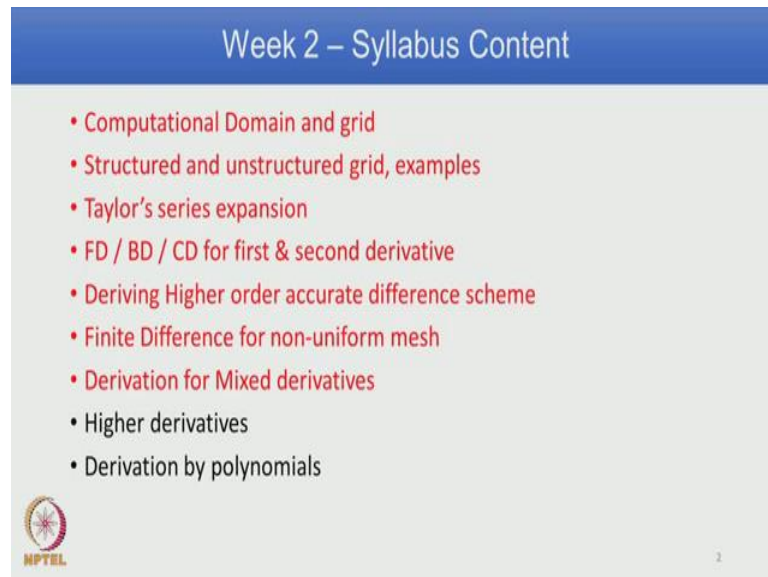


Foundation of Computational Fluid Dynamics
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Lecture - 10

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Week 2 – Syllabus Content

- Computational Domain and grid
- Structured and unstructured grid, examples
- Taylor's series expansion
- FD / BD / CD for first & second derivative
- Deriving Higher order accurate difference scheme
- Finite Difference for non-uniform mesh
- Derivation for Mixed derivatives
- Higher derivatives
- Derivation by polynomials

 NPTEL 2

My greetings to you all, we are now to the last class for this week, which is module five. And so far, we have seen about domain, different types of grid, how to obtain Taylor's series expansion from Taylor series expansion, how to obtain different difference formula and higher order accurate scheme, and how to obtain finite difference scheme on non-uniform mesh. Also obtaining difference formula for mixed derivatives. Now, today's class, we will particularly see how to get higher derivatives and getting finite difference formula by other procedure, particularly we are going to see by polynomial procedure. So, we have seen so far all these.


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Higher Derivatives

We had seen so far

- first and second derivative
- Forward / Backward / Central difference
- Higher order scheme
- Mixed derivative

We also have equations with term **Higher (like third) derivative**



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And we also have equation with higher order terms, for example, if you consider vorticity transport equation or vorticity stream function formulation that we had seen last week. It has a fourth order based on stream function. So, we should know how to evaluate or how to obtain finite difference formula for any order as well.


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Finite Difference Formulations for Higher derivatives

The Taylor series expansion of $f(x+\Delta x)$, $f(x+2\Delta x)$ and $f(x+3\Delta x)$

$$f(x+\Delta x) = f(x) + \Delta x \left(\frac{\partial f}{\partial x}\right) + \frac{\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad \text{Eq.1}$$
$$f(x+2\Delta x) = f(x) + 2\Delta x \left(\frac{\partial f}{\partial x}\right) + \frac{4\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{8\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad \text{Eq.2}$$
$$f(x+3\Delta x) = f(x) + 3\Delta x \left(\frac{\partial f}{\partial x}\right) + \frac{9\Delta x^2}{2!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{27\Delta x^3}{3!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad \text{Eq.3}$$

Multiply Eq.1 by 3 and subtract from Eq.3 we get,



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And this we had seen towards end of last class, we repeat here for the sake of continuity. So, Taylor series expansion it is written for three different spacing, f of x plus Δx , f of x plus $2\Delta x$ and f of x plus $3\Delta x$. By now you are familiar, how to write Taylor

series expansion in any direction that is either forward or backward, you are also familiar with the procedure to get any difference formula. So, writing the equation for three different spacing, x plus Δx , x plus $2\Delta x$ and x plus $3\Delta x$. And what we are interested is the last term that is the third derivative term $\Delta x^3 f'''(x)$, and the term is there in all the three equations, equation one, equation two and equation three. So, we have to do some kind of arithmetic operation, manipulation to get rid of the term first derivative as well as second derivative. So, basically do two arithmetic operation the beginning, considering the equation one and three. So, multiply equation one by three and subtract it from equation three, which is actually for f of x evaluated at x plus three Δx .

