Computational Fluid Dynamics
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Module - 3
Lecture – 22
Basics of CFD-Finite Difference Methods

Today we will start the third module of this particular course, and in this module we are going to look at numerical solution of the governing equations which we have derived in the second module. We are also going to look at the concepts of Finite Difference Methods which enable us to convert a partial difference equation into an algebraic equation. So, part A of this module which may take about a week's worth of classes is on Finite Difference Methods and how we can make use of this - Finite Difference Methods to find approximations for the partial derivatives that occur in our governing equations.

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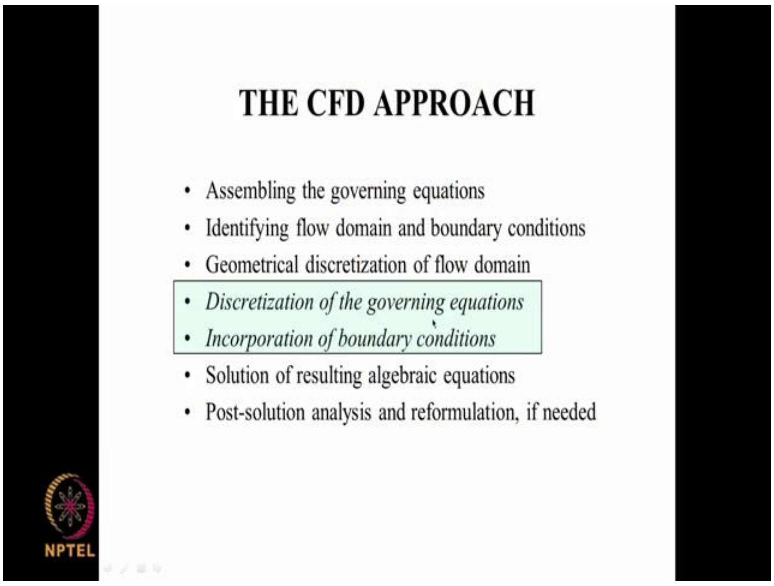

The basic concept of a CFD approach is something that we have a already seen in the very first week, where we tried to calculate the flow through a rectangular that and we saw that day that in those lectures that there are certain steps that we take while doing a CFD solution.

So, first one is assembling the governing equation and then the next is identifying the flow domain and boundary conditions and third is geometrical discretization of flow domain. So, these are the things that we can now say we have some idea about these things and we have seen in the second module what kind of governing equations are there. For example, the equation of navier stokes equation for an incompressible flow constitutes a set of 4 equations with 4 variables.

So, these are supplemented by a flow domain and the boundary conditions and initial conditions that go with it. We have a mathematical problem in which we have enough number of equations to solve for the number of variables and we go into the solution from the formulation of the problem into the solution part. So, we have also noted that these governing equations are coupled non-linear equations and that in the general case there is no analytic solution for these and which is why we would like to do a numerical solution.

So, when we do a numerical solution we go away from trying to define, find the value of phi at any x y z t into defining the value, finding the value at grid points. So, this is where we have this idea of geometrical discretization of the flow domain where we identify, we spread a large number of points throughout the flow domain and at these points we would like to find the flow variables and the flow variables are like the u velocity component, v velocity component, w velocity component, pressure, temperature, concentration, enthalpy, whatever else that is associated with the flow and whatever else that can be derived from these things.

For example, the shear stress, the heat transfer coefficient, the mass transfer coefficient, the net force acting on it all these things are derived quantities that we have a set of fundamental variables - for example, in the case of incompressible flow without any heat transfer of a simple single component fluid. We have 4 equations - the 3 momentum equations and 1 continuity equation, describing the four variables u v w and p. So, we would like to find out the values of these variables at these points grid nodes spread throughout the domain.

So, once we have identified why we want to find the variables and what variables we want to find then it comes to how to do this, how to find these things from the equations that we are giving. So, that aspect of this is what we are going to discuss in this particular part and we make use of finite difference approximations to get an approximate equivalence for the derivatives that occur in the governing equations, and when we substitute this approximations the governing equation becomes a set of algebraic equations. And in the process we also make use of the boundary conditions.

