Computational Fluid Dynamics
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Lecture - 24
Higher order and mixed derivatives

In the last lecture we have seen how to derive an approximation for a first derivative of any order of accuracy.

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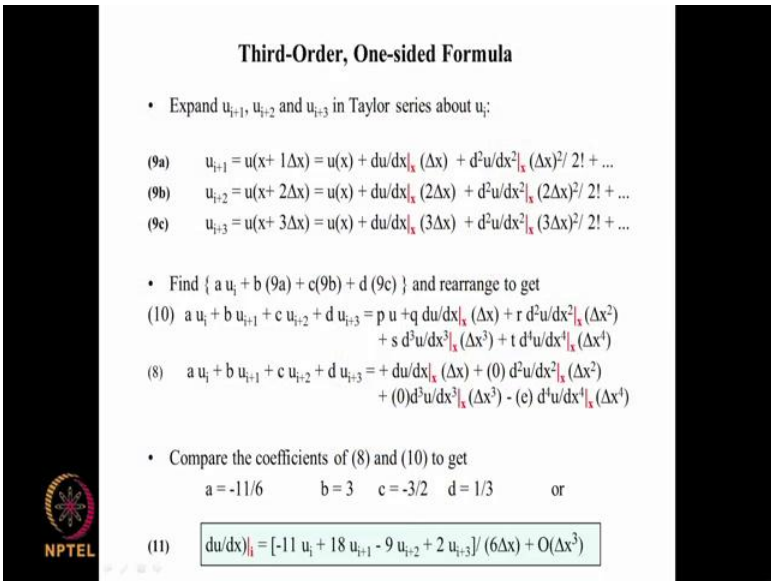

For example we have derived here an approximation for the first derivative at i of third order accuracy involving four successive values of i, equispaced values of the function u at i i plus 1 i plus 2 i plus 3. This is done for a first derivative, but in a governing equation we have not just the first derivatives but also higher derivatives.

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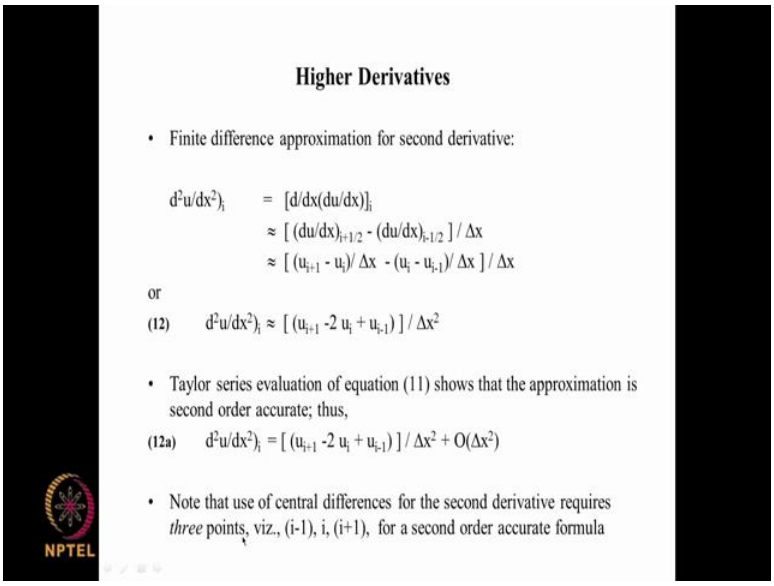

For example we have second derivative. If you have a derivative like dou square u by dou x square and we have to derive a (Refer Time: 00:00) difference approximation for that at that particular point i, then it is pretty straight forward we can write this second derivative as d by d x of d u by d x at i. Now if you call d u by d x as a function f for example, d of by d x at i can be written as d u by d x at i plus half minus d u by d x at i minus half divided by delta x. Now at this stage we are evaluating u only at i i plus 1 i minus 1 i plus 2 like that, we are not actually evaluating at i plus half. So we should not be writing like this, but fortunately this is not for u it is only the value u that is being evaluated at the grid nodes.

We are not yet evaluating u, so we can write this approximately using central differencing because the derivative d u by d x which is our f whose derivatives d of by d x we want at i is being evaluated as function f at i plus half minus function at i minus half so that is on the right side on the left side of the point i, divided by the special distance between i plus half and i minus half is delta x. This is one way of expressing d by d x of f at i where f is d u by d x, so we writing d square u by d x square as d by d x of d u by d x and then we can write this approximation. This is a central differencing approximation.