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Finite Difference Formulations for Higher derivatives

$$3f(x+\Delta x) - f(x+3\Delta x) = 2f(x) - \frac{3\Delta x^2}{1!} \left(\frac{\partial^2 f}{\partial x^2}\right) - \frac{4\Delta x^3}{1!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad (4)$$

Multiply Eq.1 by 2 and subtract from Eq.2 we get,

$$f(x+2\Delta x) - 2f(x+\Delta x) = -f(x) + \frac{\Delta x^2}{1!} \left(\frac{\partial^2 f}{\partial x^2}\right) + \frac{\Delta x^3}{1!} \left(\frac{\partial^3 f}{\partial x^3}\right) + \dots \quad (5)$$

Solving the above two equations for $\left(\frac{\partial^3 f}{\partial x^3}\right)$ we get,

Multiply Eqn (5) by 3 and add it to Eqn. (4)

$$\left(\frac{\partial^3 f}{\partial x^3}\right) = \frac{f(x+3\Delta x) - 3f(x+2\Delta x) + 3f(x+\Delta x) - f(x)}{(\Delta x)^3} + O(\Delta x)$$

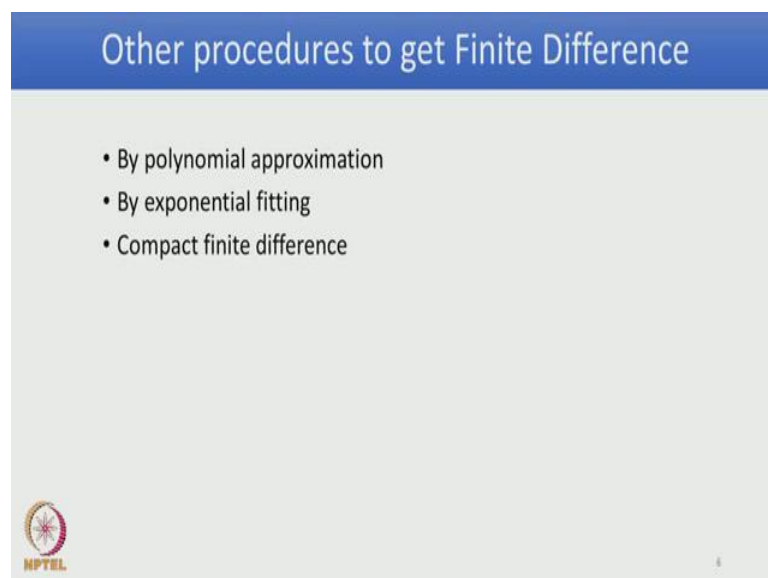
So, if you do that, you get this equation, three times f of x plus Δx that is the first equation and this is the third equation term, so we have a term on left hand side, remaining term on the right hand side. You can actually see term by term and verify this expression is correct, and numbered this equation as four. We do one more operation that is multiplying equation 1 by 2 and subtract it from equation two, so we get f of x plus $2\Delta x$ minus two times f of x plus Δx this is coming from the first equation that is why we have the coefficient two here, so we said multiply equation by two, so we have term on the left hand side, and then remaining terms on the right hand side, and we numbered this equation as five. Once again we have to get only third derivative Δx^3

f by Δx cube is still have the second derivative term in both equations four as well as five.

So, one more small arithmetic operation that is multiply equation five by three and add it to equation four. So, if you do that, so the equation five you have the term Δx square whose coefficient is actually one, so if you multiply this by 3, and added to corresponding term in equation four, they both get cancelled. And finally, you get after rearrangement, finally, you get expression for Δx cube f by Δx cube and which is given here and you can recognize that it requires three additional points in the forward direction with respect to the function value itself, so f of x is the point of interest at unique function values at $x + \Delta x$, $x + 2\Delta x$ and $x + 3\Delta x$.

And this is forward difference formula of order Δx . And you can just follow the procedure as we did for first derivative and second derivative; you can also obtain backward difference formula and this is also possible to obtain either forward or backward higher accuracy. So, in this case, it is of order Δx , you can consider higher terms in the Taylor series expansion replace them, do again arithmetic operation, follow all the algebraic care, it is possible to obtain any order of accuracy and in any direction forward or backward.

