Computational Fluid Dynamics

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Module No. # 01

Lecture No. # 32

Discretization of Convection-Diffusion Equations:

A Finite Volume Approach (Contd.).

In the previous lecture we were discussing about the exact solution of a one dimensional problem and let us continue with that. To recapitulate, we had convection diffusion - steady state convection diffusion equation d d x of rho u phi is equal to d d x of gamma d phi d x.

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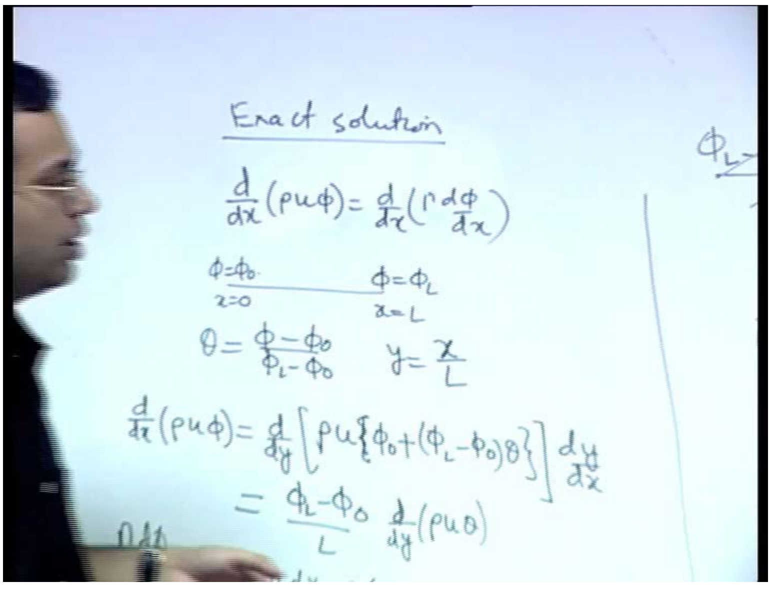

We tried to impose the boundary condition that at x equal to 0 phi equal to phi 0 and at x equal to l phi equal to phi l. Then, we introduced a non dimensional variable theta as phi minus phi 0 by phi l minus phi 0 with an intension that theta lies between 0 and 1 and similarly a non dimensional x which also lies between 0 to 1 that is y equal to x by l.

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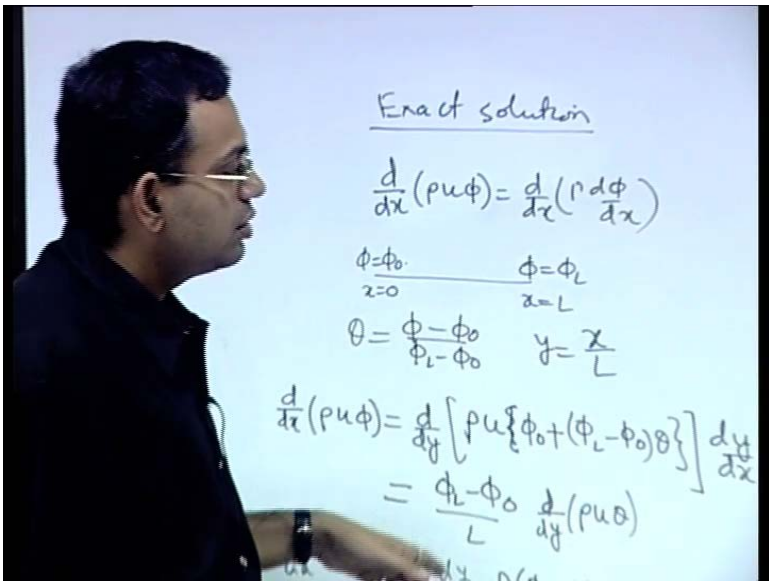

With these transformed coordinate system or rescaled coordinate system so to say, we obtain the following governing differential equation: d d y of p theta is equal to d d y of d theta d y, where p is the pellet number based on the length scale l. That is the f by d where f is equal to rho u and d is gamma by l. We have assumed during these derivations that, gamma is a constant. Now, corresponding boundary conditions are at y equal to 0; theta equal to 0 and at y equal to 1 theta equal to 1. So, let us try to solve this equation.