Now, this d u by d x at i plus half which is midway between i and i plus 1, can again be written in the form of central differencing involving values to the left of i plus half which is u i and to the right of i plus half which is u i plus 1. You can write this as u i plus 1 minus u i divided by the distance between i and i plus 1 which is delta x. So this whole thing is an approximation for d u by d x at i plus half. Similarly, d u by d x at i minus half can again be represented using central differencing around point i minus half, so that is to the left of i minus half is u i minus 1 to the right of i minus half is u i so u i minus u i minus 1 divided by delta x. This whole thing is approximation for d u by d x at i minus half and this whole thing is divided by delta x so we have this divided by delta x.

Now if you then expand this and then bring them together then you have an formula d square u by d x square at i has being given by u i plus 1 minus 2 u i because the delta x is the same and you have minus u i here and minus u i here, so you have minus 2 i plus u i minus 1 this minus and this minus together will give you plus like this, and this is an approximation for the second derivative at point i involving points u i and the point the value of u at grid point to the left of i and to the right of i, so, u i plus 1 u i minus 1 and u i. This is a symmetric difference u by formula, so our central differencing formula for dou square u by dou x square at i.

And in deriving this we have not made anything about to Taylor series and all that. So, what is the order of accuracy for this approximation? If you want to do that then you are writing it like; this you can express u i plus one in terms of Taylor series expansion around point i, you can also put u i minus 1 expand it in terms of u i and derivatives at of u at i and all that around point i, and then substitute them into this and then you will see that the difference between this and the right hand side which is the truncation error is of second order accuracy.

Through Taylor series expansion just like the way that we used here and substituted this in order to get an x of formula of the this type. Now we are going from this formula and substituting into this and then see what are the terms that are coming here and then what is the leading term that is left out. In the in a reverse way we can find out the order of accuracy for any given finite difference approximation for any derivative. We can do that and it is a fairly straight forward thing to do.

So, Taylor series evaluation of equation 12 shows that the approximation is of second order accurate and therefore we can write dou square u by dou x square at i equal to u i plus 1 minus 2 u i plus u i minus 1 divided by delta x square plus terms of the order of delta x square. This is a second order approximation for second derivative. And what we would like to point out here is that this central difference approximation for the second derivative requires three points that is; the evaluation of u at i minus 1 i and i plus 1. Whereas, for the first derivatives central difference required u i plus 1 and u i minus 1, only two neighbouring values.

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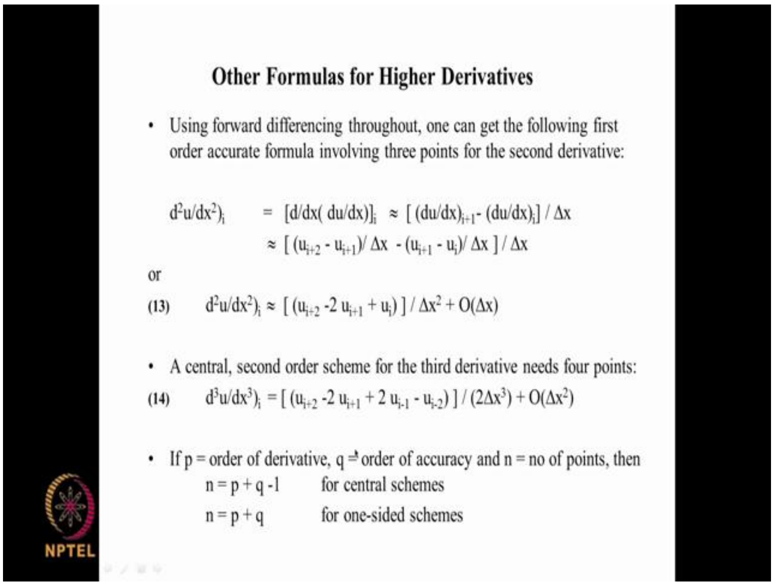

So, we can also have other formulas for higher derivatives it is just not necessarily that this is only way. For example, when we are at the edges of the domain then we may not be able to use central differencing because that there may be no grid point to the left of i, the point where we want to evaluate or they may not be anything to the right side of this. In such a case we had to go for one sided differencing.

