Computational Fluid Dynamics

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Module no. # 03

Template for the numeric solution of the generic scalar transport equation

Lecture no: #09

Finite difference approximation of p th order of accuracy for q th order derivative

Cross-derivatives

Examples of high order accurate formulae for several derivatives

On the governing equation that we are solving the Navier-Strokes equation have only highest derivative of the second derivative.

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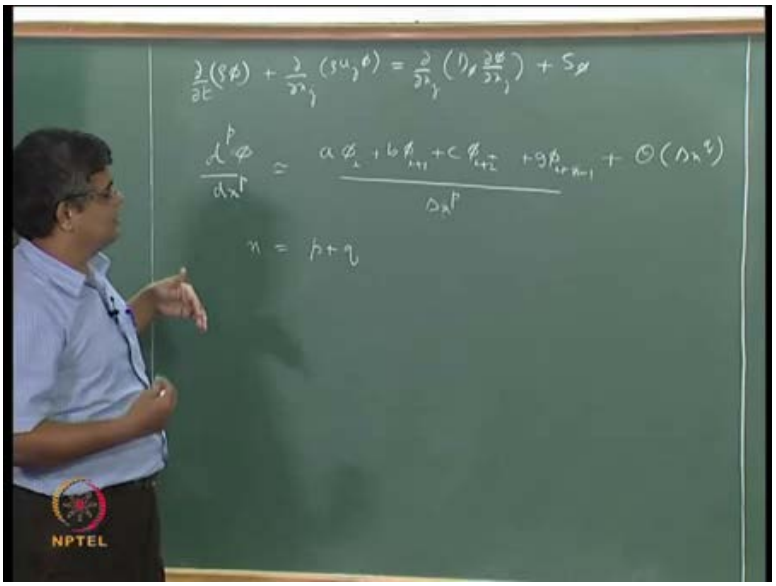

In the diffusion term, it is, it is sometimes necessary for us to get even a higher derivative. So, we will try to seek a method, by which, we can write a finite difference approximation of a desired accuracy for any derivative as required by the problem.

So, we are looking at, at, a solution like this d p phi by dx p. So, that is a p th derivative of q th order can be approximated as a phi i b phi i plus 1 plus c phi i plus 2 plus say g phi i plus n by delta x to the power p - where n is the number of points which are required for this. It should be n minus 1. If put like this, then n is equal to p plus q for this forward differencing, and if you take points both on to the left and to the right of it, for example, i minus 1 i i plus 1 i plus 2 and so on, we would be able to have n which is equal to p plus q minus 1.

So, this general rule says that for a p th order derivative, for a q th order accuracy, the number of points which are equispaced which should be brought in to this formula is fixed by n being equal to p plus q for a one sided formula and p plus q minus 1 for a, for a central differencing formula.

Now, the question is we can write it down like this, but what are the values of these coefficients of a b c d e and so on? Without the values of the coefficients, this approximation is useless for us. We know that it is we can write it like this, but as it is, it is the prescription is not complete without a method by which we can determine the values of a b c d e.

So, let us, let us try to find that method. The method is, is, very simple. You know that this is the formula that we are seeking and we expand each of these in terms of Taylor series expansion, in terms of Taylor series, about the point i and then we put all of them together, then compare the coefficients with what we are expecting here, and by comparing coefficients. We will have a certain number of equations and as many equations as there are unknowns here, and using that, we should be able to find a values of this.

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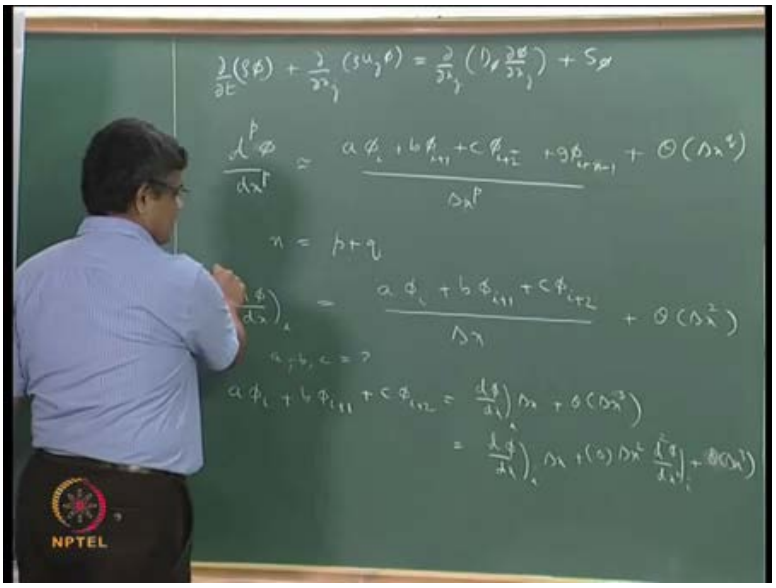

We will illustrate this for a simple case of a first derivative d phi by dx at i expressed in terms of written as a phi i plus b phi i plus 1 plus c phi i plus 2 divided by delta x for dimensional consistency, and as per our formula p is equal to 1, first derivative and n is equal to t 3 i i plus 1 and i plus 2 and this is a forward difference approximation, because we have i i plus 1 and i plus 2. So, n is 3 and p is 1. So, q is equal 2. So, this gives us a second-order accurate approximation, and the question is what are a b and c?

If we are able to determine the values of a b and c for this approximation, then wherever we have a first derivative, we can substitute this approximation and we can be confident that we have a second-order at that approximation. Now, how do we find this?

In order to find this, we rewrite this equation as a phi i plus b phi i plus 1 plus c phi i plus 2 is equal to d phi by dx at i times delta x plus terms of the order of delta x square. This is nothing but restating of this. We have put delta x here. So, when we multiply terms of the order of delta x square with this, for example, we take this one here and multiply by this, we shall be getting delta x cube. So, we can also write like this that d phi by dx at i times delta x plus 0 times delta x square times d square phi by dx square at i plus terms of the order of delta x cube.

So, by this, we are saying we have delta x, a term of the order of delta x which is here and any terms of delta x square will be 0 and delta x cube terms will be non zero. So, this is what this expression actually means. In this expression, in this formula that we are

treating, we have phi i and phi i plus 1 and phi i plus 2. So, let us write Taylor series expansion for each of these around the .point i plus 1.