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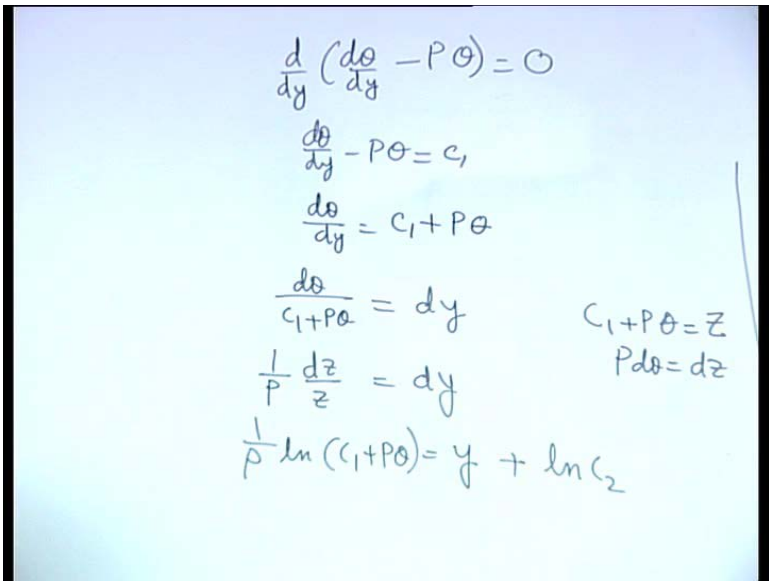

You have d d y of d theta d y minus p theta is equal to 0 from which we get d theta d y minus p theta is equal to c 1. So, d theta d y is equal to c 1 plus p theta. So, d theta by c 1 plus p theta is equal to d y. So, you can make a change of variable c 1 plus p theta equal to say z; so, p d theta equal to d z. So, 1 by p d z by z is equal to d y; that means 1 by p l n of c 1 plus p theta is equal to y plus some constant of integration say l n c 2. You can write this as l n c 1 plus p theta is equal to p y plus p l n c 2 remember p is a fixed parameter which is like a constant for this particular problem. So, p l n c 2 we can call this as sum c 3 l n c 3.

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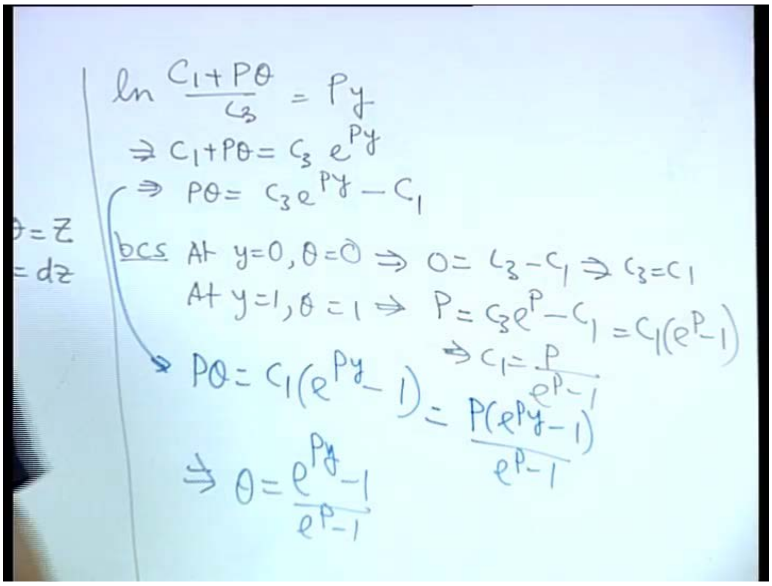

So, l n c 1 plus p theta by c 3 is equal to p y. It implies c 1 plus p theta is equal to c 3 e to the power p y or p theta is equal to c 3 e to the power p y minus c 1 what were the boundary conditions at y equal to 0 theta equal to 0. From this boundary condition you get 0 is equal to c 3 minus c 1 and at y equal to 1 theta equal to 1. From this we get p is equal to c 3 e to the power p minus c 1 c 3 and c 1 are equal from the first boundary condition. So, this is as good as c 1 e to the power p minus 1. So, c 1 is equal to p by e to the power p minus 1. So, this we can use in this solution. So, p theta is equal to c 1 e to the power p y minus 1 in place of c 1 you can write p by e to the power p minus 1.

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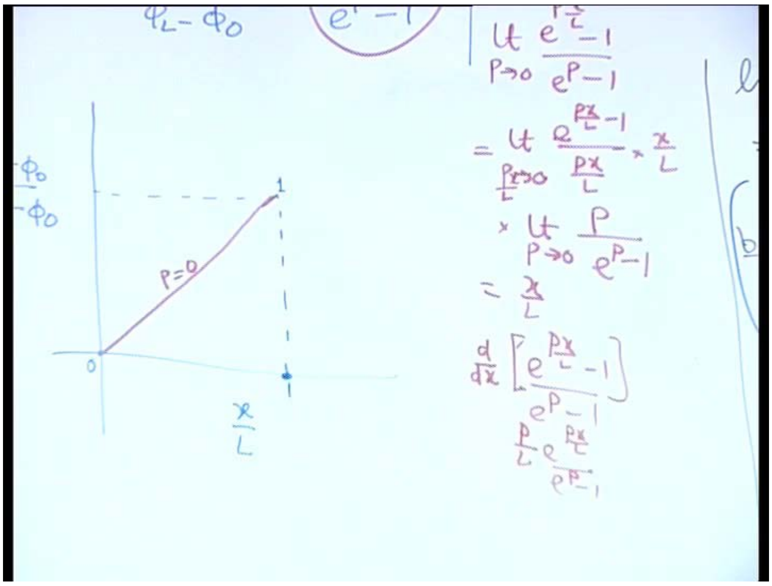

So, p e to the power p y minus 1 by e to the power p minus 1 hence the solution theta is equal to e to the power p y minus 1 by e to the power p minus 1 or in terms of the original variables phi minus phi 0 by phi l minus phi 0 equal to e to the power p x by l minus 1 by e to the power p minus 1.

