? The purpose that it serves is that if I wrote phi e is equal to phi p.

This would have implied that this is the discretization for phi using the first order upwind scheme. Right. Now, QUICK or CD2 both have higher formal accuracy than the first order upwind scheme. However, they develop some numerical oscillations at times. So, we are aware of both the issues that on one hand they have better formal accuracy; on another hand first order upwind scheme which is able to satisfy the boundedness property all the time is not necessarily satisfied by schemes like CD2 or QUICK.

So, this adjustment terms that we have over here are accounting for better accuracy, but at the same time, the root of those oscillations also lie there in some manner. So, can we just extract that root of the problem associated with oscillations but still maintain higher formal accuracy? That is the question to pose. Let us try to gradually take it forward. So, that we can try to find an answer to this.

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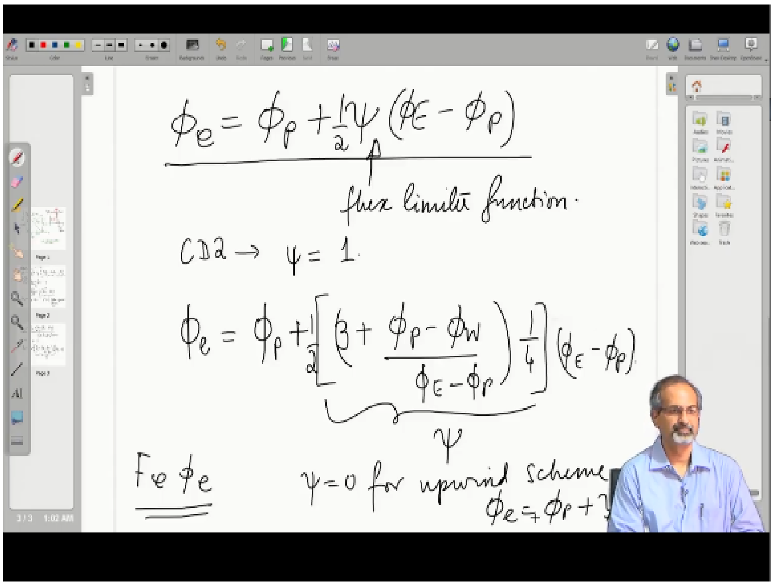

So, now that we saw two schemes behaving that way, we could write it like this perhaps that we should hopefully be able to write down the different schemes that we have in a form like this. Why we are concerned with a function that should be half Psi times phi e - phi p. You are introducing a function which we often called as the flux limiter function.

Now, as you can understand that the flux limiter function for the CD2 scheme happens to be 1 because if you just replace Psi by 1, you get back CD2 scheme. What is this Psi for the QUICK scheme? Are we aware of that? Let us try to work it out for the QUICK scheme. Let us try to lay it in this form phi p + half off and then if you do a little bit of algebra then you can put it in this form.

So, that you have an expression for the Psi which is your flux limiter function for QUICK. Right. So, this entire expression within the square bracket is the Psi expression for QUICK. Right, which we are calling as the flux limiter function. So, this portion of the expression involving Psi. What is it? It is like an additional convective or advective flux. Right. So, when I use this in the advection diffusion equation.

This will actually be used as F e times phi e. Is it not? Which will account for the advective flux at the east face of the selfie. Right. So, if I have an additional term, in addition to phi p accounted by that Psi portion of the expression, then that must be an additional advective flux contribution. Right. So, that additional contribution is actually carrying some information about the gradient of the transported quantity phi at the east face.

The moment, I take a difference phi e - phi p. I am actually talking about a gradient at that it is East face. So, I am addition additionally incorporating some gradient information in the phi e expression through that Psi part of the entire expression. Right, So, that gradient expression is improving the formal accuracy, but I have to just ensure that it additionally does not create the problem with numerical oscillations. Right.