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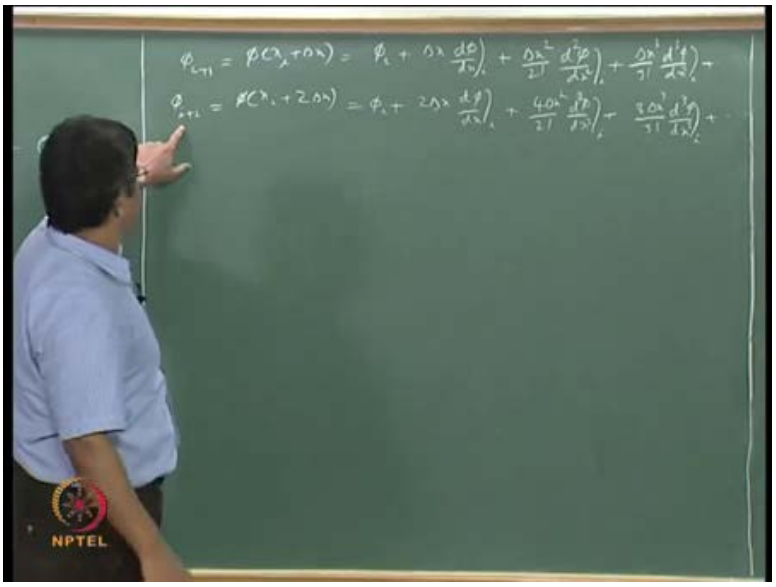

So, we can say that phi i plus 1 is nothing but phi of x i plus delta x as per our terminology and this is equal to phi i plus delta x times d phi by dx at i plus delta x square by factorial 2 times d square phi by dx square at i plus delta x cubed by factorial 3 third derivative at i plus so on. Since we are looking at terms going up to delta x cubed, we need to retain at least this term.

We can also retain higher terms, but they are not really necessary for us. Similarly, we can write phi i plus 2 is nothing but phi at x i plus 2 delta x. That is what we mean by i plus 2 and this can be written as phi i. Where ever we have delta x here, we substitute 2 delta x. So, that is 2 delta x times d phi by dx at i plus 2 delta x whole square. So, that is 4 delta x square by factorial 2 d square phi by dx square at i plus 2 delta x cube. So, that is 8 delta x cube by factorial three times d 3 phi by dx 3 at i plus so on.

So, this is phi i plus 2 and this is phi i plus 1, and what we are looking at is a times phi i plus b times phi i plus 2 plus c times phi i plus 3.

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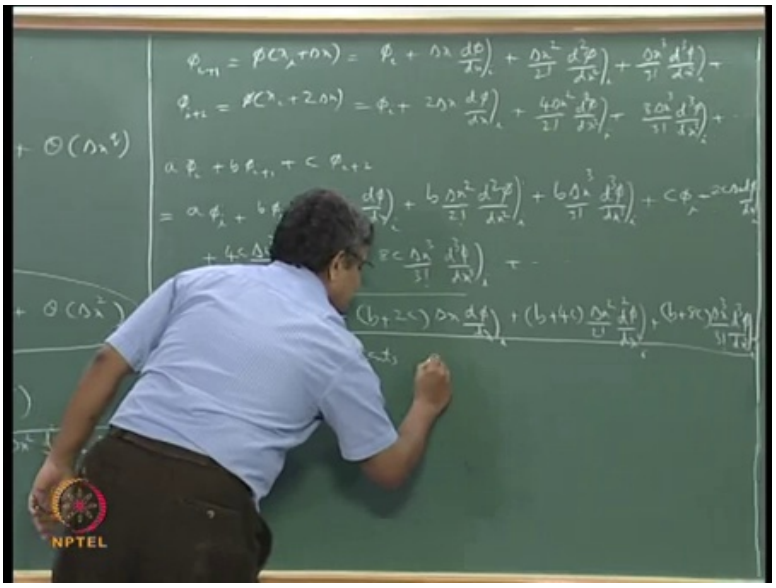

So, we can therefore write a phi plus b phi i plus 1 plus c phi i plus 2 as a phi i. You multiply this whole thing by b and bring it here; so, that is b phi i plus b times delta x d phi by dx, we will just, plus b times delta x square by factorial 2 times d square phi by d x square at i plus b times delta x cubed by factorial 3.

Third derivative, we will, for the time being neglect the higher order terms, we will include that if necessary plus we have c i plus c times phi i plus 2. So, we will multiply all this by c here. So, that is c phi i plus 2 c delta x d phi by dx at i plus 4 c delta x square by factorial 2 d square phi by dx square at i plus 8 c delta x cubed by factorial 3 times third derivative and so on.

And let us bring like terms together. So, we can write this as a plus b plus c here times phi i, and what is the next term? d phi by dx. So, that is b plus we have 2 c times delta x d phi by dx plus we have d square phi by dx square is b here and we have 4 c, 4 c delta x square by factorial 2 d square phi by d x square at i plus we have d 3 cube d cubed by dx cubed is b plus 8 c delta x cube by factorial 3 d 3 phi by dx 3 at i plus so on like this. So, this a phi plus b phi i plus 1 plus c i plus 2 is this and it is also equal to this.

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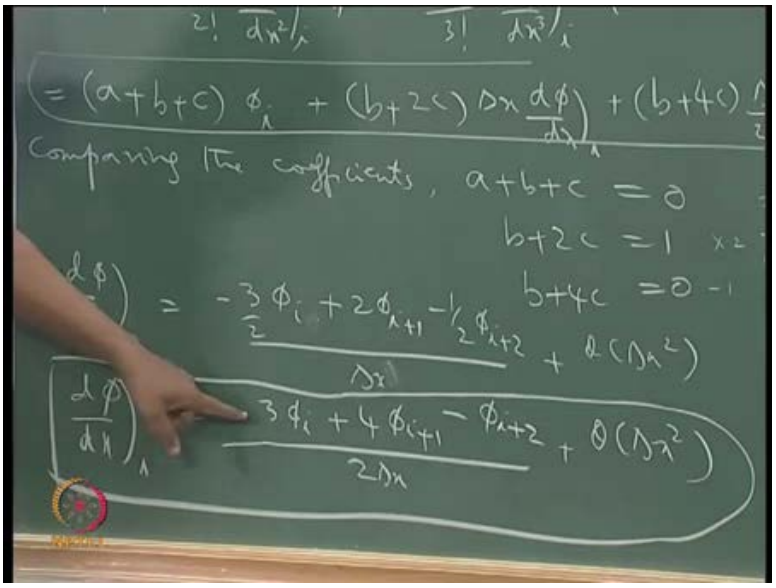
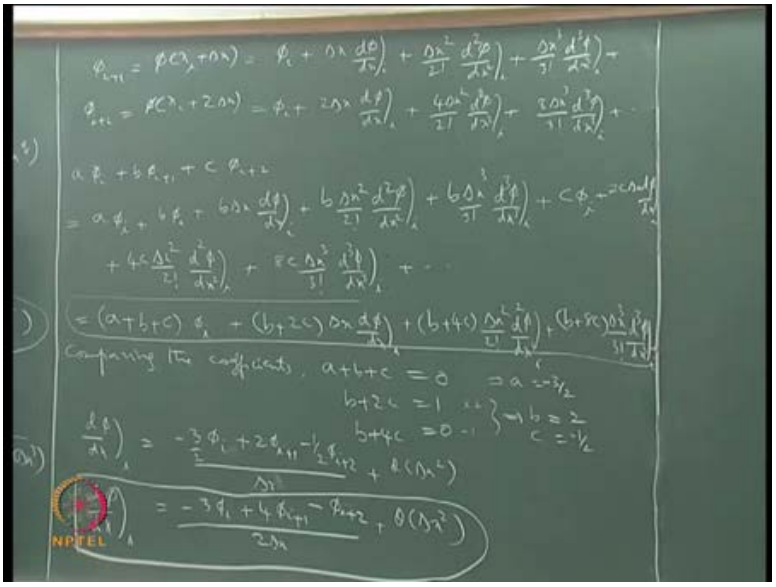


So, we compare the coefficients on the right hand side of this and this expression and we can see that here there is no phi i term. So, comparing the coefficients of this one with this one here, we see that a plus b plus c must be equal to 0, and this is d phi by dx times delta x; we have d phi by d x times delta x at I; so, b plus 2 2 c is equal to 1 and 0 times delta x square times d square phi by dx square. So, we have b plus 4 c is equal to 0 and we will have terms of b plus 8 c which is non-zero. Essentially, what we are saying.