So, we are going to stress on the Discretization of the governing equations on a given grid and Incorporation of the boundary conditions, together; and when we do this together we will get a system of algebraic equations and we will go on to the solution of this algebraic equations later. But the focus of this particular lecture and the coming lecture in this module is on the guiding principles which tell us how to do that discrete, how to write approximations for the partial derivatives using the finite difference approach, and what kind of approximations are admissible, and what kind of approximations are not really the good way of going about it.

So, we are going to look at the two concepts, two steps the discretization of the governing equations and the incorporation of boundary conditions.

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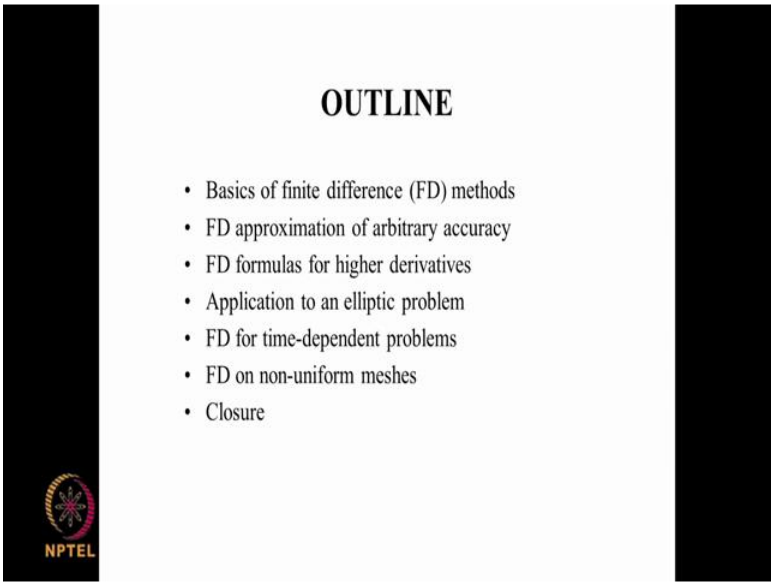

So, the outline for this set of lectures is that we look at the basic ideas behind the finite difference approximations and we also touch up on the idea of deriving an approximation of a given order of accuracy. Because we will see that there is no single unique approximation, there can be many choices and accuracy is one parameter which distinguishes one choice of approximation from another choice.

Obviously, we would like our approximation to be accurate and we would like to need a come up with a method by which we can write a finite difference approximation of arbitrary accuracy. We will see what we mean by accuracy and arbitrary accuracy. And once we do these two things we look at finite difference formula approximations for higher derivatives and we apply these basic ideas to an elliptic problem and then, we see how we can make use of these approximations to convert an elliptic partial differential equation into set of algebraic equations. And then we touch up on time dependent problems which bring in additional complexities associated with writing the finite difference approximation. Finally, we look at finite difference approximations on non-uniform meshes.

So, non-uniform meshes are the once that are practically used, but the basic ideas can be easily understood with a uniform mesh and it is in this context when we talk about geometrical discretization of the flow domain as far as the initial modules are concerned we are looking at simple (Refer Time: 08:17) in mesh. So, that is we have a rectangular mesh with uniform grid spacing in the x direction and y direction and therefore, the boundaries of flow domain are x equal to constant, x equal to constant, y equal to constant and y equal to constant.

So, they can be fit in a rectangular shape flow domain. So, for something like this it is pretty trivial to fit a uniform mesh with a delta x spacing in the x direction and delta y spacing in the y direction. If you know the width divided by a number of intervals that we have will give us delta x and similarly, the height divided by the number of intervals in the y direction will give us delta y. So, using this we can illustrate the basic concepts of finite difference approximations and we can also look at why certain approximations are good and certain others are not good. So, all these things we will discuss in the context of uniform mesh, but we will also touch up on how the finite difference approximations can be derived from non-uniform meshes.