So, let us try to understand that what would Psi be for the upwind scheme straight forward the Psi would be 0. Why is it? Because phi e is equal to phi p and therefore, it is 0 times Psi. That is plain and simple. Now, if I were even improving the formal order of accuracy of the first order upwind scheme by going in for a say a second order upwind scheme, which we often call as the LUD scheme or the linear upwind differencing scheme.

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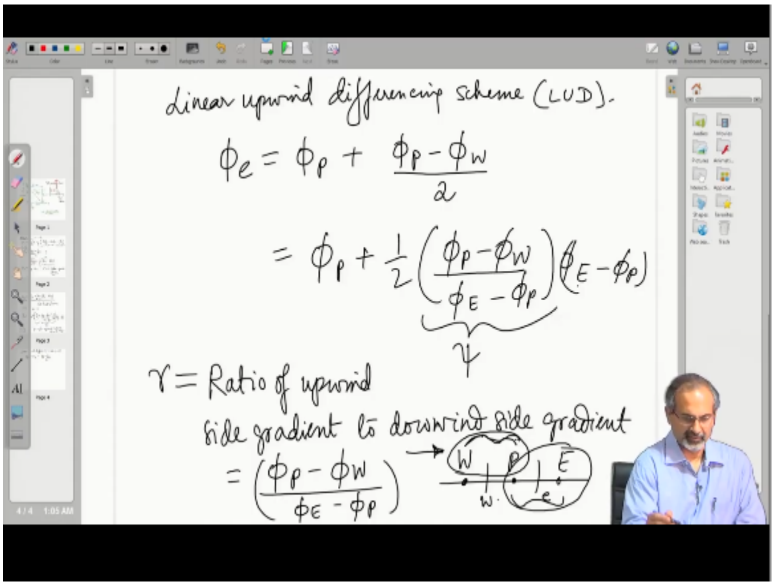

The expression would actually come out to be phi e = phi p + phi p - phi w by 2. This is how it is going to work out. Right. Okay. So, you can work it out later on yourself and try to check for yourself that this can work out as phi p + half of phi p - phi w by phi e - phi p into phi e - phi p. Alright. So, we have an expression for Psi for the linear upwind different scheme this way. Okay.

So, we have definition of a ratio r which is the ratio of upwind side gradient to downwind side gradient. Which for the direction of flow from left to right would be defined as phi p -

phi w by phi e - phi p. So, we have to just keep track of the grid. This is our grid. This is small e. This is small w. So, phi p - phi w involves these two nodal points. phi e - phi p involves these two nodal points.

So, ratio of upwind side gradient to downwind side gradients. So, flow is moving in this direction. So, this is the upwind side; this is the downwind side. So, that is how this ratio is defined.

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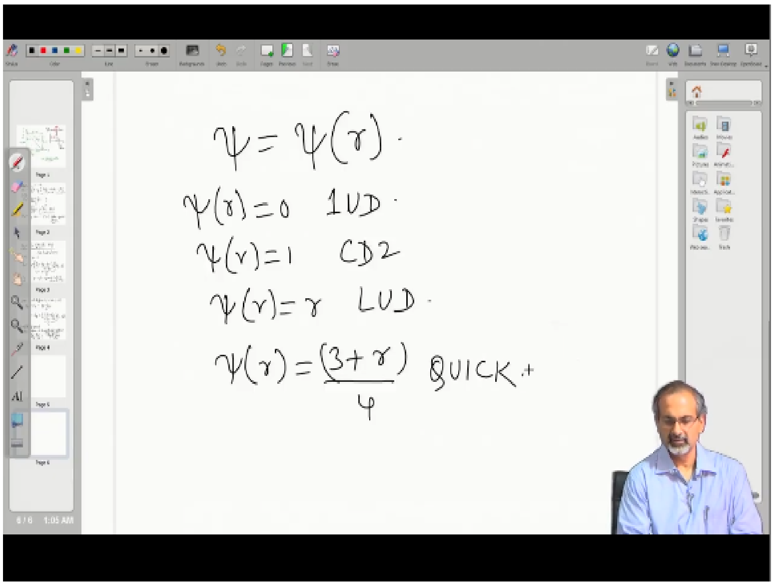

And we will find that Psi would incidentally become a function of r. Now, Psi r is 0 for upwind difference, first order upwind difference. Let us put it as first order UD. Psi r is equal to 1 for CD2. Psi r is equal to r for the LED scheme. Psi r is equal to 3 + r the whole by 4 for QUICK. This, you can check for yourself. Now, can there be a diagrammatic representation of the information here.