You can see that the exact solution is having a profile which is exponential in nature. So, how phi varies with x? phi varies with x in an exponential manner; the possible failure of the central differencing scheme or the upwind scheme under certain conditions is because of the criticality in capturing an exponential behavior. If you are considering linear piecewise linear profile assumption, that means, that assumption is a linearised representation of the exponential profile. So, that may be true; that may be correct only when the higher order terms in the Taylor series beyond the linear term are actually negligible.

We have discussed about this issue earlier that for an exponential term. So, if you have say e to the power x all higher order derivatives of these are e to the power x. So, in the Taylor series repeatedly this will come multiplied by delta x sometimes delta x's square by factorial 2 delta x cube by factorial three like that.

If e to the power x itself is not negligible then the higher order terms are negligible only when these are small; that means, when delta x is really very small and delta x is an important component that contribute to the cell packet number that is this 1. So, if delta x is small then only the cell packet number is small and we have seen that smallness should be less than or equal to 2 in terms of its magnitude so that, you can successfully employ the central differencing scheme without any physical inconsistency.

We will look into that in much more details by considering this as a standard profile. So, let us try to make a plot of this profile the first is what happens in the limit as x y or limit as packet number tends to 0. So, the limit as packet number tends to 0 will essentially talk about the small packet number considerations. So, limit as packet number tends to 0 e to the power p x by l minus 1 by e to the power p minus 1 you can multiply both numerator and denominator by p or p x by l to be specific because e to the power x minus 1 by x in the limit as x tends to 0 is 1 that this into limit as p tends to 0 p by e to the power p minus 1 when p tends to 0 p x by l also tends to 0. So, it is a product of these 2 limits the first limit will give x by l and second limit will give 1.

So, when p tends to 0 the theta is equal to y that is phi minus phi 0 by phi l minus phi 0 is equal to x by l. So, it is a straight line passing through the origin this is p equal to 0 what happens if p is greater than 0 what will be the nature of the slope of the graph. So, if you find out what is d d x of e to the power p x by l minus 1 of course, by e to the power p minus 1 is there. So, p by l e to the power p x by l by e to the power p minus 1; when p is greater than 0 then denominator is positive, numerator is also positive p by l the multiplier itself is positive. So, the slope of this variation is positive; that means, you can have a curve of this type this is p greater than 0.

If p is less than 0 on the other hand the denominator what will be the denominator. So, in essence the slope will just be reversed and it may be something like this the rate of change will be reversed. So, to say it is not directly the, exactly the slope in that sense because you can see that from the first value. Then it will increase and here also you can see that from the first value it increases and comes to this, but the nature of variation here the concavity. So, to say it is not just the slope you have to also consider another order derivative, but I have just calculated one order derivative, but you have to calculate one more order derivative because it is necessarily not just the slope, but the concavity of the function that changes.

These are not very important limits; we will not therefore spend more time in calculating the second order derivative and looking for the concavity and convexity. What we will do is, we will consider the special limits when p is very large. See, we have seen that for small p the central difference scheme works nicely for the large p we have seen that upwind scheme may be a physically pertinent scheme. To see the corresponding consequences here we will consider a large packet number limit to begin with. So, just for p greater than 0 and p less than 0 remember that mere slope considerations are not good enough. One has to look into the concavity and convexity of the functions to come up with these variations which we have not gone through in details because these are not of our interest.

Our interest is packet number tends to infinity; a large packet number when packet number tends to infinity. We can divide this into two parts: one is when x by l is small another is when x by l is large. When x by l is small that is tending to 0 then, what happens? Numerator is e to the power tending to infinity into tending to 0; p tends to infinity x by l tends to 0, but p into x by l is finite. So, e to the power some finite minus 1; that is a finite number where as in the denominator it is e to the power infinity minus 1 that is the denominator tends to infinity, but the numerator tends to a finite limit. So, this ratio tends to 0.

Therefore, for small values of x by l this will tend to 0 what happens for large values of x by l when it becomes when x by l is, you cannot say x by l is indefinitely large maximum value is 1. So, when x by l tends to 1 that is x by l large when you say; that means, it is maximum limit it tends to 1 then this ratio tends to 1. So, when it goes close to 1 there is a jump from this towards 1. So, this is packet number much greater than 1- very large.