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Next, we are going to see another procedure. So, far we have seen how to obtain difference formula only from Taylor series expansion,, but there are also other

procedures, polynomial approximation of a function, exponential fitting procedure, and there is also a different class of finite difference scheme what is known as compact finite differences scheme. So, as the name indicates, you are able to obtain higher order accuracy scheme by considering only less number of points and there is a procedure available to get this higher accuracy scheme by considering only less number points and that is what is given as compact finite differences scheme. We are not going to talk about compact finite difference schemes, we will see how to obtain by polynomial approximation.

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Finite Difference using Polynomials

- Approximating the function f as a polynomial
- Calculating the coefficients by substitution of function values
- Consider a 2^{nd} order polynomial approximating the actual function

$$f(x) = Ax^2 + Bx + C$$

f_i f_{i+1} f_{i+2}
 i $i+1$ $i+2$
 Δx Δx
 $2\Delta x$

So, the way to do is, there are three steps one is approximating the function f as a polynomial; so when you say polynomial the; obviously, question is what degree it is required. So, depending on the degree, the polynomial; obviously, one will get different accuracy scheme, and the polynomial will have expression with coefficients and you can obtain or evaluate the coefficient values substitute in the function subsequently to derivatives then you will get difference formula. So, in this exercise, we are going to demonstrate that procedure by considering second order polynomial and that is shown here, function f of x is approximated by second order polynomial as given here $Ax^2 + Bx + C$. This is your schematic graphical representation of the function; this is the point of interest f of i at i , neighboring points in the forward direction $i + 1$, which is the distance of Δx , and $i + 2$, which is at distance of two Δx from the point i or it is a distance of Δx from the point $i + 1$.

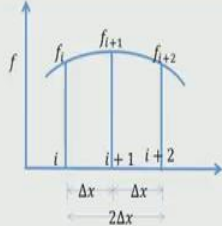
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Finite Difference using Polynomials


Therefore,

$$f(x_i) = f_i = Ax_i^2 + Bx_i + C$$
$$f(x_{i+1}) = f_{i+1} = Ax_{i+1}^2 + Bx_{i+1} + C$$
$$f(x_{i+2}) = f_{i+2} = Ax_{i+2}^2 + Bx_{i+2} + C$$

For $x_i = 0$; $x_{i+1} = \Delta x$; $x_{i+2} = 2\Delta x$



Substituting we get,

$$f_i = C$$
$$f_{i+1} = A(\Delta x)^2 + B\Delta x + C$$
$$f_{i+2} = A(2\Delta x)^2 + B(2\Delta x) + C$$


So, if you evaluate that function that is we have described quadratic polynomial function, evaluate that function at three different point that we have shown i , $i + 1$, $i + 2$. So, the same function is repeated for different nodal points, f of i is $A x^2$ plus $B x$ plus C ; similarly for f of $i + 1$, and f of $i + 2$. Why we want to do this expressing the function at three points, because we have three coefficients A , B , C for the quadratic polynomial that we have consider $A x^2$ plus $B x$ plus C . So, you can immediately get the idea, if it is polynomial with the degree five then you need to get the expression or function value evaluated at five nodal points.

Now, you need to evaluate coefficient A , B , C . So, first what we do, we find out these function values at specific location. Say if we consider x of i as zero, because that is your point of interest then x of $i + 1$ is at distance of Δx , and x of $i + 2$ is at distance of two times Δx with respect to i . So, it is to be clear, it is only at a distance of Δx from $i + 1$, whereas, it is at distance of two times Δx from i . Once again for simplification, we have consider only uniform mesh that is why it is two times is coming here. And next we are going to see how to for non-uniform mesh also. So, if you substitute these values, that is x of i , x of $i + 1$, x of $i + 2$ in this expression, we get three equations for three coefficient A , B , C .

So, on substitution so x of i is equal to zero, first value; you substitute to the first equation A , B will go to zero, remaining term only C and that is directly related to f of i

as f of i equal to C . Then we substitute for the second equation, f of i plus 1 equal to $A \Delta x^2 + B \Delta x + C$; similarly for third equation, $A x$ of x at i plus 2 is replaced with two times Δx and square is there, so it is A two times Δx square plus B two times Δx plus C . So, if you solve, you already have value for C as equal to f of i that is also you can substitute then remaining two coefficients A and B are evaluated by suitable arithmetic operation between these two equations.