So, we will have three equations here for the three unknowns - a plus b plus a b c here and we can eliminate c from this. So, that gives us if you multiply this by 2 and subtract this, then we get b is equal to 2 and c is equal to minus half so that b is 2 and 4 times this is minus 2; that is correct, and. So, from this, we get a equal to 2 minus of this is 3 by 2. So, we have a equal to 3 by 2, b equal to 2 and c equal to minus half; a is minus 3 by 2 so that minus 3 by 2 minus 1 by 2 will cancel out with this.

So, therefore, we can write this expression here as d phi by dx at i is equal to a is minus three by 2 phi i plus, we have the, we can take the 2 here minus 3 by 2 plus 2 phi i plus 1 minus half phi i plus 2 divided by delta x square delta x plus terms (( )) out of delta x and we can write the same thing as minus 3 phi i plus 4 i plus 1 minus phi i plus 2 by 2 delta x. This is the one sided forward differencing approximation for the first derivative of second order accuracy involving three points - phi i phi i plus 1 and phi i plus 2 with coefficients of minus 3 plus 4 and 1 minus 1 and the whole thing divided by 2. So, these

are the three coefficients. So, this method that we have written down here is very generic and you can do this like what you were trying to do, that is, for the third derivative of second order accuracy. So, you need to put two more points and then we need to expand this to have more number of points here and there will be phi i plus 3 and phi i plus 4. (Refer Slide Time: 16:39)



We have to write down phi i plus 3 phi i plus 4 and then multiply by the appropriate coefficients and then put the whole thing together and obviously going to be more terms in this and we can compare the coefficients of this approximation and what we mean by seeking an approximation like this. By comparing the coefficients, we will have a system of equations which we need to solve simultaneously to get the values of the coefficients. So, in this way, we write down the approximation for any derivative of desired accuracy either in the forward mode or in the central mode or, in, in the backward mode.

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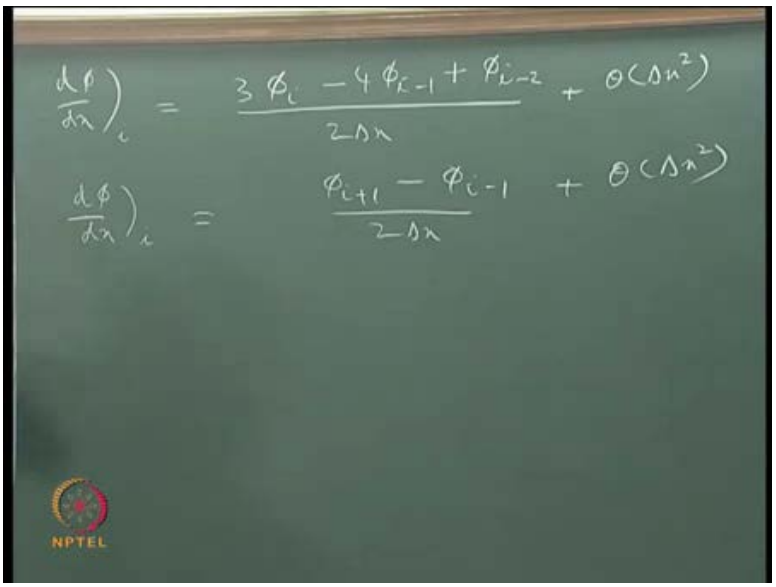

So, let us, this is a very generic method. Using this for any derivative, we can find a finite difference approximation of a given accuracy. So, just to bring home the point, let us write down some interesting formulas. We have here a forward differencing second order accurate formula for the first derivative, which can be useful at one extreme.

We can also write a backward differencing formula of second order accuracy for the first derivative and this will be 3 phi i minus 4 i minus 1 plus phi i minus 2 divided by 2 delta x and this is second order accurate. And so, using this, you can get a second order accurate approximation and we also know that d phi by dx at is given by phi i plus 1 minus phi i minus 1 by 2 delta x.

So, using these set of formulas, these set of formulas, you can maintain consistently second order approximation for interior points for one boundary, at the bottom boundary, that is, at the top boundary and the bottom boundary using this. So, this is for a first derivative.

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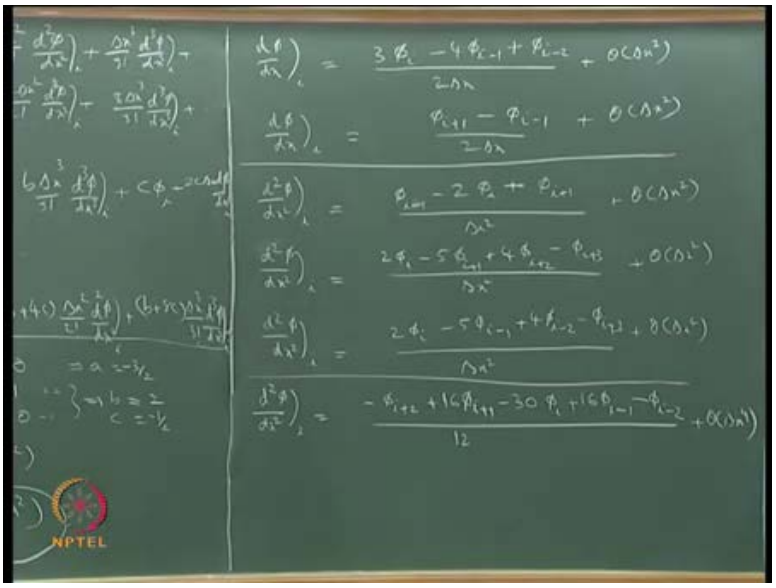

We can similarly write for a second derivative, we know the central difference formula; we have already derived. This is phi i minus 2 plus 2 phi i plus phi i plus 1 by delta x square and this is a second order accurate formula. Forward difference formula for second order accurate formula is 2 phi i 4 phi i plus 2 minus phi. This is again a second order accurate forward differencing formula for the second derivative.

You can see that p is equal to 2 and q is equal to 2. So, that is second derivative and second order accurate formula. So, the number of points that we want are 4. You can see that there are four points – i, i plus 1, i plus 2 and i plus 3, and we can also write a backward differencing formula of second order accurate thing for the second derivative. This will be very similar, and just for the point of illustration, we can also write a fourth order accurate central differencing formula for the second derivative and this is minus phi i plus 2 phi i plus 1 minus 30 phi i plus 16 phi i plus 1 minus 30 phi i plus 16 phi i minus 1 minus phi i minus 2 this whole thing divided by 12 plus terms of the order of delta x 4.