So, we are going back to the same old dou square u by dou x square at i, and it is being written as d by d x of d u by d x at i. And that is written now using forward differences. So that is d u by d x at i plus 1 minus d u by d x at i divided by delta x. This is a forward difference approximation of d by d x d by d x of d u by d x at i. F or example, here you have i and you have i plus 1 and i minus 1 and the distance between the two is delta x. Earlier we had this one at i plus half and this one at i minus half so that we made it central, now we making it forward here. Now d u by d x at i plus half can again be evaluated using forward differences at i plus 1 as u i plus 2 minus u i plus 1 divided by delta x. So, this is a forward difference approximation for the first derivative at i plus 1 not at i.

Similarly, this expression here can be evaluated using forward difference as u i plus 1 minus u i by delta x, that we know. The difference between this and this is that this is being evaluate at i plus 1 therefore we substitute for i here as i plus 1, so i plus 1 plus 1 that gives i plus 2 and i plus 1 here. So this whole thing is divided by delta x square. And when you simplify this you get a different approximation d square u by d x square at i is given as u i plus 2 minus 2 u i plus 1 plus u i plus 1 plus u i divided by delta x square. And you can go through a Taylor series expansion or you can say ok I have use consistently forward difference here and forward difference here, so therefore the whole thing is going to be first order accurate or you can do that or you can formally expand this in a Taylor series expansion. And then demonstrate that this is only first order accurate approximation.

So, compare to the previous one where we have a second order accurate approximation for the second derivative at i involving three points here, but this three points are spread on either side. Here we have three points again, but all the three points are to the same side of u i, therefore this can used for example at a left boundary where you have u i minus 1 is not brought into picture. A central second order scheme for third derivative needs four points. So, what we have done here for the second derivative you can also do for a third derivative and one can show derive using similar kind of arguments for example, writing d 3 u by d x 3 at i as d by d x of d square u by d x square at i and then substituting the formulas there. In that way you can do that and then you can come up with formula like this.

Or you can also put this as a u i plus 2 and b u i and all that thing and then we can tried to evaluate the coefficients a b c d by comparison just like u by we have done in the previous lecture, and then come up with the coefficients here. You can see that here you again have for the third derivative at i we have a second order accurate approximation involving four points i plus 2 i plus 1 i minus 1 and i minus 2 and you have i minus 1 i plus 1 and i minus 2 and i plus 2, so that is symmetric around point i and that gives us second order accurate approximation.

So, we can see that as you go from second order approximation you have three points here, and here you have third derivative at the same point second order accurate and you have four points here. The number of points which appear in the finite difference approximation increases as either the order of derivative increases or the order of the accuracy that remanded increases. And it also depends on whether we using one sided or two sided formulas. So there is a general formula that can be derived, that if p is of the order of the derivative and q is the order of accuracy of the finite difference approximation that is preside and n is the number of points that appear in the approximation then n is equal to p plus q minus 1 plus central differencing formulas, and it is equal to p plus q for one sided formulas.

So, if you fix the value of n then a central schemes using the same number of points will be more accurate than a one sided scheme. And if you want more accuracy from the one sided formulas then you have to use more number of points, and more number of points will slightly make your matrix bigger and make the competition slightly higher. But otherwise it is about the same thing. And I would also like to point out here you have this coefficients 1 minus 2 plus 2 minus 1 and this all add up to 0 here. And again here you have coefficient of minus 2 here plus 1 plus 1, so they all add up to 0. So, in all these finite difference formulas on these uniform grids here we get something like this.

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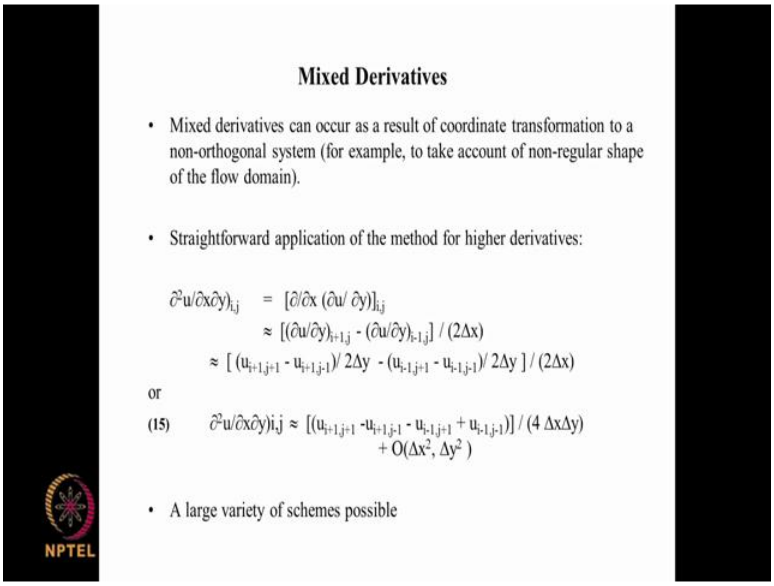