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Finite Difference using Polynomials

The coefficients are

$$C = f_i$$


$$B = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2(\Delta x)} \quad \text{and} \quad A = \frac{f_{i+2} - 2f_{i+1} + f_i}{2(\Delta x)^2}$$

$$f(x) = Ax^2 + Bx + C$$

Now, $\frac{\partial f}{\partial x} = 2Ax + B$

At $x_i = 0$; $\frac{\partial f}{\partial x} = B = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2(\Delta x)}$

which is second order accurate forward difference expression



And if you follow that procedure, you get expression for coefficient A and B and that is what is shown here. Coefficient value B as expressed in terms of i plus 2, i plus 1 and i as this way; and similarly for coefficient value A is expressed in this form. Now, come back to the polynomial expression that we have taken, quadratic polynomial function that we have taken, so f of x is $A x$ square plus $B x$ plus C . So, if you substitute values for A , B , C , you actually have function evaluated based on function values in the subsequent forward points. So, you want first derivative, take the first derivative $\text{d}f$ by $\text{d}x$, and do the derivative on right hand side two times $A x$ plus B , C goes to 0. Now, if you substitute for A and B in this expression from this expression that we obtained for coefficient A and B , substitute B and substitute for A into this expression, we get $\text{d}f$ by $\text{d}x$ evaluated at x of i , this is our point of interest. And we already defined x of i to be 0, so the first term goes to 0, and we have only B here, so $\text{d}f$ by $\text{d}x$ evaluated at i is same as B and that expression is here and repeated here for first derivative.

Now, the question is how to know what is the order of accuracy in this scheme, we know from the Taylor series procedure, how to obtain order of accuracy. Now, what we do in this expression, we substitute f of i plus 2 from the Taylor series expansion, similarly f of i plus 1 from the Taylor series expansion, f of i is same that is on the right hand side. And we also know dof by dou x evaluated by different procedure by different order of accuracy and so on. So, we replace dof by dou x and replace all these term in Taylor series expansion and compare terms on either side left hand side and right hand side, finally, you get that this scheme is second order accurate forward difference expression. Though explain, how to obtain the accuracy it is not shown here, what is important is to know that this is second order accurate forward different scheme and you can also recognize immediately, we have consider two neighboring points with respect to i , that is i plus 1 as well as i plus 2. And you can also recognize this expression from the first exercise obtained from Taylor series expansion. Now, we have shown for the first derivative dof by dou x from this polynomial. So, if you do one more time derivative, then you will get second derivative, so $\text{dou square f by dou x square}$ is given here.

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Finite Difference using Polynomials


The coefficients are

$$C = f_i$$

$$B = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2(\Delta x)} \quad \text{and} \quad A = \frac{f_{i+2} - 2f_{i+1} + f_i}{2(\Delta x)^2}$$

$$f(x) = Ax^2 + Bx + C$$

$$\frac{\partial^2 f}{\partial x^2} = 2A = \frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2}$$

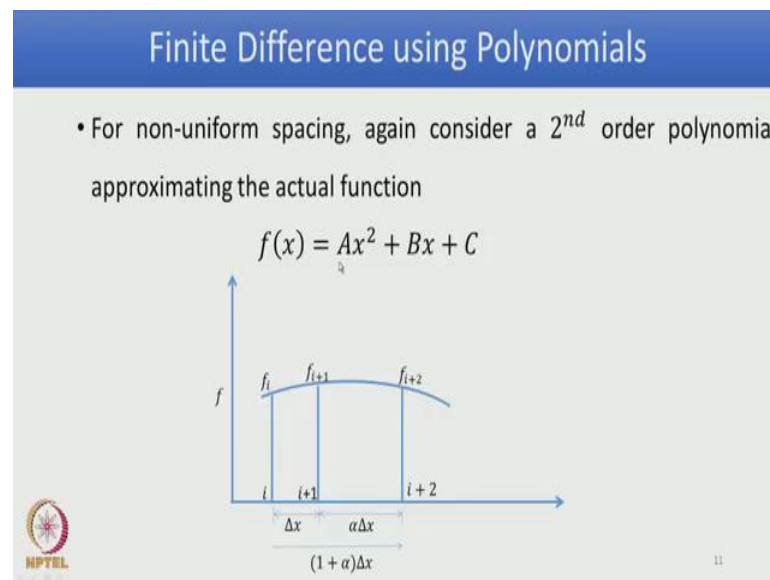

 which is first order accurate forward difference expression

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Do second derivative, so $\text{dou square f by dou x square}$ and that is what is shown here. So, $\text{dou square f by dou x square}$ is basically two times A , because B also goes and A is already here that we obtained coefficient for A , and this two two gets cancelled then we have only the remaining term for the coefficient; A and this is actually the second derivative forward difference formula obtained from polynomial procedure. And once

