

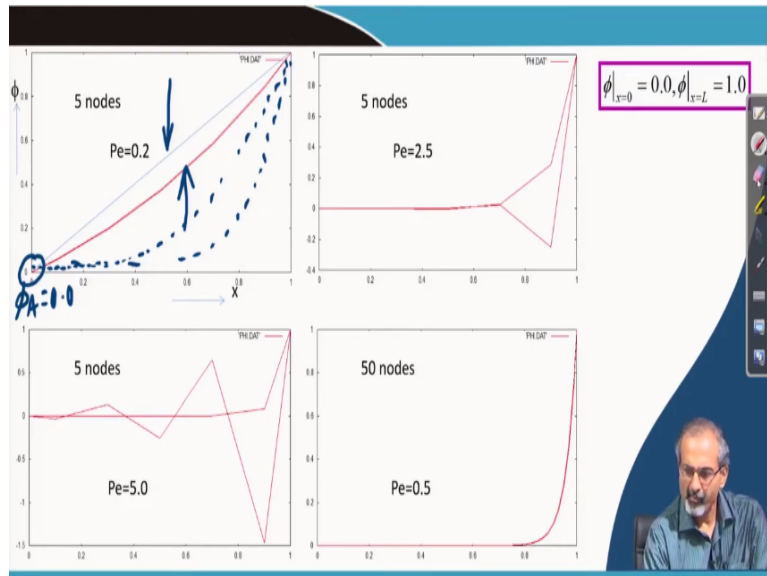
Introduction to CFD
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Lecture - 36

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

Let us continue with discussion of the one dimensional convection diffusion equation.

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So, last time we saw a result for the central differencing scheme with two values at the boundaries. So, the left boundary had a value of 1, the right boundary had a value of 0. And then the flow was moving from the left to the right, and then we try to see for different Peclet numbers, how the phi distribution look like in the domain. That means, how was phi transported in the domain. So, we relook at another result.

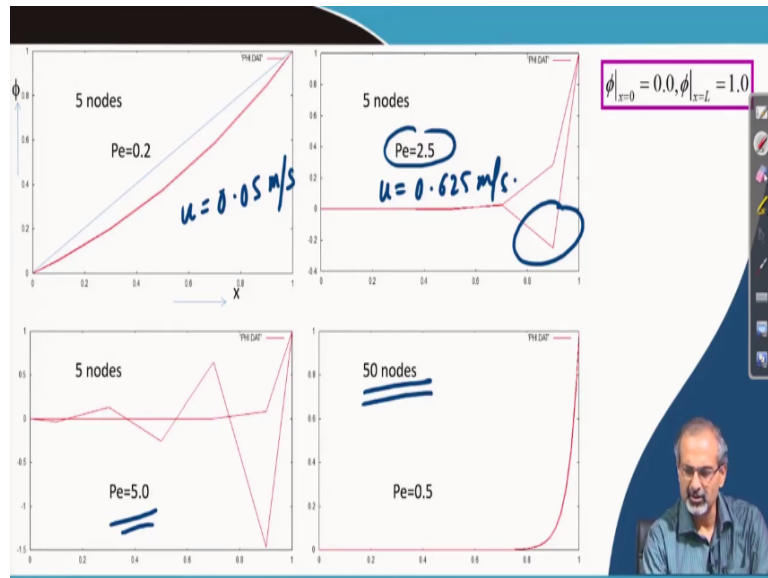
And here if you notice carefully that the boundary values have been just swapped. So, on the left end now you have a value of 0 on the right end you have a value of 1, and therefore as you can understand there is that as advection becomes stronger. There will be a stronger sweep of the left end value towards the right. Right. So, if that is the situation for low Peclet number as you can see here that the blue curve is the is the only diffusion case that means no advection. Right.

So, then there would be a linear distribution of phi from the left to the right end. Right. However, the moment there is an advection effect. You have a sweep down of the curve.

Why is it? Because the left end value the phi A is equal to 0. So, what it would try to do is keep the value of phi closer to 0 as the advection becomes stronger. So, as u becomes larger, you will see the trend would be that the curves will start looking like this.

That means there is a stronger and stronger sweep of the phi A value towards the right as advection becomes stronger. Alright.