Similarly, a large negative number if the packet number is a large negative number then, what happens for small x by l? That its numerator is first consider the denominator when packet number tends to minus infinity. This tends to minus 1 and numerator. What is the limit of that numerator? Consider the upper limit; if you are more comfortable with that when x by l is large tends to 1.

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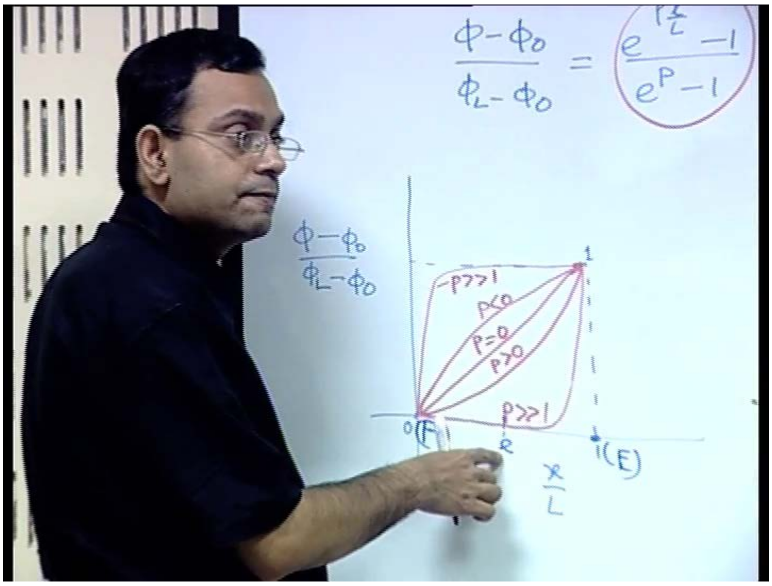

Then in that limit it will tend to 1. So, it will tend to 1 in that limit. So, it is effectively like a sort of image with respect to p equal to 0 this is minus p much greater than 1 the behavior here is similar to the behavior here. So, what is important for us to appreciate is that what happens for mod of packet number much greater than 1 which is true for this one as well as this one. This is tending to minus infinity and this is tending to plus infinity, but both are large in magnitude. So, when both are large in magnitude you see what happens.

Let us say that this is the grid point p this is the grid point e. So, this is the grid point this is the control volume phase small e. So, you can see that phi small e equal to phi p if packet number is much greater than 1 very large. So, this is like the upwind scheme and packet the line packet number equal to 0 confirms to the case when the central difference scheme is exactly working that is it is solely governed by the diffusion there is negligible advection.

So, one limit is negligible advection another limit is very strong advection and when there is very strong advection you see that the sum total of the flux the advection flux and diffusion flux gives phi small e equal to phi capital p this is considering both advection and diffusion.

In the upwind scheme that is substituted only in the advection term in the diffusion term you have an additional central differencing and that is why upwind scheme over predicts diffusion because the diffusion term it could have been set to 0 only the advection term was good enough to represent this physical scenario in the upwind scheme, but one also puts the diffusion term in the upwind scheme and that is how it can over predict diffusion.

So, in a case when it is a large packet number, the upwind scheme is supposed to represent a very strong advection, but it is also representing some diffusion by central differencing that diffusion is negligible actually in the physical sense for very large packet number ok. Now, remember that although we are talking about an exact solution here this exact solution can hardly be prevailing in reality because in many cases it is not such a simple case as one dimensional steady state convection diffusion problem with constant properties also it is not always that you have fixed a specified value of phi as the boundary conditions at that two ends therefore, the problem that we have considered is a very simplified version of something which can deviate significantly from the reality.

Despite that, it gives us a good insight it shows that if you have a variation if you have some arbitrary value of phi at two grid points i and j as phi i and phi j and if it is a one dimensional variation then how phi will vary in between the values of phi i and phi j say sum value phi i for i and sum value phi j for j. So, in between how it will vary that it can predict.

Now, taking this as a profile, one can device a scheme for numerical solution of may be more complicated problems if possible and that particular scheme where it considers this exponential profile is called as exponential scheme. So, let us look into the exponential scheme.

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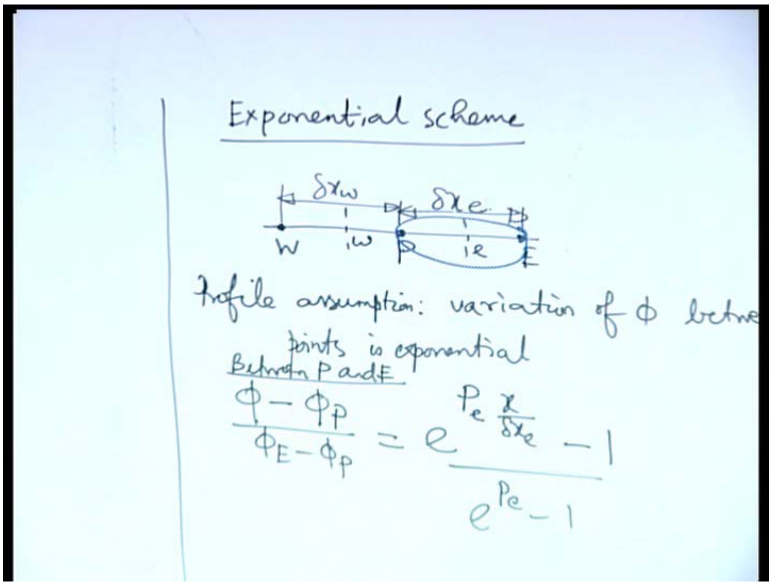