again we follow the procedure of expanding this function from Taylor series on the left hand side, and obtaining the difference formula from Taylor series and compare the coefficients then you get the idea of order of accuracy of this scheme. And in this case it is first order accurate forward difference scheme for the second derivative.

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Now, we have seen before, we also have a situation of non-uniform mesh, so we should find out how to do by polynomial procedure for non-uniform mesh also. So, function is given, again second order polynomial function $A x^2 + B x + C$. And graphical representation for non-uniform mesh, so i is the point of interest, $i + 1$ is an immediate neighbor point which is at distance of Δx ; and $i + 2$ is the next neighbor point, which is at distance of $\alpha \Delta x$ with respect to $i + 1$, and at distance of $(1 + \alpha) \Delta x$ with respect to i point. So, we follow the same procedure expressing this quadratic polynomial that we have assumed at all the three points then find out the procedure, how to estimate these coefficients A , B , C .

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Finite Difference using Polynomials

For $x_i = 0; x_{i+1} = \Delta x; x_{i+2} = (1 + \alpha)\Delta x$

$$f_i = C$$

$$f_{i+1} = A(\Delta x)^2 + B\Delta x + C$$


$$f_{i+2} = A((1 + \alpha)\Delta x)^2 + B((1 + \alpha)\Delta x) + C$$

We get,

$$C = f_i$$

$$B = \frac{-f_{i+2} + (1 + \alpha)^2 f_{i+1} - (\alpha^2 + 2\alpha)f_i}{\alpha(1 + \alpha)(\Delta x)}$$

And

$$A = \frac{f_{i+2} - (1 + \alpha)f_{i+1} + \alpha f_i}{\alpha(1 + \alpha)(\Delta x)^2}$$

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So, at x of i , which is the point of interest, the function is the x value is zero; and x of i plus 1 is Δx , and x of i plus 2 is one plus α times Δx . Now, if you substitute in function, then we get expression like this, and we already noticed that C is related to f of i itself, and f of i plus 1, and f of i plus 2 are also expressed like this. We are interested to find out coefficient values of A and B , and C is substituted as f of i , now between these two equation, you can solve and get A and B , and you get expression for B as shown here, and expression for A as shown here.


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Finite Difference using Polynomials

Now, $\frac{\partial f}{\partial x} = 2Ax + B$ and $\frac{\partial^2 f}{\partial x^2} = 2A$

Therefore,

At $x_i = 0; \frac{\partial f}{\partial x} = B = \frac{-f_{i+2} + (1 + \alpha)^2 f_{i+1} - (\alpha^2 + 2\alpha)f_i}{\alpha(1 + \alpha)(\Delta x)}$

$$\frac{\partial^2 f}{\partial x^2} = 2A = 2 \left[\frac{f_{i+2} - (1 + \alpha)f_{i+1} + \alpha f_i}{\alpha(1 + \alpha)(\Delta x)^2} \right]$$

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So, we use these values C, B and A, and substitute in polynomial expression that we have consider. And we are interested in the first derivative then it gets reduced to $2 A x$ plus B, if you are interested in the second derivative, it gets reduced to $2 A$. So, substitute for A and B, and substitute for A here, so subsequently you get first derivative evaluated at x of i, because that is the point of interest at i, x will have a zero value, so if you substitute that the term is only B for first derivative and that is shown here. Similarly, for the second derivative, it is two times A, and evaluate, we have already evaluated coefficient value for A, and you substitute we get this.

So, entire week what we have seen important aspect of CFD, the first step that is how to obtain finite difference formula by two different procedure from Taylor series expansion procedure and from polynomial procedure, and first derivative, second derivative third derivative, uniform mesh, non-uniform mesh and how to obtain higher order accuracy scheme and so on.

Thank you.