So, this is a fourth order accurate formula for a second derivative involving central differencing, because you have i plus 2 and i minus 2 i plus 1 i minus 1 and i here, and So, we have p is equal to 2 here and q is equal to 4 and n must be equal to p plus q minus 1, that is, 5 and we see here five points - 1 2 3 4 5. So, this again satisfies our requirement. And another point to note is that, with these kinds of formulas for with

uniform mesh spacing, all the coefficients here will add up to 0. So, you have 16 plus 16, that is, plus 32 minus 31 minus 32. So, they all add up to 0 here, and if you look at it here, minus 5 minus 1; so, that is minus 6 4 plus 2 plus 6. So, that is 0, and the same thing here, this is minus 2 plus 1 plus 1, and here, again plus 1 minus 1 minus 4 3 plus 1 4. So, that is a quick check for us to see that our derivation of these coefficients is correct.

So, in this way, we can get an approximate formulae for any derivative, any desired accuracy which is applicable right now for, for, uniform spacing. With our capability now to represent any derivative with an equivalent finite difference approximation, we are ready to discretize our governing equation, but we need to do some more things.

So far we have been talking only about d phi by dx, d square phi by dx square, d cube phi by dx cubed and so on, but sometimes we also have to deal with mixed derivatives, that is, d square phi by dx dy.

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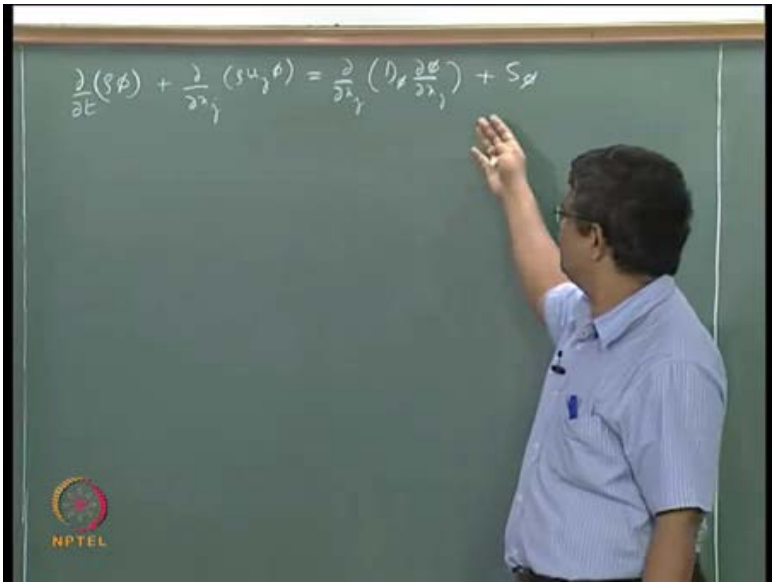

When we deal with strictly orthogonal coordinate system and look at our governing equations like the generic scalar equation, we would not have any mixed derivatives; we will have either d square phi by dx square or d square phi by dy square or d square phi by dz square, only the normal derivatives will be present, but if we were dealing with a non orthogonal coordinate system, for example, to consider the possibility of a flow domain which does not fit in to this fixed coordinate lines, orthogonal coordinate lines, in such a

case, we will have, we have to transform these equations from orthogonal to non orthogonal coordinate system, in which case, we will have mixed derivatives.

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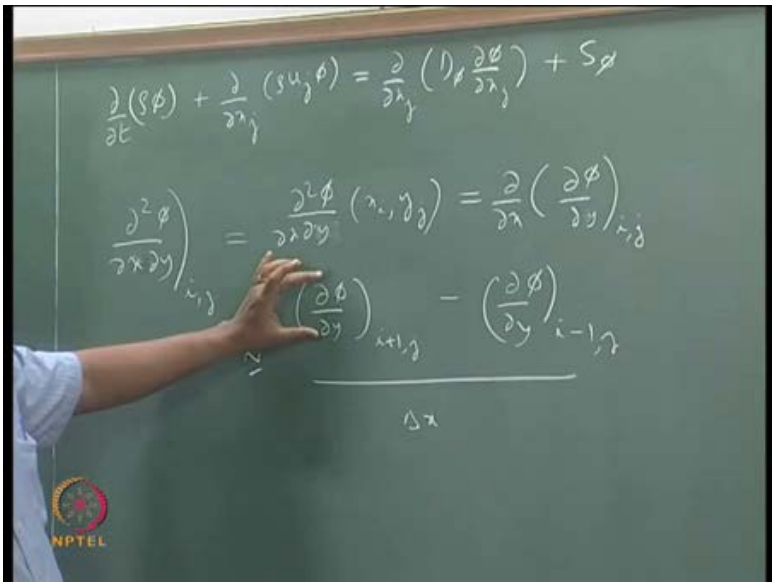

So, we will have a derivative, for example, dou square phi by dou x dou y. So, this type of term will also appear in the governing equations. Writing the finite difference approximation for this kind of derivative is relatively straightforward. Although, later on we will see that treatment of the mixed derivatives is always a headache. When we try to look at CFD solution, we will just try to see why it may be so starting with, when we look at the, the, finite difference approximation points. So, let us just see how we can write dou square phi by dou x dou y.

Now, since we are dealing with two coordinates, we need to have two indices – i, j; this obviously means that dou square phi by dou x dou y at x i y j and we are assuming uniform grid spacing of delta x in the i i direction and delta y in the j th direction.

So, we can write this as dou by dou x of dou phi by dou y at i, j and we can write this as dou phi by dou y at i plus 1 minus dou phi by dou y at i minus 1 divided by delta x. So, in, so doing, we are making use of central difference approximation for the derivative with respect to x. So, this is obviously an approximation; so, we can write this approximately as this. And since we are dealing only with the derivative in the x direction, the index j does not change; so, this is i plus 1 j and i minus 1 j by delta x.

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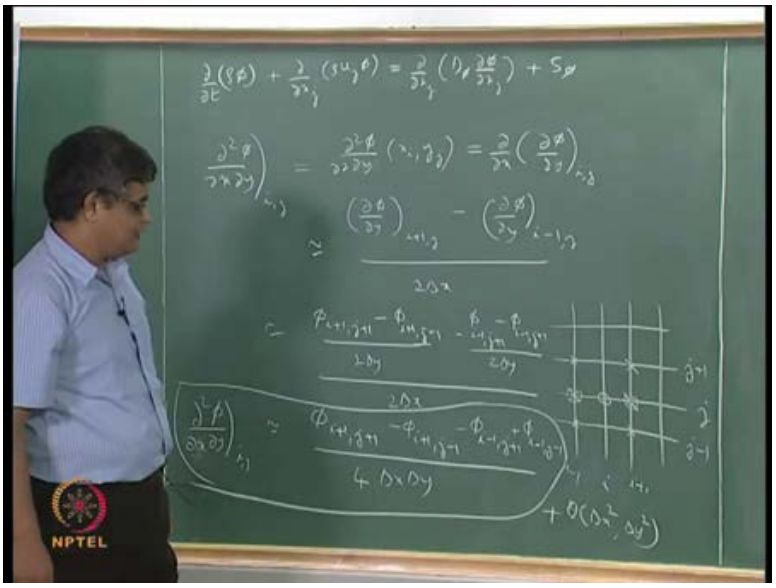