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So, here you have a case of $u = 0.05$ meters per second. Here, it is like $.625$ meters per second, like we had done for the previous example. And moment you exceed the Peclet number of 2.5 , you see an oscillation again. And then with the same number of nodes if you push it to 5 again there are similar oscillations. And the problem is resolved by putting in more number of nodes.

The only difference between this case, and the previous case is, how you have swept the boundary values, and what effect it has on the curve, the nature of the phi distribution. In one case, it was moving up upwards from the perfect diffusion case. In another case that means in this case, it is moving downwards from the perfect diffusion case. So, this is the difference we need to note.

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Scarborough (1958)* has shown that a sufficient condition for a convergent iterative method can be expressed in terms of the values of the coefficients of the discretized equations:

a_p is the net coefficient of the central node P, which includes the effect of S_p for boundary nodes & summation in the numerator of the expression is taken over all the neighbouring nodes indicated by suffix (nb).

$$\left\{ \begin{array}{l} \sum |a_{nb}| \leq 1 \\ |a_p| < 1 \end{array} \right.$$

at all nodes
at one node at least

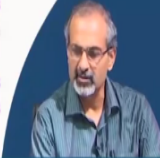
□ If the differencing scheme produces coefficients that satisfy the above criterion the resulting matrix of coefficients is diagonally dominant. To achieve diagonal dominance we need large values of net coefficient a_p , which is possible when S_p is always negative. If this is the case $-S_p$ is always positive and adds to a_p to produce a large positive net coefficient.

□ Diagonal dominance of coefficient matrix helps satisfy the 'boundedness' criterion. This implies that in the absence of sources the internal nodal values of property ϕ should be bounded by its boundary values.

□ An essential requirement for boundedness is that all coefficients of the discretised equations should have the same sign which is usually all positive. The physical implication of this is that an increase in the variable ϕ at one node should result in an increase in ϕ at neighbouring nodes.

□ If the discretisation scheme violates boundedness requirements, most often the solution does not converge at all, or, if it does, then it contains 'wiggles' (undershoots and overshoots) which is a signature of numerical instability.

*Scarborough, J. B. (1958), Numerical Mathematical Analysis, 4th edn, Johns Hopkins University Press, Baltimore, MD.



Last time we had talked about the Scarborough criterion, which is the sufficient condition for a convergent iterative method for solving a system of equations. So, we again revisit this in the form of few important bullet points here. So, we have done the calculations earlier we already have the knowledge of this condition which was checked. And we notice that if the criteria is satisfied what it does is that the resulting matrix of coefficients is diagonally dominant.

That is the condition that it ends up producing. And that is ensured when you have large values of net coefficient a_p , and that is possible only when you have S_p , having very large negative values. And of course, when it is diagonally dominant, it remains bounded. The boundedness criterion is satisfied. And if you do not have sources in the internal regions of the flow, then it also means that the internal modal values of ϕ should remain bounded by boundary values.

That means they cannot ever exceed the boundary values cannot become larger or smaller than the boundary values, and all the coefficients of the discretized equations should have the same sign, preferably positive. And if these conditions are ensured then you will always have oscillation free solution. That means a bounded solution. However, if you are not able to satisfy this condition, then what happens is you end up producing wiggles, which is typically the signature of numerical instability.

And wiggles are essentially undershoots and overshoots beyond the expected value of the analytical solution. So, these are the important points which we would like to recapitulate

again. And these are very important because the boundedness nature of the solution depends on satisfaction of this criteria.

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Conservativeness: The central differencing scheme uses consistent expressions to evaluate advective and diffusive fluxes at the control volume faces.

Boundedness: Satisfied for $Pec < 2^*$.

Transportiveness: Value at node P is influenced by all neighbours to calculate the advective and diffusive flux. Hence the scheme does not recognise the direction of the flow or the relative strength of advection relative to diffusion. It does not possess the transportiveness property at high Pec .

Accuracy: It has second-order formal accuracy.