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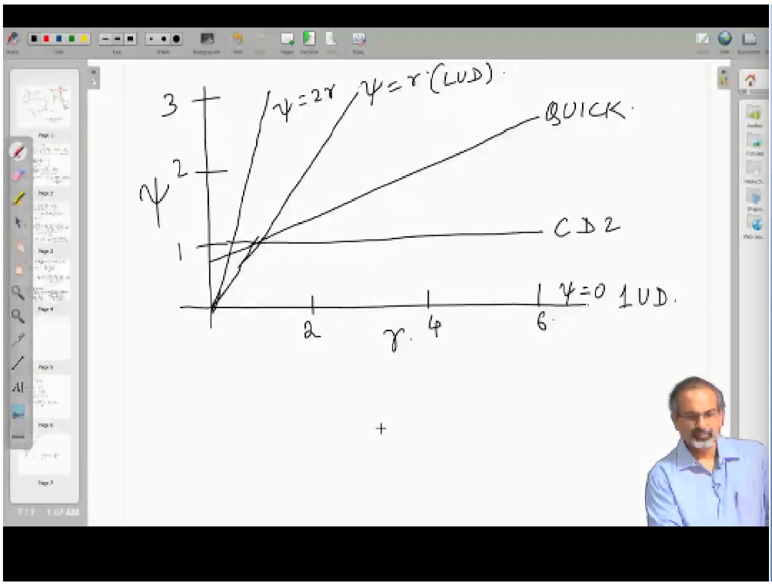

Yes of course, you can make Psi r plot this way and you will find that it is easy to show the variations this way and all the schemes that we discussed would actually be representable in this manner. So, this could be like Psi = r which is the LUD scheme. This would be the QUICK scheme and this would be the CD2 scheme and of course, Psi = 0 is the first order upwind difference scheme which lies along the x axis itself.

So, this is how the different schemes actually figure in the Psi arc length. Right. Now, how can we define a region in the Psi r plane. So, that we can get schemes which are devoid of oscillations. Now, what are the properties that oscillation free schemes have to satisfy?

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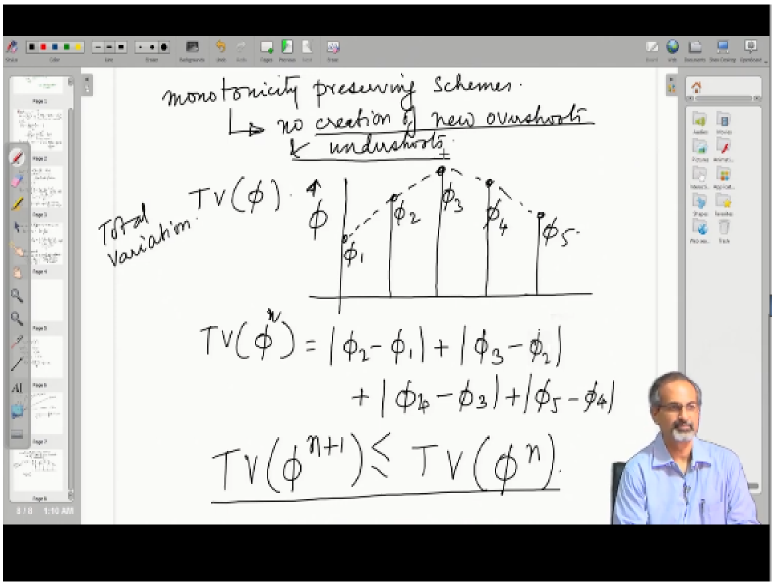

So, if you look at that we come to the property of monotonicity preserving schemes. Of course, higher order schemes which satisfy the monotonicity preserving property. What does that mean? It means that given a solution at a certain time instant a monotonicity preserving scheme will not create any new local extrema and values of the existing minimum would not decrease any further.