So, now we have to write finite difference approximations by dou phi by dou y at i plus 1 j and dou phi by dou y at i minus 1 j. So, let us just have an idea of what we are talking about here. This is our uniform grid and let us say that this is our point, this is i here and this is the j th column; this is our point i j and we have expressed i plus 1 j here; this is the point at which d phi by dy has to be evaluated and this is the point at which this has to be evaluated. So, let us mark these points like this and we can write dou phi by dou y at i plus 1 j at this point in terms of phi value here and phi value here using central differencing. So, we can write this as keeping in mind this and this. So, this is j plus 1 and this is j minus 1 and this is i plus 1. So, we can write dou phi by dou y at i plus one j as phi at i plus 1 j plus 1 minus phi at i plus 1 j minus 1 divided by this distance which is 2 delta y. So, we can write this expression as i plus 2 j plus 1 minus phi i plus 1 j minus 1 by 2 delta 1. Similarly, dou phi by dou y at i minus 1 j, this is i minus 1 and j here, can be expressed as phi value at j plus 1 minus phi value at j minus 1 divided by this 2 delta y and both the phi values are evaluated at i minus 1.

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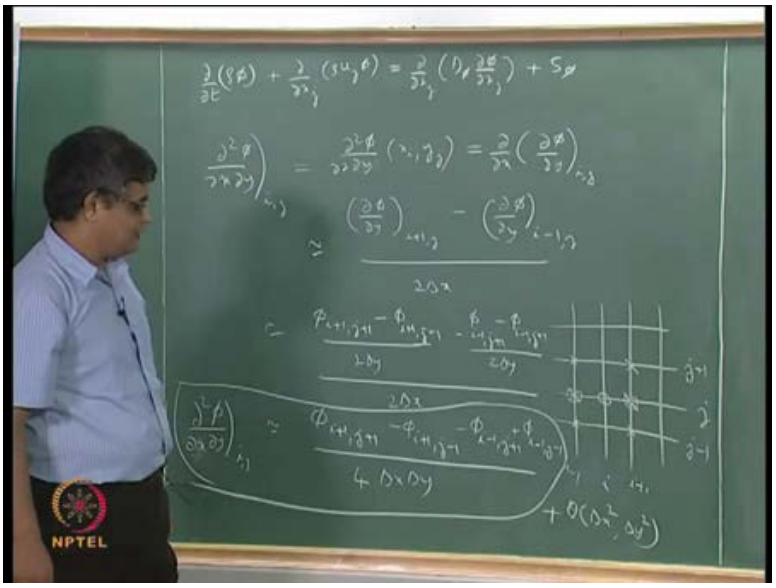

So, we can write this as minus of phi i minus1 j plus 1 minus phi i minus 1 j plus 1 divided by 2 delta y. This whole thing divided by delta x. This whole thing divided by here, it is 2 delta x, because the spacing is 2 delta x. So, this should be 2 delta x.

So, this will give us phi i plus 1 j plus 1 minus phi i plus 1 j minus 1 minus phi i minus 1 j plus 1 plus phi i minus 1 j minus 1 divided by 4 delta x delta y. So, this is an approximation for the mixed derivative dou square x dou square phi by dou x dou y at point i j. What will be the accuracy of this? We have consistently used the central differencing here and central differencing here, so, we can expect an overall accuracy of second order in both x direction and y direction. We can verify this using Taylor series expansion. We can verify each of this we can expand each of these about Taylor series about point i, j and then show that this is second order accurate in, in, both delta x and delta y.

So, this is one particular thing, and when we look at the final formula here, the value of d phi by d y dou square phi by dou x dou y at point i j is expressed in terms of the values at the four corners immediate, immediate, corner points of this rectangle here and also importantly there is no contribution of the value of phi i j in this. So, that is an important thing when we write down the full set of equations for the whole thing and then put convert the whole thing in to an equivalent algebraic equation.

It is important that in the final finite difference approximation for this equation, the contribution from the cell point at which we are doing the discretization. For example, we are evaluating this term at i j and this term at i j and the source term also at i j. So, the contribution of this particular point should be predominant.

This is expressed in the condition of diagonal dominance, which we will see at a later stage. That diagonal dominance condition is necessary for us to use good iterative methods like the Gauss siedel method, which we have already used only when you have diagonal dominance, can we expect that Gauss siedel method to guarantee us a converged solution; otherwise, it, it, may not give us that convergence. So, it is desirable to have a strong contribution from the central point here, whereas, in the discretization of this using eminently acceptable central difference formulas which we had been advocating in so far with the second order accuracy. In this approximation, we have no contribution from the point i j itself. We have only points contribution from the four corner points.

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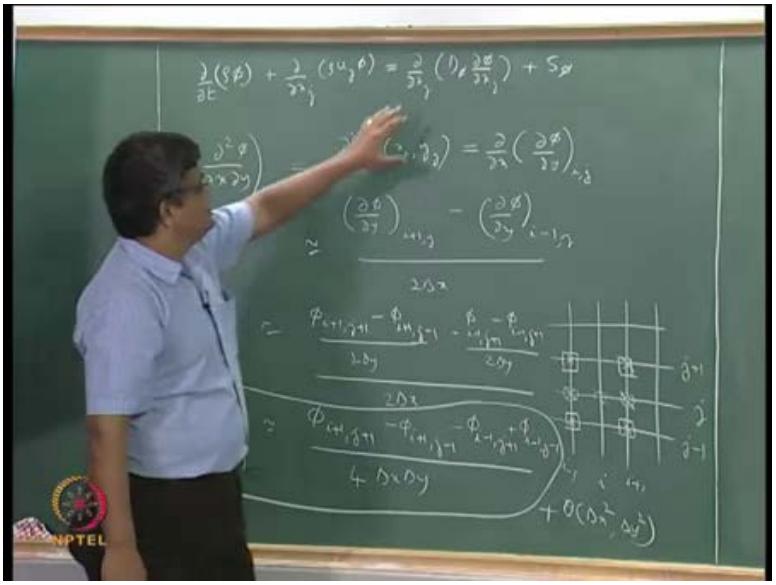

So, if we were to have this term in the equation here, then the discretization of the cost derivative or the mixed derivative will tend to destabilize the overall iterative solution. So, that is why mixed derivatives are a headache; we have to treat them like something of a deferred correction method, or we must find formulae for the for the mixed derivatives, in which, the contribution from this point also arises, and if you do that, then

we can retain the contribution from this point and we can put away the contribution from the off diagonal terms on to the right hand side and in a deferred correction way, which improves the rate of convergence of the overall iterative method.