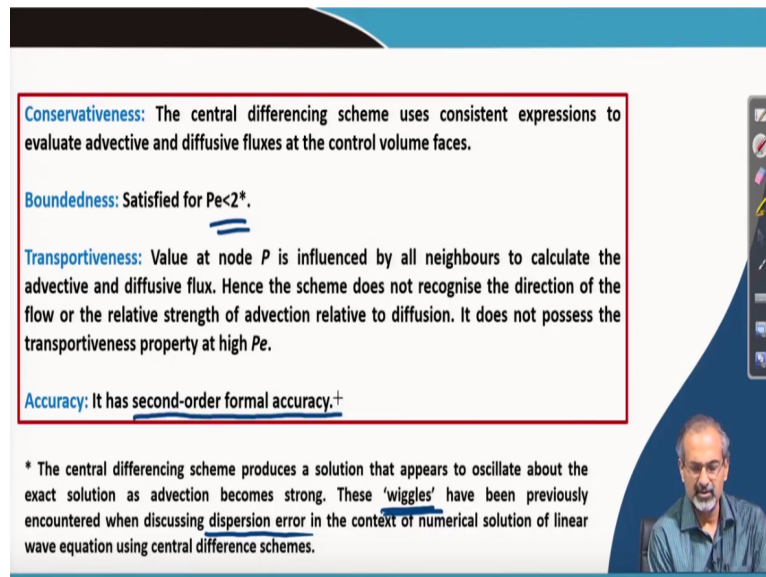
* The central differencing scheme produces a solution that appears to oscillate about the exact solution as advection becomes strong. These 'wiggles' have been previously encountered when discussing dispersion error in the context of numerical solution of linear wave equation using central difference schemes.

Just having a quick overview of the different properties of the central differencing scheme. So, the conservativeness is ensured because you have consistent expressions. You know, solving for the values at the interfaces. Why is it consistent? Because, let us say, we will make a quick sketch here that is if we have a node P here and node E here, and an interface E , where you are trying to reconstruct because you are doing a linear interpolation.

It will always depend on P and E , whether it is the east face of P or the west face of E . So, that is what is meant by consistent expression for the value of ϕ at the point E . Similarly, if you are calculating the, the derivatives, they are also found in a consistent manner because they just depend on ϕ_E and ϕ_P , and they are divided by the distance separating them, and that is essentially the derivative.

Whether you are looking at that point E as the east face of P or the west face of E . So, consistent expressions are used in the scheme. The scheme satisfies the boundedness criterion for Peclet number < 2 .

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Transportiveness: Value at node P is influenced by all neighbours to calculate the advective and diffusive flux. Hence the scheme does not recognise the direction of the flow or the relative strength of advection relative to diffusion. It does not possess the transportiveness property at high Pe .

Accuracy: It has second-order formal accuracy.[†]

* The central differencing scheme produces a solution that appears to oscillate about the exact solution as advection becomes strong. These 'wiggles' have been previously encountered when discussing dispersion error in the context of numerical solution of linear wave equation using central difference schemes.

And if you violate them, then you would see wiggles, and even may remember that we saw similar wiggles when we were talking about dispersion error in the context of numerical errors when we studied the linear advection equation, or wave equation. There we had seen wiggles with central differencing as far as transportiveness is concerned. When we are calculating the values at the cell interfaces, we are putting equal weightage on the neighboring nodes.

That means we are not paying attention to the direction of transportation, and that is essentially the reason why the solution becomes bound unbounded beyond a certain range of Peclet number if you do not pay attention to the flow direction. So, there is an issue with transportiveness of this scheme, and it has second order formula accuracy, which we have discussed adequately even before.

So, these are the characteristics of the central differencing scheme.

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(B) First order upwind (FOU) scheme (or 'donor cell' scheme) for advective fluxes and CDS for diffusive fluxes

$u_w > 0 (F_w > 0), u_e > 0 (F_e > 0)$
 $\phi_w = \phi_P, \phi_e = \phi_P$

$u_w < 0 (F_w < 0), u_e < 0 (F_e < 0)$
 $\phi_w = \phi_P, \phi_e = \phi_E$

Let us move on to the next numerical scheme of interest for us, which is the first order upwind scheme or the donor cell scheme for advective fluxes, and we continue to use the central difference for diffusive fluxes. And it is rather simple to define how first order upwind works. That means when the velocity is from left to right. Then if you have points, the node points like this, and cell interfaces, like this define.