In the exponential scheme what we are thinking of is that, if you have the grid points p e w small e small w like this then, the variation of phi between grid points is exponential that is the profile assumption. So, the profile assumption is there are two different variations that we consider for each control volume one for phi between capital w to capital p another between capital p to capital e.

For phi between capital p to capital e let us say we consider this portion. So, capital p is like x equal to 0 capital e is like x equal to l. So, l is delta x e. So, here what is the profile phi between capital p and capital e? What is the profile phi minus phi p by phi e minus phi p? So, this is just like phi minus phi 0 by phi l minus phi 0 is equal to e to the power packet number now based on delta x e; so, e to the power p e into x by delta x e minus 1 by e to the power p e minus 1.

Till now we have seen profiles like piecewise constant piecewise linear instead of that just consider this as another profile assumption now with this different profile assumption we have we now have to derive the finite volume discretization corresponding to this chosen control volume.

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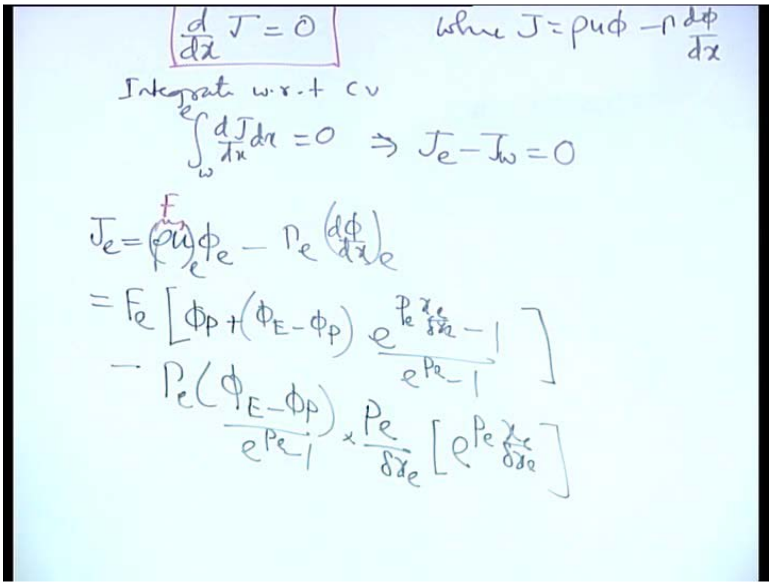

What is our governing equation? d d x of rho u phi is equal to d d x of gamma d phi d x. So, this in short form you can write d j d x equal to 0 where j is the total flux rho u phi minus gamma d phi d x. So, let us consider d j d x equal to 0 as our governing differential equation what will be the first step when we consider the finite volume discretization integrate with respect to the control volume. So, integral of d j d x d x from small w to small e equal to 0 that gives j e minus j w equal to 0.

So, let us calculate j e and j w what is j e rho into u is f. So, it is f e phi e. So, f e in place of phi e we can write you substitute x equal to x e to get phi equal to phi e. So, phi p plus phi e minus phi p into e to the power p e x e by delta x e minus 1 by e to the power p e minus 1 minus gamma e d phi d x is first you take the common part phi e minus phi p by e to the power p e minus 1 into p e by delta x e e to the power p x by delta x e at x equal to x e. So, we differentiate this and substitute x equal to x e.

Then we can observe that we have gamma e by delta x e in this term. So, gamma e by delta x e is d e and p into d e is equal to f e. We have 1 p that multiplied by d makes it f e. So, you have f e phi p plus phi e minus phi p into e to the power p e x e by delta x e minus 1 by e to the power p e minus 1 minus phi e minus phi p by e to the power p e minus 1 that multiplied by f e into e to the power p e x e by delta x e. So, you have a term phi e minus phi p into e to the power p x e by delta x e by e to the power p minus 1 that multiplied by f e and that term gets cancelled with this term the last term there that is also same as this with a minus sign.