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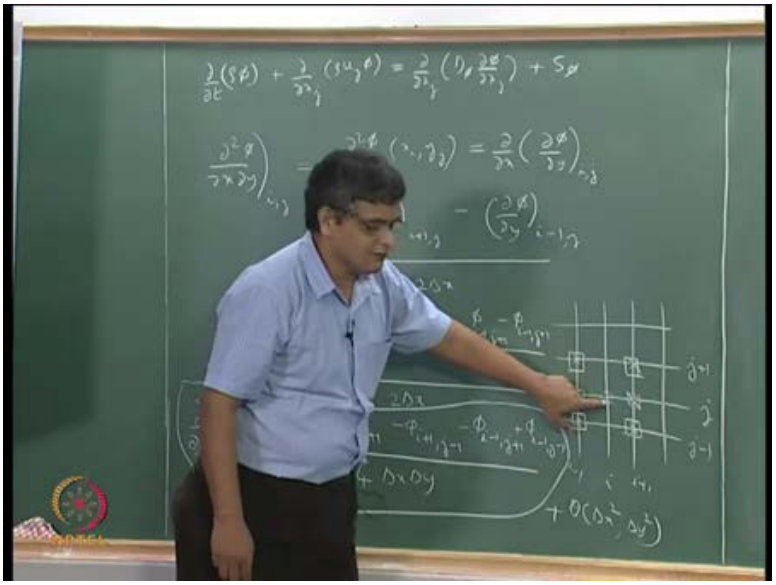

So, what we want to take home at this particular point is that the mixed derivatives can also be discredited using the methods that we have outlined earlier, but mixed derivatives gives rise to an overall formula, in which, the point at which we are evaluating the derivative does not come in to the picture in this particular discretization formula.

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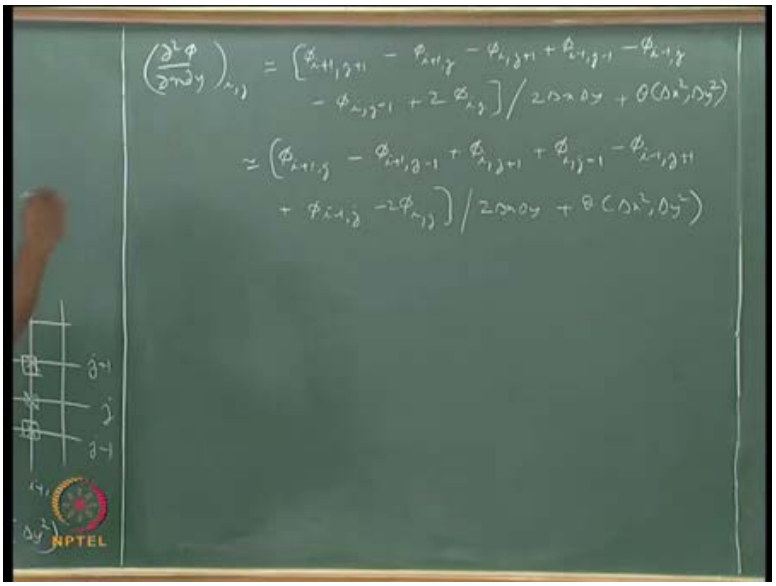

There are other formulas which I will write down and which will be left as an exercise for the reader dou square phi by dou x dou y at i, j can also be represented as phi i plus 1 j plus 1 minus phi i plus 1 j minus phi i j plus 1 plus phi i minus 1 j minus 1 minus phi i minus 1 j minus phi i j minus 1 plus 2 phi i j this whole thing divided by 2 delta x delta y plus terms of the order of delta x square delta y square.

So, this is one formula. We will take a look at it just now, but we will write one more formula - a different formula is phi i plus 1 j minus phi i plus 1 j minus 1 plus phi i j plus 1 plus phi i j minus 1 minus phi i minus 1 j plus 1 plus phi i minus 1 j minus 2 phi i j. This whole thing divided by 2 delta x delta y and this is also a second order accurate formula in both delta x and delta y. So, this can be derived using the methods that we have discussed. Let us look at the corresponding computation molecule for this, for these two formulas.

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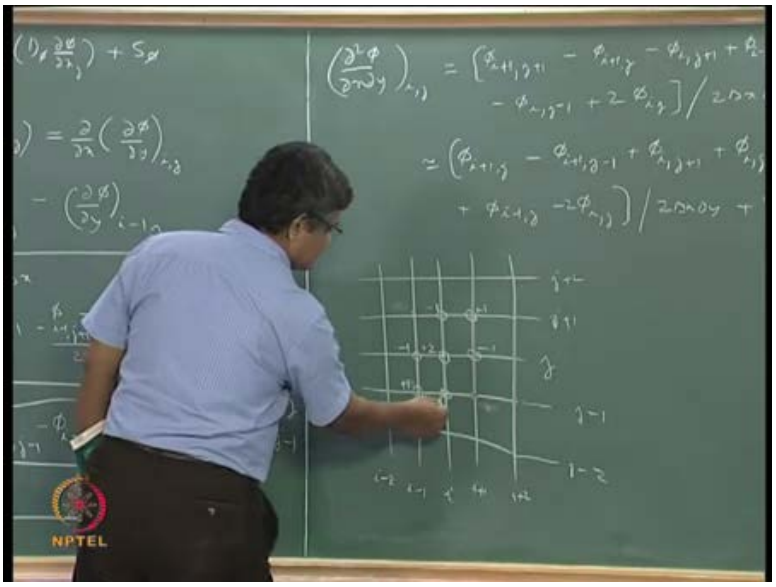

Again we have the x y z grid here. Let us take the center line to be i here and this is j. So, we are looking at this particular point here, and so, this is j plus 1 j plus 2 j minus 2 j minus 1 and this is i minus 1 i plus 1F i plus 2 and i minus 2. So, in such a case, in this formula, let us call this as formula B and formula C and formula A.

We know that in formula A, we have these four points and 0 contribution from this and we have plus 1 for this corner point i plus 1 j minus 1 i plus 1 j minus 1 is and i minus 1

minus 1 j plus 1 is minus 1 i minus 1 j plus 1 is this. This is minus 1 and i minus 1 j minus 1 is plus 1.

So, we have a contribution of plus 1 from these two corner points and minus 1 from these two corner points for formula a. Now, what about this 1 here? Here we have i plus 1 j plus 1. So, this is i plus 1 j plus 1 that has 1 here i plus 1 j i plus 1 j is this 1 here and this has a contribution of minus 1. So, let us just start with these 2 i j minus i j plus 1. So, this is i j plus 1, sorry, yes, this is minus i j plus 1 minus i plus 1 j is this. So, this is i plus 1 j is minus 1 and then i minus 1 j minus 1, i minus 1 j minus 1, is this, and here, this has plus 1 i minus 1 j i minus 1 j is minus 1 i j minus 1 i j minus 1 is this one; this is minus 1 and plus 2 i j; so, this is 2.

So, we have contribution from this, from this. So, the second derivative here is expressed in terms of 1 2 3 4 5 6 7 points here and it is oriented towards plus direction. So, it is inclined like this and minus 1 minus 1 minus 1 minus 1. So, this is plus 4 plus 1 plus 1 plus 2; so, that is plus 4. So, they all cancel out and this molecule is different from this molecule, where it has plus 1 plus 1 plus 1 minus 1 and minus 1 for this.