Now, what we have done for the second derivative and third derivative we can also do for a mixed derivative. What we mean by mixed derivative? For example, a term like dou square u by dou x dou y. Since mixed derivative require at least two variables x and y here independent variables we are not talking about a partial derivative dou square u by dou x dou y at point i j.

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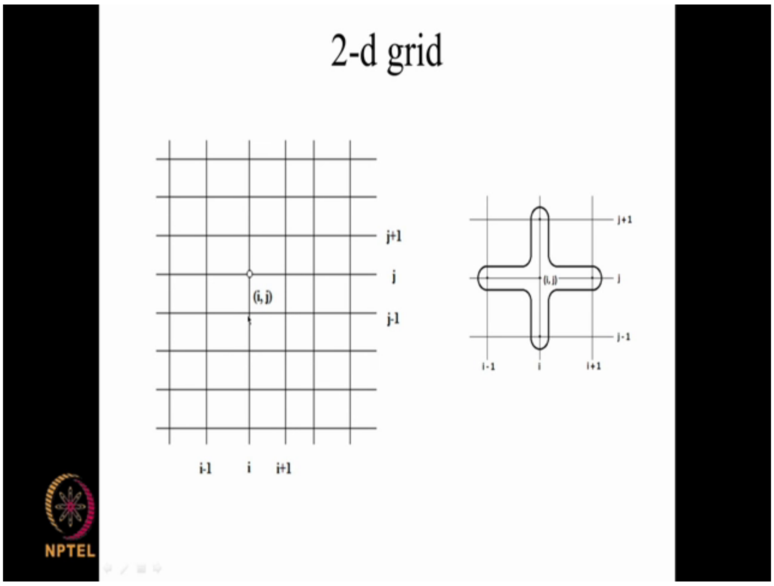

So, we are looking at a two dimensional grid like this, you have x direction y direction and you have delta x delta x. In this case it is more generic with a non uniform spacing here. The coordinate direction x i here all these points have the same x i and all these points have the same y j and the intersection of these defines the point i j here. And this is coordinate line having y j, y j plus 1 and y j minus 1 and i plus 1 and i minus 1 coming here. And so the thing which is surrounding this is given here, you have point i j here and if you have a formula which will see involving these four points then you have a competition molecule like this.

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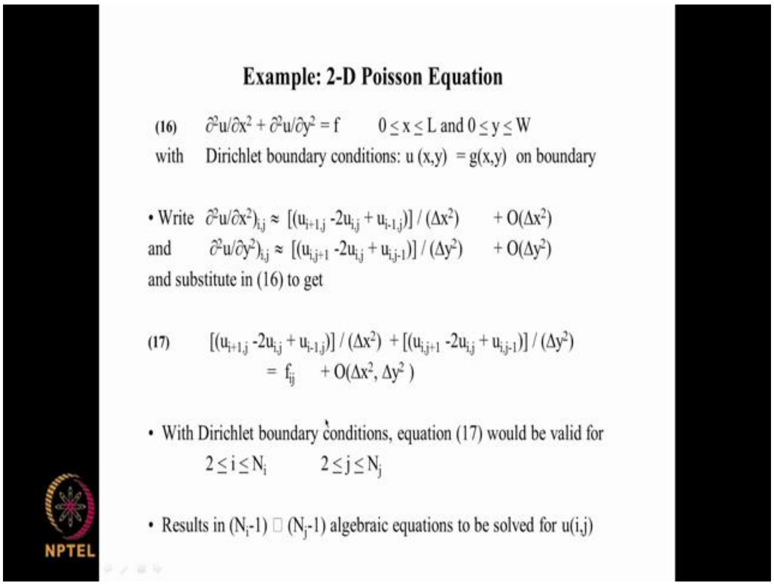

So, we are looking at variation of u in this two dimensional space and we are specifically looking at a mixed derivative like; dou square u by dou x dou y and at point i j, because there are two indices here two independent variables x and y special variations then you initially give i for the index in the x direction and j for the index in the y direction. So using that we can put it like this. And now we can write dou square u by dou x dou y assuming continuous function and all that we can write this as dou by dou x of dou u by dou y at point i j.