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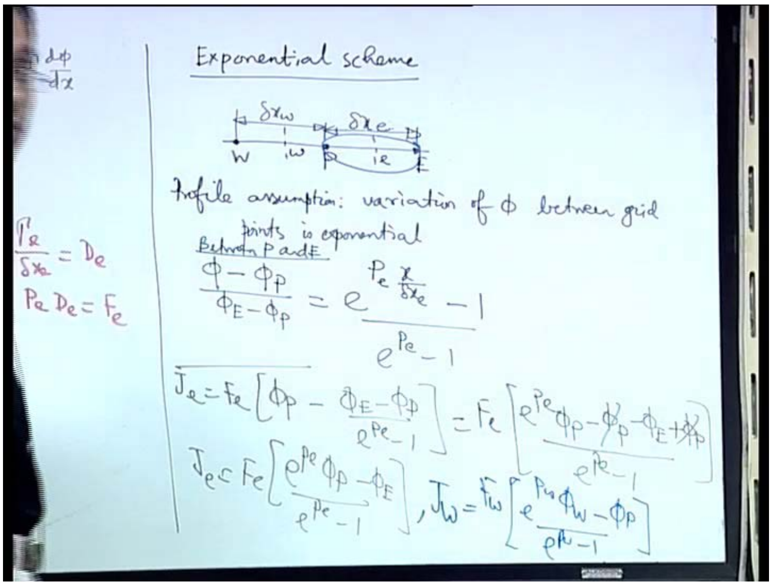

Keeping that in view, you can write j e is equal to f e into phi p minus phi e minus phi p by e to the power p e minus 1. So, it becomes f e e to the power p e phi p minus phi p minus phi e then plus phi p by e to the power p e minus 1. So, 1 phi p gets cancelled. So, you have j e is equal to f e e to the power p e phi p minus phi e by e to the power p e minus 1. If this is j e, what is j w? In place of f e, we will have f w e to the power p w; in place of p it will be w e to the power w into phi w minus phi p by e to the power p w minus 1 and the discretization equation is j e equal to j w.

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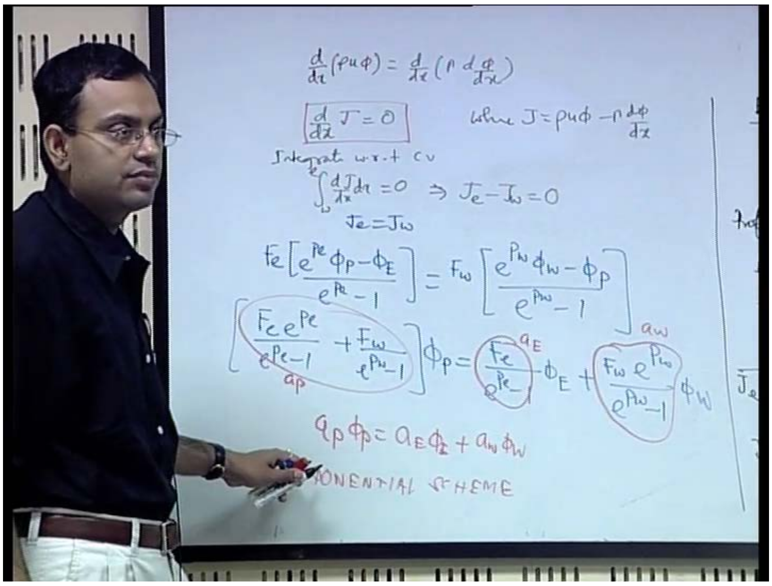

So, f e e to the power p e phi p minus phi e by e to the power p e minus 1 is equal to f w e to the power p w phi w minus phi p by e to the power p w minus 1. If we collect all the terms f e e to the power p e by e to the power p e minus 1 plus f w by e to the power p w minus 1 this times phi p is equal to f e by e to the power p e minus 1 phi e plus f w e to the power p w by e to the power p w minus 1 phi w this is of the form a p phi p is equal to a e phi e plus a w phi w, where this is equal to a p this is equal to a e this is equal to a w.

This particular scheme where the coefficients are exponential functions of the cell based packet numbers this is called as exponential scheme. So, exponential scheme is a discretization scheme which is derived on the basis of the analytical solution of a simplified case 1 dimensional steady state problem. The name exponential scheme stems from the fact that you have exponential variation of the coefficients as a function of packet number cell packet number.

Now, the exponential scheme is actually in conceptual terms is very ideal because it is based on a variation where it confirms to the analytical solution for a special case, but even if that special case does not hold physically it should have the same qualitative characteristics and in that way this is actually very ideal, but still people seldom use the exponential scheme for numerical implementation question is why.

The reason is that exponential computation is computationally very expensive. So, in the exponential scheme you have to calculate coefficients which are exponential functions and calculating exponential functions is effectively like calculating a large number of terms in the exponential series each of the terms has a numerator and a denominator where you have multiplications in that denominator and exponential calculations involving such series summations is therefore, quite expensive in nature.

To get rid of the problem, our next objective will be to see that can we have a scheme where we represent the essence of the exponential scheme without using exponential functions or in a better way using just piecewise linear functions can we represent the behavior of the exponential scheme let us try to do that.