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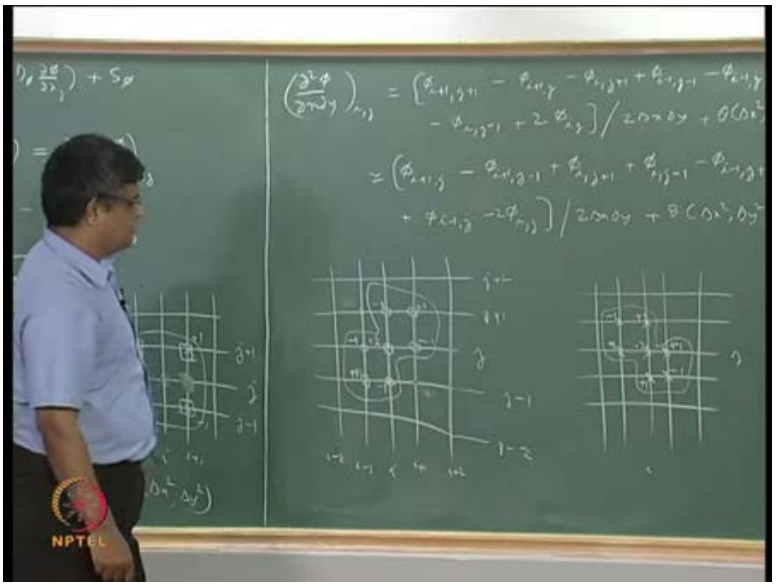

Now, let us see what this molecule here says 3 4 5. Again, we have i here and j here. So, we are looking at this 1 and here is i plus 1 j. So, i plus one j is this one with a plus, plus, 1 i plus 1 j minus 1, so, that is, this 1 here with a minus 1 and i j plus 1 i j plus one is is

this with plus 1 i j minus 1 is this 1 plus 1 minus i minus 1 j plus 1. So, is this that is with minus 1; i minus 1 j is this one, so, this is plus 1 and this is minus 2.

So, here we have. So, we have these points coming in the picture, and here, we have these points coming here and here it is these 4. So, this is inclined towards positive x and positive y site, and here, it is more like negative x and y side here. And otherwise, the computational molecule looks the same, but the difference between this approximation and this approximation is that here the central point has 0 weightage and here it has the highest weightage and here also it has the highest weightage, but still this is not wholly satisfactory because the central point does not have the preponderous weightage, where by that we mean that the central point has a weightage which is equal to the sum of all of them, all the rest put together or at greater than that.

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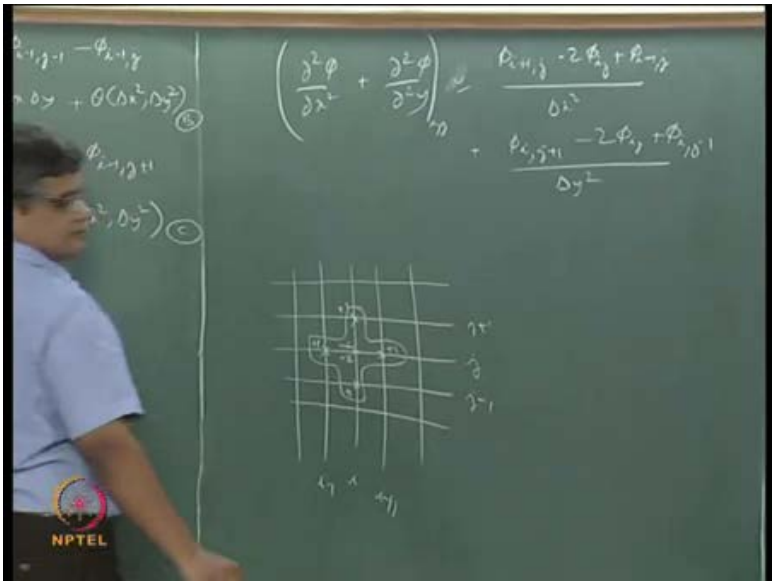

So, when you say preponderance, the value here should be greater than all of them. It does not happen for an interior point, but at least it should be as much as the sum of all the other points which does not happen in for the cross derivative, but let us also for the sake of interest, for the sake of comparison, let us take the normal derivatives coming from a the diffusion term in a two-dimensional case and we can write the approximations using the same central differences for this and this will be as we have seen phi i plus 1 j minus 2 phi i j plus phi i minus 1 j by delta x square.

So, that is approximation for this, and for this, we will have plus phi i j plus 1 minus 2 phi i j plus phi i j minus 1 divided by delta y square. So, the central difference approximation for second derivative in x and second derivative in y, the sum together will be like this and if we examine the computational molecule for this, this is the i, j and we are evaluating this whole thing at i, j, which is the same for all of these. So, in this particular case, if you look at the central point here, the computational molecule for this you have plus 1, that is, let us put this i plus 1 i minus 1 j minus 1 and j plus 1. So, the cross derivative here as plus 1 minus 2 for the central point and plus 1 for this and weightage coming from the cross derivative in y direction is j plus 1 here, this is plus 1 minus 2 and plus 1.

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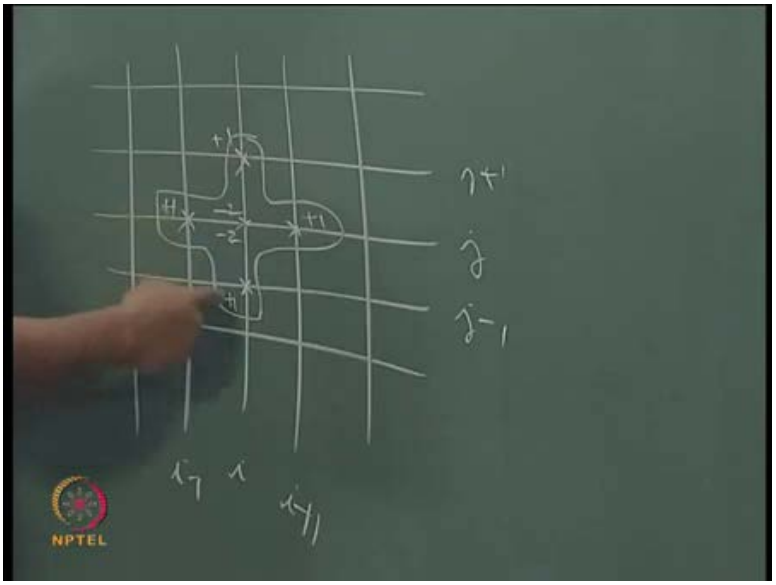

So, we have a computational molecule which is like this. So, for the two normal derivatives, we have a total contribution of minus 4 for the central point and for all the other points also it is minus 4. So, we can say that the center point weightage is as much as the weightage of all the other points put together in absolute sense.