So, at the cell interface e when the flow is moving from left to right, you would assign $\phi_e = \phi_P$ that means, this information percolates, to the point e and ϕ_W is assigned to the cell face w. So, that is how it works. Why if the flow changes direction and moves from right to left, then it just reverses. That means now the value of ϕ from the capital E node will be assigned to the face e, and the value of ϕ from capital E point will be assigned to the cell face small w.

So, that is how the first order upwind discretization will work. So, if you try to work out the coefficients of the first order upwind scheme. You can certainly do it the way we did it for the central differencing scheme, but we will just keep a few steps and go over to the final expression straightaway.

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Internal nodes $F > 0$ +ve velocity (left to right)

$$\phi_p \left[\underbrace{D_e + F_e}_{a_w} + \underbrace{D_w}_{a_e} + (F_e - F_w) \right]$$

$$= \phi_w [D_w + F_w] + \phi_e [D_e].$$

node 1

$$S_u = \phi_A [2D + F].$$

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

So, for internal nodes, how do we do it? We do it this way, ϕ_p . This is your a_w . This is your a_e . Remember, we are treating the case of $F > 0$ that means, positive velocity or moving from left to right that kind of situation. So, in that set in that sense, a_e is D_w and then we will be left with $F_e - F_w$. This is equal to ϕ_w . This is how it will work for internal nodes.

For node 1 that means the left boundary node, you can show that S_u will work out to be ϕ_A times $2D + F$, and S_p is equal to minus of $F + 2D$.

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node 5 $S_u = 2D\phi_B$ $F_e = F_w$

$$S_p = -2D$$

node	a_p	a_e	S_p	S_u	$a_p = a_w + a_e - S_p$
1	0	D	$-(2D+F)$	$(2D+F)\phi_A$	$3D+F$
2,3,4	$D+F$	D	0	0	$2D+F$
5	$D+F$	0	$-2D$	$2D\phi_B$	$3D+F$

+ve -ve

And for node 5, you can show that S_u is equal to $2D$ times ϕ_B . While S_p is equal to $-2D$. Here again, we need to mention that you know, these expressions are all identical this comes from continuity and D_e and D_w 's are not distinguished anymore. They are just treated as

these. So, then you will get expressions of this kind for the first order upwind. Now we will go over to the expression for the coefficients.

Make the table and see what happens. So, the format of the table is known to us already. We have done it in detail for the central differencing scheme already. And now, let us do it for the first order upwind. So, we continue to refer to 5 nodes. And the expressions come up like this. Sorry. So, what I wrote over here is essentially S P. So, we treat this as S u. So, there is a small mistake instead of rewriting it all over. Please take note that this is S u.

This is S P. So, slightly swapped. a P is $3D + F$ $2D + F$, and $3D + F$ here. So, we are done with the coefficients. We need to notice certain important things. As you can see all these terms are positive, which is very favorable. Again, the S P's are all negative which is also very favorable. So, it seems. The first order upwind scheme will have no issues with boundedness.

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Case 2 $Pe = 2.5$

Nodes	a_w	a_E	S_p	S_u	a_p
1	0	0.5	-2.25	2.25	2.75
2,3,4	1.75	0.5	0	0	2.25
5	1.75	0	-1	0	2.75

$\frac{S.C.}{\text{node 1}} \rightarrow \frac{0.5}{2.75} < 1$ $\frac{\text{node 5}}{1.75} < 1$
 $\text{nodes 2,3,4} \rightarrow \frac{1.75 + 0.5}{2.25} = 1$

So, we will go straight away to check for the Case 2, which we did for the central differencing because as you can understand that Case 2 was a little more difficult case to handle for central differencing. Case 1 was easier. So, let us check how first order upwind does for the Case 2 directly. If it does well, we can be rest assured that it will do well for Case 1 also. So, Case 2 is the Peclet number 2.5 situation.

And for that if you do the calculations, what do you get? Let us find out the values. So, here we find these values for a W, these values for a E, these values for S P and S u finally a P.

And you can notice that if you have large values of a P, a big contribution is coming from the $-S P$. And if that happens, satisfying Scarborough's criterion becomes that much more easier.