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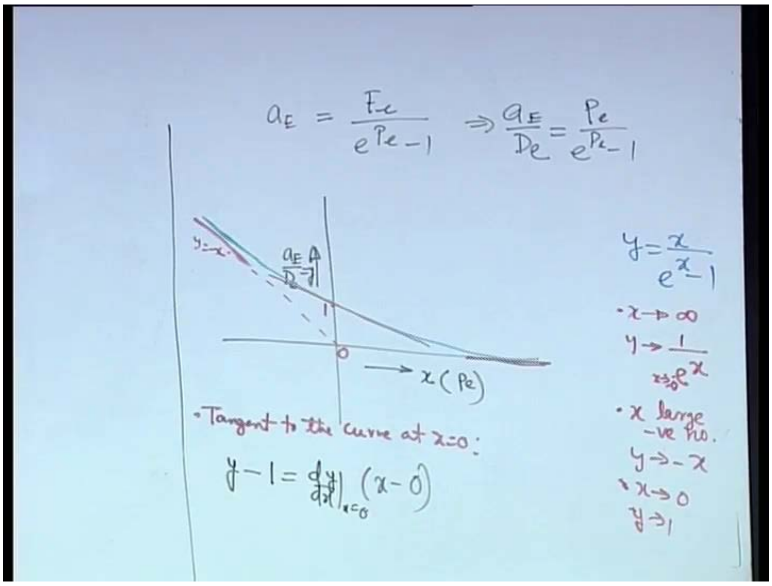

In the exponential scheme we have this coefficient a e is equal to f e by e to the power p e minus 1 if we represent it with a non dimensional way then how can we represent this in a non dimensional way we can divide it by d e because f e by d e will become p e which is a non dimensional number. So, a e by d e just a non dimensional representation of a e is p e by e to the power p e minus 1. Let us try to make a sketch of a e by d e which we give a name y as a function of x which we call as packet number.

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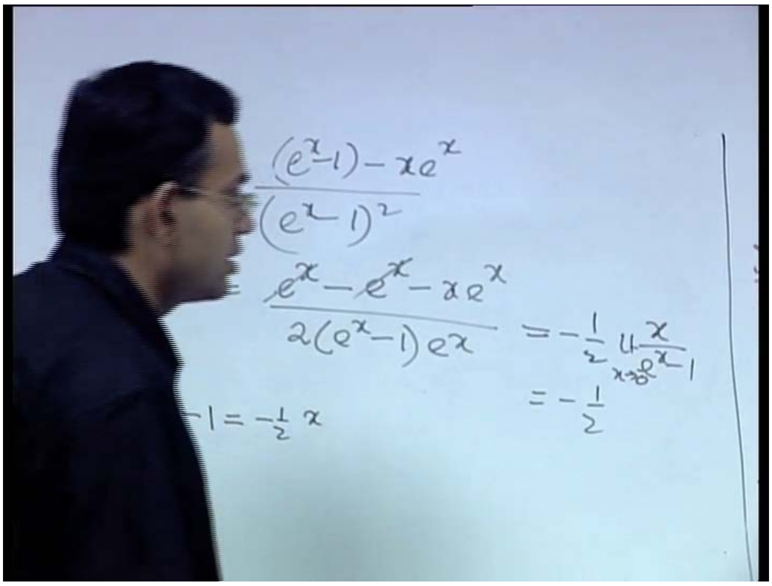

Our variation is y equal to x by e to the power x minus 1 let us consider some special limits let us consider first the limit as x tends to infinity when you have x tends to infinity see it is \infinity by infinity form. So, you can use the l'hopital's rule for calculating the limit. So, y will tend to 1 by e to the power x as x tends to infinity. So, it will tend to 0.

So, when it tends to infinity tends to infinity for a numerical purpose means just something very large. So, when x tends to something very large y tends to 0 when x is a large negative number then what happens the denominator e to the power x is e to the power minus infinity that tends to 0 see tends to minus 1 therefore, in that case y tends to minus x it depends on how large or how small the magnitude of x is. So, we can say y tends to minus x. So, if you tend to draw y equal to minus x. So, this is that limit and what is the value of the function when x tends to 0? So, in the limit as x tends to 0 y tends to 1 that is the limit x tends to 0 x by e to the power x minus 1. So, if you want to make a sketch of the function the function is expected to behave in this way the green colored line and these red colored two lines are the two asymptotes that is tangents to the function at infinity.

Now, if we want to represent this green line by piecewise straight lines see 1 piecewise straight line 1 piece of the straight line is this 1 when it tends to infinity another piece of the straight line may be y equal to minus x when it tends to minus infinity, but in between we have to consider another straight line and that straight line can be considered as the linearization of this function at x equal to 0.

How do we align? Raise a function we tend to represent the tangent to the curve at that particular point at which we want to linearism. So, if we want to linearism it at x equal to 0 we are basically interested to draw the tangent to this green line at x equal to 0. So, tangent to the curve at x equal to 0 what is this y minus y 1 that is 1 is equal to d y d x at x equal to 0 into x minus x 1 that is 0. Next let us calculate, what is d y d x at x equal to 0.