So, this will, in a way this can satisfy at least the weak form of diagonal dominance, which is required for the convergence of the iterative method like the Gauss siedel method, but when you come to the cross derivatives, in this, the weightage for the central point at which we are evaluating the derivative is 0, and here, it is something and here it is something, but it is not preponderant; it is not even, it would not even satisfy the weak

form of diagonal dominance. So, when we deal with the discretization of an equation which is written in orthogonal coordinate frame, in which, there are no mixed derivatives, then we can expect to get a discretized equation which satisfies the weak form of diagonal dominance. Therefore, the standard method like gauss siedel iterative method can be applied for the solution of that algebraic equation a phi equal to b provided we do the source term linearization in an intelligent way, but when we have the same equations, the same governing equation written in a non orthogonal coordinative system, then we will have the cross derivative terms, and when you discretize the cross derivative terms, then we will have the difficulty of the non preponderance of the central. So, this will, if you directly implement it into the discretized equation, then the resulting discretized equation which is A phi equal to b will not satisfy the even the weak form of diagonal dominance. So, in that case, we cannot apply the standard iterative methods like Gauss Siedel methods or Jacobi method for the solution of A phi equal to b. Resulting from the discretization of a governing equation written in non orthogonal coordinate system.

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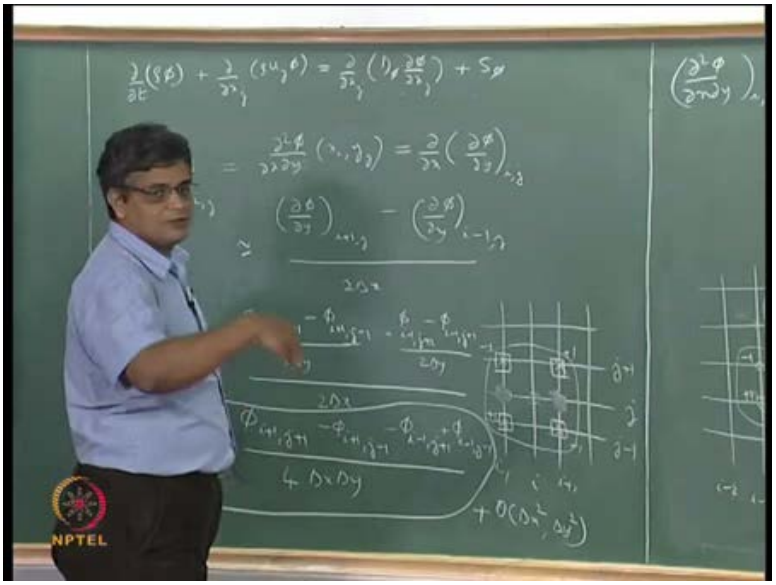

So, we have to use something like a deferred correction method, in which, the contribution from all the off diagonal terms is put on to the right hand side in to the b side of the equation and so that we can preserve the diagonal dominance of the matrix A.

We will discuss this more in detail later on, but what we want to say is that the moment you put some of the phi terms from the left hand side that is a phi equal to b in to the right hand side, that is, in to b, then you lose the, the, rate of convergence of the iterative method. So, that will lead, that will, that will make you, make a compromise on the rate of convergence, and sometimes, if the off diagonal terms are preponderant, then this may lead to divergence of the numerical.

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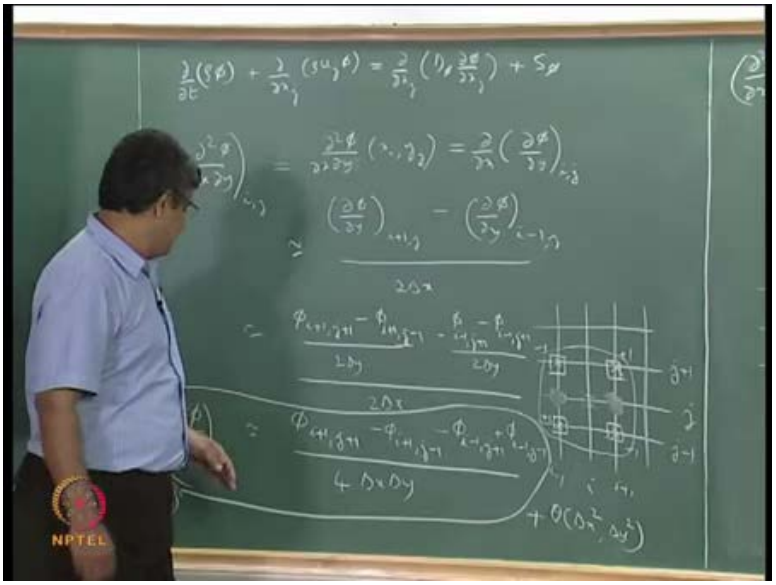

So, to the extent possible, we would like to deal with the equation in an orthogonal coordinate frame, but when you are dealing with complex geometries, it is maybe necessary to go in to non orthogonal coordinates, in which case, the presence of mixed derivatives becomes a necessary evil. Now, we can deal with it for the deferred correctional approach, but we can, we can, we cannot avoid these, we can try to mitigate their effect by having a grid which is not highly distorted, because in a highly distorted mesh, the preponderance of the cost derivative terms will become even more critical. So, in which case, even if you do a deferential correction approach, you may not get a convergence. So, that is why when we generate a grid, it is important to make sure that the grid is not very highly distorted so as to give rise to a numerical problem. So, and all that boils down to how we discretize, how we, what kind of finite difference approximation we write for the derivatives which appear in the equations and what is the result in the computational molecule and what is the weightage of the central point at which we are doing the discretization with respect to the other points. So, it, it all boils

down to the computational molecule, and whenever we write a finite difference approximation for each term in this, the overall resulting equation here should be put up in the computational molecule and see we should check whether or not we are satisfying the preponderance of the coefficient associated with the central, central, grid point. So, this is important in this.

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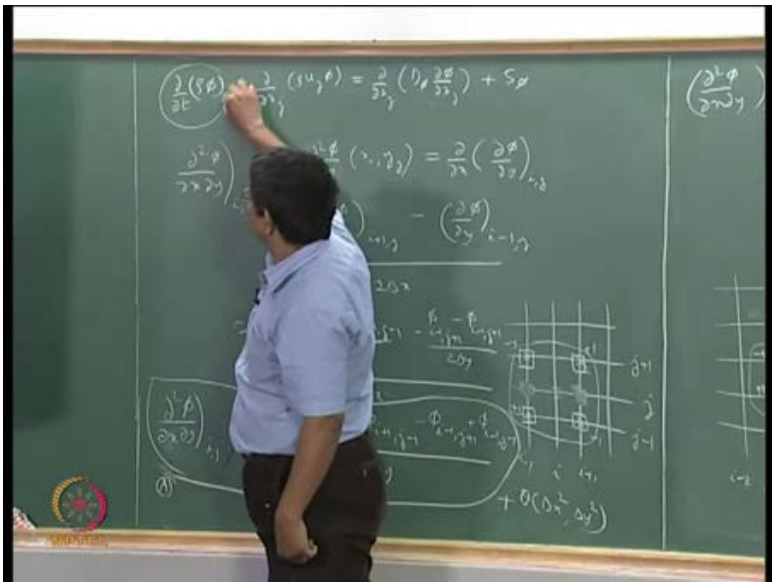

At this stage, we are now almost at a point where we can tackle the conservation equation. We still have the term coming from the time derivative that brings in the question of explicitness implicitness. Once we tackle that, we will be in a position to look at discretizaiton for the generic scalar transport equation.