So, there you can keep the, you know, summation of mod neighbored coefficient times by a P below 1. Right. So, let us check the Scarborough criterion. So, for node 1, what is it worked out to be? .5 by 2.75, which is <1 . Then for nodes 2, 3, 4, what do we have? We have $1.75 + .5$ by 2.25, which is precisely 1. And then again for node 5, you have 1.75 by 2.75 which is <1 . So, even for the Case 2 it has satisfied the Scarborough's criterion.

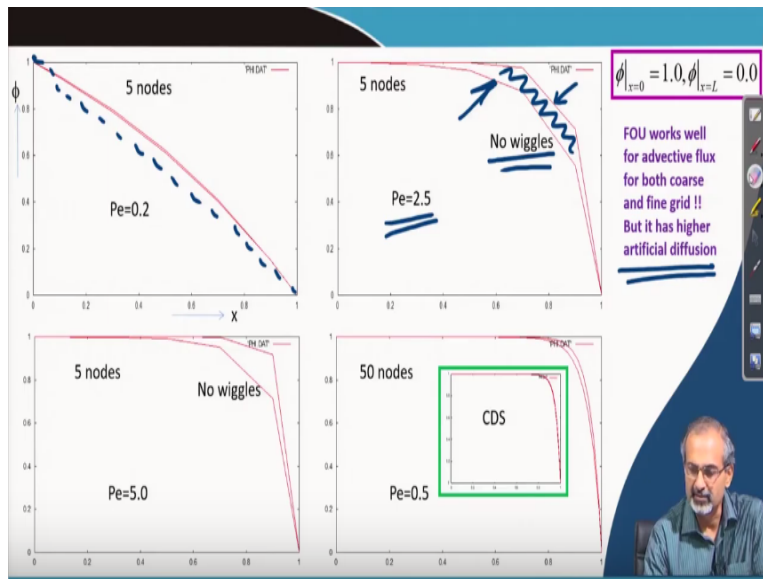
So, you can expect that there will be no oscillations in the solution. Before accepting it straight away. Let us try to look at some numerical results.

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(B) First order upwind (FOU) scheme (or 'donor cell' scheme) for advective fluxes and CDS for diffusive fluxes

$$u_w > 0 (F_w > 0), u_e > 0 (F_e > 0)$$
$$\phi_w = \phi_P, \phi_e = \phi_P$$
$$u_w < 0 (F_w < 0), u_e < 0 (F_e < 0)$$
$$\phi_w = \phi_P, \phi_e = \phi_E$$

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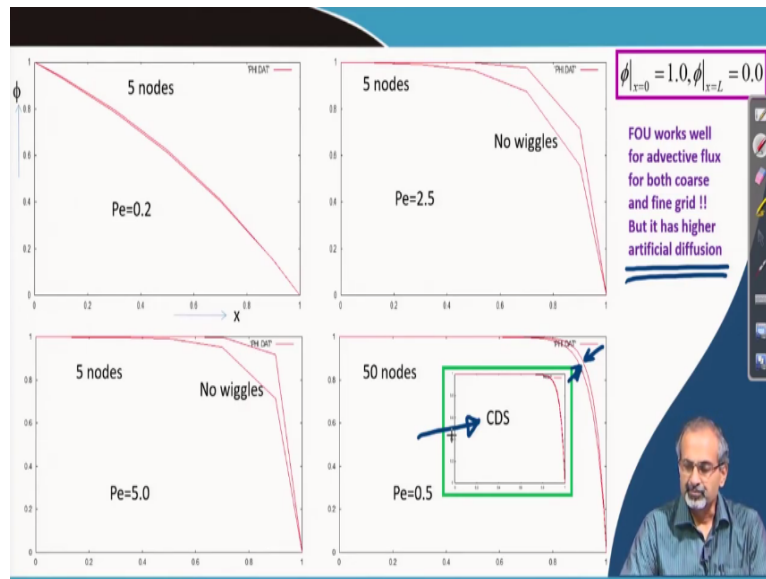
So, here is the solution coming from first order upwind scheme. And precisely the same cases, which we treated for the central differencing scheme one by one, we can see. And here the left boundary value is $\phi_A = 1$, right boundary value is $\phi_B = 0$. We have not shown the pure diffusion solution but you can imagine that it will be line as a straight line here connecting ϕ_A and ϕ_B .