The values of the existing maximum would not be increasing any further. Alright. So, this brings the idea that if such a property is actually satisfied by a numerical scheme, there would be no creation of new overshoots and undershoots. This brings in the concept of total variation of a variable file. What does that mean? If I have a variable file whose values are indicated this way at different points, discrete points and these are the values of the variable phi for those points at a certain instant of time.

Let us mark these values as phi 1 to phi 5. Let us see. So, the total variation of the property phi at, let us say the nth time instant would be given by the sum of the modally of the differences of phi as we move from one point to the other covering the entire range of phi that we can see. So, that gives the total variation. The idea is that monotonicity preserving schemes would never allow the total variation to increase with time.

It would be kept bounded, which means that if I go to the next instant the total variation of that next instant will be certainly less than equal to the total variation which was there at the nth time instant. Alright. If this happens, you will never see creation of new overshoots and undershoots. So, this was a very, very important concept in developing schemes devoid of oscillations, but still retaining higher order accuracy.

The main aim was to keep second order accuracy as the target and build schemes which are devoid of oscillations.

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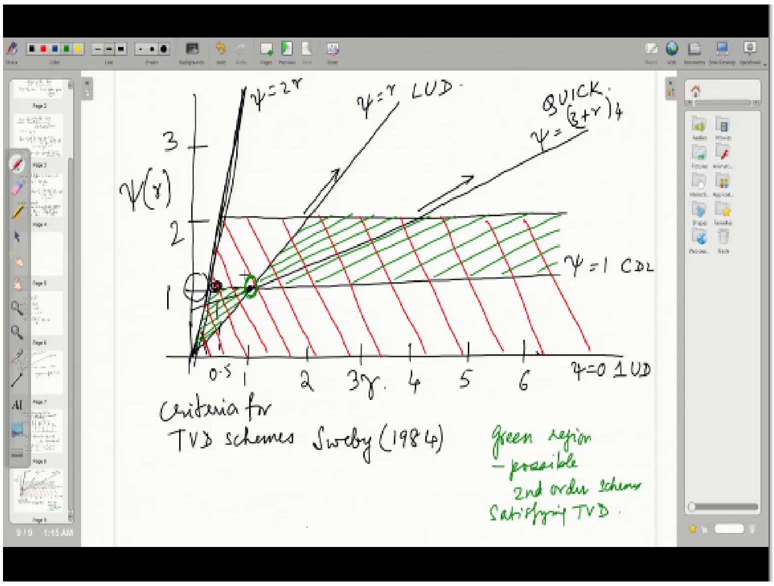

So, we go back to the phi r plot once more or other the Psi r plot once more and we try to look at those regions carefully will shade a certain region now, which is going to be a very important reason for us. So, if you locate a point which is at 1 1 that is a very, very important point for us. Before we do that we draw a line which has the equation Psi is equal to 2 r. So, ideally, it should cross through 0.5 here.

So, that is Psi is equal to 2r. The Psi = r, of course, will pass through 1 1 because it has a 45 degree incline in the x axis which is incidentally r. Psi is equal to r means, this is the LUD scheme. The QUICK scheme again passes through the point 1 1. Remember that this is 3 + r by 4. So, that is QUICK. The CD2 also passes through 1 1. So, this is Psi = 1 and of course, this is Psi = 0 which is first order upwind.

So, these are the schemes we already know of, and now, we are going to shade a certain region. Let us try to use a shade like this, where the first draw a bounding line here and we tried to shade the region. So, the criteria to be fulfilled by TVD schemes was first very widely investigated and reported by Sweby in 1984. A very famous paper and it was indicated that the shaded region that we have on top, the red shaded region satisfies the TVD property.