So, d y d x is e to the power x minus 1 whole square into e to the power x minus 1 into derivative of x that is x minus x e to the power x as x tends to 0 it assumes a 0 by 0 form. So, 1 can use the l'hopital's rule. So, you have to differentiate the numerator that is e to the power x plus x e to the power x minus, sorry, this x is not there; first x.

First x is not there right. So, e to the power x minus e to the power x minus x e to the power x divided by 2 into e to the power x minus 1 into e to the power x. So, these 2 get cancelled out e to the power x also gets cancelled out. So, minus half x by e to the power x minus 1 in the limit as x tends to 0. So, that is equal to minus half. So, y minus 1 is equal to minus half x that is the representation of the tangent to the curve at x equal to 0.

So, if we now represent this curve by three straight lines one is this tangent then the others will be the lines which are y equal to 0 and y equal to minus x. So, what will be the domains when these lines are functional; that means, you have this total curve represented by three lines over certain domains some of the line out of the three lines any one line represents the function. So, let us see that what is the domain over which it does. We have to find out what are the points of intersection of these lines. So, this point is y equal to intersection of y equal to minus x with y equal to 1 minus half x. So, minus x equal to 1 minus half x; that means, x equal to minus 2. So, this point corresponds to x equal to minus 2. Similarly, what about this point. So, it is a intersection of y equal to 0 with y equal to 1 minus half x. So, this is y equal to 1 minus half x; so, this is 2.

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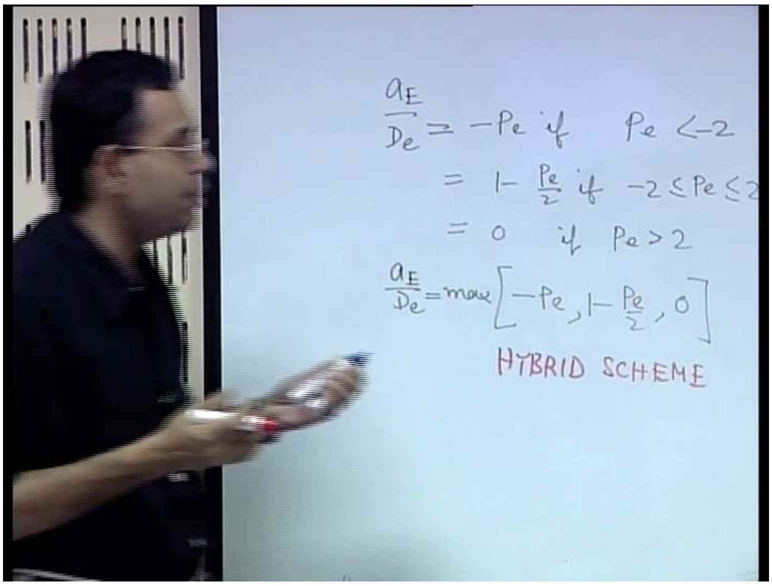

You can represent this total function as follows a e by d is equal to minus p if p is less than minus 2 is equal to 1 minus p e by 2 if p is between minus 2 to 2 and is equal to 0 if p is greater than 2. So, it is like a combination of central difference scheme and up winding scheme see 1 minus p by 2 this is like the central difference scheme a e by d e is 1 minus p e by 2 we have seen that that is nothing but the discretization of the central difference scheme. So, you can combine these together and write a e by d is equal to max of minus p e 1 minus p e by 2 and 0.

How it is possible? If you look into this variation, now you can see that you can divide it into three parts considered the left most part that is pellet number between minus infinity and minus 3. Then you can see that out of these three piecewise straight lines the left straight line has gives the maximum value because if you extrapolate this straight line or this straight line out of these three, this one gives the maximum value. If you consider the middle range you can see that this straight line gives the maximum value. If you consider the right range you can see that this straight line gives the maximum value.

So, if you use the max function now, the max function has three arguments. Out of these three arguments, you can use the maximum of the three. So, in a very short form you can write it as the max of these three. This particular representation is known as hybrid scheme; it is nothing but a piecewise linearization of the exponential scheme the whole idea is you avoid exponential calculation, but try to represent the physical nature of the exponential function by some piecewise straight lines. See you have basically used the asymptotes and the tangents to the function to represent a similar function as that of the exponential function without involving any exponential calculation; that is the benefit behind it. But, the only problem is that it sets of the diffusion to 0 at packet number equal to 2. Beyond that, you have a e by d equal to 0; that means, the diffusion is set to 0. Whereas, it in reality it does not do so; at such a small value of x it does. So, at a value of x which is somewhat larger than this one, a better solution may be you have different curve fitting of this function not just a piecewise linear representation. That we will see in the next class; thank you.