And we can see that the troublesome case which began with Peclet number 2.5 is indicated here. So, you do not have any wiggles. But the trouble with first order upwind scheme is of course visible here, the analytical one lies on top. And the one from first order upwind scheme lies below. And clearly, there is a gap. Yeah. And why is it so? It is due to artificial diffusion.

You are aware that first order upwind scheme does have a significant artificial dissipation or diffusion and that is what is responsible for the gap between the analytical solution and the numerical solution. But nevertheless, there is no wiggles, which was a major issue with the central differencing solution. Now, if you push it to Peclet number 5 case even there you see no wiggles, which was making central differencing very unbounded filled with undershoots and overshoots.

Here, on the contrary, you find no wiggle whatsoever. But diffusion error again remains there. And what happens if you try to solve it using much larger number of nodes, the 50 nodes case. Here of course there will be no wiggles that we knew.

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But the point is that you find that even with large number of nodes, there is a gap between the analytical solution, and the numerical solution, which is again due to the artificial diffusion. And the insert you see that in central differencing scheme, there was virtually no gap between the analytical solution, and the numerical solution, which was due to its superior formal accuracy and essentially no diffusion.

Now, we went through two different schemes now already to look at solutions of one dimensional advection diffusion equation. So, we remember earlier, we had discussed about the exact solution of the (19:37) equation. In that case, we found that you know the solution comes out in the form of exponents.

And we just recollect that solution once more. And then we are proposing whether we can explore a scheme where we can actually use that exponential distribution. Because that is expected to give us much superior match with the exact solution at least in the one dimensional case, right. So, that is the motivation with which let us discuss a bit about a scheme, it is called as the exponential scheme.

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Exponential Scheme

$\frac{d}{dx}(\rho u \phi) = \frac{d}{dx}(\tau \frac{d\phi}{dx})$
 $\frac{d}{dx}(J) = 0 \leftarrow$
 $J = \rho u \phi - \tau \frac{d\phi}{dx}$
exact solution

$\frac{\phi - \phi_P}{\phi_E - \phi_P} = \frac{e^{\rho u \frac{x}{\Delta x_e}} - 1}{e^{\rho u \Delta x_e} - 1}$

$\int_w^e \frac{dJ}{dx} dx = J_e - J_w = 0$
 $J_e = J_w$

And the motivation behind the scheme is the exact solution of the one dimensional advection diffusion equation. And for that we will actually draw a small grid here in order to define the parameters which will be of use to us to come up with a derivation of the scheme. So, between the nodes P and E if we use the exponential scheme, then you may remember that from the exact solution we can write the distribution of phi in this region in this form.

So, this is essentially coming from the exact solution. What we have done is use the exact solution in this span between P and E. Alright. So, this holds good between P and E. We can similarly write it between another set of (()) (21:25) nodes. Now, we recall that our governing equation was this, right. So, this governing equation let this be written in a more compact form.

Let us call this as J where J is essentially rho u phi minus gamma d phi d x. Alright. So, this governing equation is now available to us in a compact form. And if you integrate this governing differential equation, let us say between limits e and w, which are applicable for the node P. Then you can write this equation in the form like this. So, J e minus J w and that should be equal to 0, which essentially means that J e is equal to J w, right.

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$$\begin{aligned}
 J_e &= (\rho u)_e \phi_e - T_e \left(\frac{d\phi}{dx} \right)_e \\
 &= F_e \phi_e - T_e \left(\frac{d\phi}{dx} \right)_e \\
 &= F_e \left[\phi_p + (\phi_E - \phi_p) \cdot \frac{e^{\frac{P_e x_e}{\delta x_e}} - 1}{e^{P_e} - 1} \right] \\
 &\quad - T_e \cdot \frac{(\phi_E - \phi_p) \cdot \frac{P_e}{\delta x_e}}{e^{P_e} - 1} \left[e^{\frac{P_e x_e}{\delta x_e}} \right].
 \end{aligned}$$

So, we can say that J_e , which needs to be not evaluated at the point e is this. And having defined the distribution of ϕ using the exponential distribution coming from the exact solution we can write this as. Okay we just do the calculation in the next step we have just put it as F_e here. Now, what is ϕ_e ? ϕ_e will be coming from the ϕ distribution that we wrote earlier for the point e .