That means, if you remain bounded within that region, the solution will never develop oscillatory tendencies. Right. So, you can see that LUD or QUICK or CD2 there would be small regions here and there maybe even larger regions here and there, where oscillations are going to come. For example, for LUD, you can understand that this is a region where instability will come for QUICK; this is the region and so on.

For CD2, there is a small region out here which will generate instabilities. Additionally, it was shown that not all the schemes under this red shaded region will actually satisfy second order accuracy. So, we are going to further shade another region here. Within the red region itself, which is going to satisfy second order accuracy which is always more desirable over first order accuracy.

So, the green region is a region for possible second order schemes satisfying TVD. Always remember that these regions are necessarily passing through this point 1 1. We are not really going into derivation of details associated with these concepts, but, it is important for us to be at least aware that which are the regions within which we need to operate in order to ensure that we have second order accuracy on one hand, again we have TVD property.

So, that we have oscillation free solution. The point that we have been trying to drive home.

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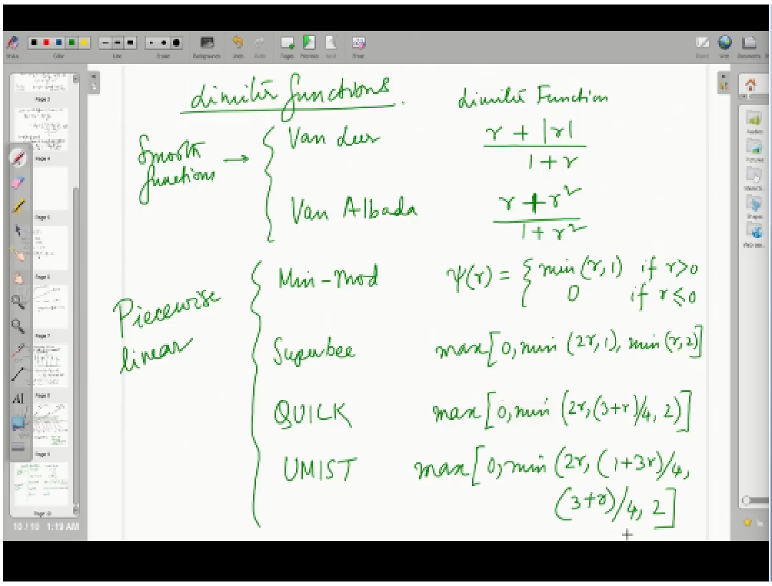

So, we will have a QUICK look at some of the possible limiter functions which are in vogue. So, off which some of the functions are smooth, while some of them are piecewise linear. So, piecewise linear functions we have seen earlier for example, hybrid scheme was a piecewise linear scheme. Again in this TVD world, we have piecewise linear schemes, again we have smooth functions.

For example, in power law, we saw smooth function. Right. So, examples of smooth functions would be the Van Leer scheme for which the Psi is given by r + mode r by 1 + r the

Van Albada scheme which is r + r square by 1 + r square. Of course, you can try plotting these functions in the Psi r plane yourself to find out that they are actually smooth and how they are showing up in that plane.

Again, you can have several piecewise linear limited functions. A very popular one is the Min-Mod. Again remember all the analysis that we did was by assuming that the flow is from the left towards the right that means towards the positive x direction. You can generate similar relations for the opposite direction as well. So, if you want to assign TVD property to QUICK, then you have to associate certain limits within which it operates.

So, one can plot all these functions and try to see that first of all they would remain within the green shaded region. Secondly, they are all going to satisfy the second order accuracy and therefore, they are going to pass through the point 1 1. So, this check can be done at your spare time. So, with this, we come to the end on this module or come to the end of this module.

And in the subsequent module, we are going to look at the incompressible two dimensional Navier Stokes equations where we would not assume the velocity field, but we would try to find ways and means which the velocity field can be solved. And then we look at the distribution of pressure, velocity in the flow field. Or we would also look at distribution of derived properties like stream function water city in the flow field. Thank you.