So, now we can evaluate this function here which is the variation of this function in the x direction, so we can write this as dou u by dou y at i plus 1 minus dou u by dou y at i minus 1 by j. We are evaluating this function here in its x derivative of this function. So, x derivative means that here we are using central differencing, so we are putting it as i plus 1 and i minus 1, in all the cases j does not change because we are evaluating the x derivative.

So, this is a central difference approximation of u by dou by dou x of this function at point i j, and because i minus 1 and i plus 1 are separated by 2 delta x you have divide by 2 delta x here. This dou u by dou y at i plus 1 j we can again evaluate this using central differences. And this time it is a variation with respect to y that is being evaluated, so we can write this as u at i plus 1 j plus 1 and u at i plus 1 j minus 1 divided by 2 delta y. In both cases i plus 1 remains constant it does not change, because it is a variation with respect to y that being evaluated. And again here it is a variation with respect to y, but at i minus 1 so you have u i minus 1 u i minus 1 and this variation with respect to y, so you have j plus 1 and j minus 1. Again j plus 1 and j minus 1 are separated by a distance of 2 delta y, so you have 2 delta y here.

Now you can simplify all these things and you could be getting an expression as given here, u i plus 1 j plus 1 minus u i plus 1 j minus 1 u i minus 1 j plus 1 plus u i minus 1 j minus 1. So you have i plus 1 j plus 1, if you now go to this particular thing here, so we are evaluating dou square u by dou x dou y at this particular point i j here. For this you have i plus 1 j plus 1 is this point and you have i plus 1 j minus 1 which is this point here and you have i minus 2 j minus 2 and you have i minus 2 j plus 2. So, the four corner points are being use to evaluate this function.

Whereas, when we had dou square u by dou x square or dou square u by dou x square we make use of only these immediate neighbours here not the corner points. The competition molecule for the evaluation of dou square u by dou x dou y the mixed derivative will bring in the corner points. Whereas, if you evaluate the second derivative of u with respect to x or y; if you are evaluating this with respect to x then it is the two immediate neighbours to the left and right will come, if it is dou square u by dou y square immediate neighbours to the top and bottom will be coming here. There is the difference in terms of what neighbouring molecules we introduce to come up with corresponding evaluation approximation for a derivative.

So, this particular feature of mixed derivative, so that is its bringing into play the corner points and not the immediate neighbours, and also the fact that dou square u by dou x dou y the approximation here does not involve the value of u at i j is again potential problem for us when we consider the whole discretized equation, but will get to that later on.

So, there is a large variety of approximation that is possible for a given derivative and for a given order of accuracy. And so we can say that at this stage we know for any derivative that may be appearing in our partially differential equations we can develop a corresponding finite difference approximation of a given order of accuracy. Now at this point we would like to mention that in our navier stokes u by equations that we have return for a Cartesian coordinate system there no mixed derivatives, we have only normal derivatives. Example; in the x momentum equation you have dou square u by d x square plus dou square u by dou x square plus dou square u by dou z square times viscosity is the viscous diffusion term that appears. So, it is always dou square u by dou x square or dou y square or dou z square. Only the normal derivatives, we do not have dou square u by dou x dou y.

But, if we do a coordinate transformation form orthogonal coordinate system like x Cartesian coordinate system or cylindrical (Refer Time: 22:06) coordinate system that kind of orthogonal coordinate system to a non orthogonal coordinate system which may happen in some special cases when we dealing with complex shapes, in such a case we have this mixed derivatives that appear. Otherwise in a navier stokes equation we only have a normal derivatives and the mixed derivatives do not come into picture. So, with this we can claim that we are now in a position to write finite difference approximation for any derivative, and therefore we are in a position to come up with a discretization scheme for a given differential equation.

So, in the next lecture we will do a tutorial on poisson equation. It is very similar to what we have done in the very first week, but will do it again with different boundary conditions just to test our understanding and also to put a knowledge of being able to derive any approximation for any derivative, we will put that into test in the form of a tutorial, that is in the next lecture.