That means here in the exponent x will be replaced by x_e that is what makes it applicable for ϕ_e . So, this is the expression for ϕ . And then we need to take a derivative. So, if you quickly do the calculation for the derivative somewhere here. Let us have a small calculation here. So, you do a $d\phi/dx$. And you can show that will be equal to, say, let us call it ϕ_L .

Rather, we call it as ϕ_P by e to the power of P_e minus 1 into P_e by δx_e into e to the power of $P_e x_e$ by δx_e . So, this would be the expression for $d\phi/dx$. Right now, if you use that for the diffusion term. What will be the calculation? Yeah. So, actually, and go back here and correct it. So, this should be ϕ_E minus ϕ_P by e to the power of P_e minus 1 into P_e by δx_e .

And then we have e to the power of $P_e x_e$ by δx_e . So, this is what we have over here. Now, you can see that one of the set of terms will actually get cancelled out.

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$$\begin{aligned}
&= F_e \phi_P + F_e (\phi_E - \phi_P) \left[\frac{e^{P_e \frac{\Delta x}{2\Delta x}}}{e^{P_e} - 1} \right] \\
&\quad - F_e (\phi_E - \phi_P) \left[\frac{e^{P_e \frac{\Delta x}{2\Delta x}}}{e^{P_e} - 1} \right] \\
&= F_e \phi_P - \frac{F_e (\phi_E - \phi_P)}{e^{P_e} - 1}
\end{aligned}$$

And you will be able to simplify this as $F_e \phi_P$ plus. So, it comes up to this and then finally, if you rearrange.

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$$\begin{aligned}
J_e &= F_e \left[\frac{e^{P_e} \phi_P - \phi_E}{e^{P_e} - 1} \right] \quad T_{\text{constant}} \\
\Rightarrow J_w &= F_w \left[\frac{e^{P_w} \phi_W - \phi_P}{e^{P_w} - 1} \right] \quad \begin{matrix} P_e \\ P_w \end{matrix} \\
J_e &= J_w \\
\left[\frac{F_e e^{P_e}}{e^{P_e} - 1} + \frac{F_w}{e^{P_w} - 1} \right] \phi_P &= \left[\frac{F_e}{e^{P_e} - 1} \right] \phi_E + \left[\frac{F_w e^{P_w}}{e^{P_w} - 1} \right] \phi_W
\end{aligned}$$

You will be able to show that J_e is equal to F_e times e to the power of $P_e \phi_P$ minus ϕ_E by e to the power of P_e minus 1. From that you can figure out that when you apply it to the west face. It could be written as e to the power of $P_e \phi_W$ minus ϕ_P by e to the power of P_e minus 1. Of course over here, we have made one assumption. As usual that γ is constant and so is the grid spacing.

Therefore, the D does not change from one big space into the other between nodes, and therefore, F anywhere remains constant because of continuity requirements. So, the ratio

Peclet number will remain constant. But if γ changes from point to point or there is non uniformness that may lead to varying values of Peclet number that you need to keep in mind.

If that is the case, then you have to assign some separate indices for Peclet number like P_e at the point e or P_w at the point w and so on. So, for simplicity here we have assumed it to be constant. Remember that J_e is equal to J_w from the governing equation. Therefore, once we set that condition and we collect all the terms together, you will get this form. Sorry. You have to write another expression here and then close the bracket ϕ_P is equal to ϕ_E to the power of P_e times ϕ_W .

So, what we find is that the coefficients of ϕ_P , ϕ_E or ϕ_W they are all functions of exponents of the cell based Peclet number. So, P_e here is the cell based Peclet number. Now, in the central differencing scheme or first order upwind scheme we never found this happening that they are exponents of Peclet number, right. So, here it comes up because we have made use of the exact solution itself to be fitted into the discrete framework.

That is why the exponential forms have come up. So, we can expect that this will function much more superiorly compared to the first order upwind or central differencing. But the problem lies elsewhere that when handling exponents numerically, it is a very cumbersome and costly issue. Because exponents involve very large series expressions, and therefore it will be extremely costly, where indices are involved.

And therefore computational costs will become sky high if you use these kinds of schemes. Therefore, due to the expense of this scheme, we cannot use the scheme, per se. Instead of that we will discuss about some reduced order forms or simplified forms of this exponential scheme in the next lecture. Thank you.