So, once we have gone through all these things we will have a good idea of what kind of finite difference approximations are possible and how these can be substituted in governing equations in order to convert them from partial differential equation into a set of algebraic equations. So, all these will do in part A. But at the end of this part A, towards end of this we will do one simple exercise to apply these concepts to typical problems that we have in a fluid flow and we show that the approximation is not so trivial as it sounds, not so straight forward as it sounds. There is much more that is required to be known in order to come up with good approximation.

So, at the end of that we will have understood what difficulties can arise in writing a finite difference approximation and we will see that all the concepts that we are talking about here will not be sufficient for us to attempt a CFD solution straight away, there can be many pit falls. So, in part B of this will go into the analysis of this discretization schemes and then we see under what conditions we might get good approximation and under what conditions we may not get good approximations, a good approximation which will lead us to reasonably accurate solution. So, that is part B and now we are looking at part A.

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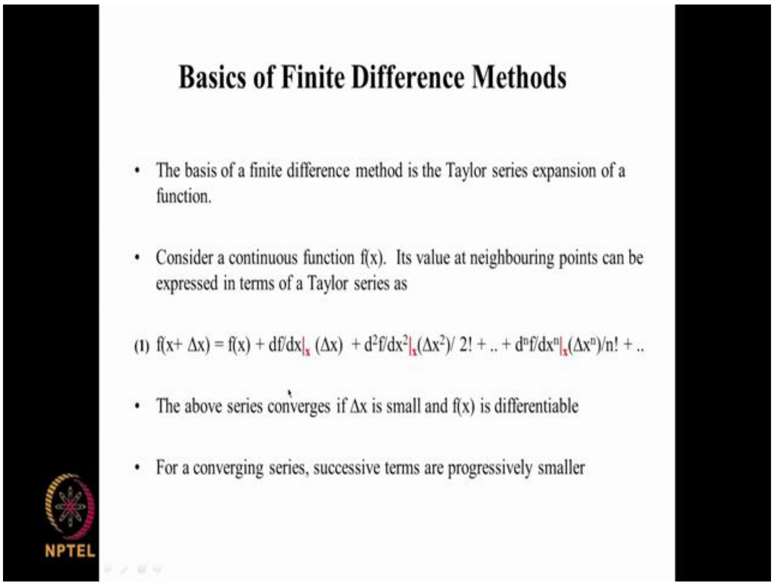

So, the basics of finite difference methods approximations are the first things that we need to know and finite difference methods are quite old not very recent they have been there for centuries and there also what we can say are out dated for CFD applications. The finite difference applications have been more or less over taken by finite volume type or finite element type of approximations because of the additional advantages that arise when we want to tackle non rectangular, non simple geometries. We will see that towards the end of this course.

But one could say that to that extent finite difference methods are dated, but still they are useful even with finite volume method we will see that even when we use finite volume of finite element method. We will have to approximate derivatives and at that point the finite difference approximations knowledge of these things becomes almost essential and even though it is simple and dated and old it serves as a point of departure to understand the concepts of CFD. We do not want to go straight away jump into the real world type of application, we would like to start with some simple things and then build up knowledge and understanding and then tackle the real world problems.

So, it is in that context, studying finite differences is also a point of departure for proper CFD studies. So, the knowledge of finite difference approximation is needed because the principle idea of CFD methods is to replace a partial differential equation which describes the evaluation or the way or the constants on how the variable can vary within our flow domain subject to physical loss. So, to replace that partial differential equation which is difficult to handle analytically and replace that by an equivalent approximation involving finite differences, so that the partial differential equation gets converted into an algebraic equation involving the variable values at this finite positions at this grid points as a variables.

And we would also like to note that finite difference techniques are one of several options for this discretization governing equations, we can have finite element methods, finite volume method is something that we have seen in the second week when we did the (Refer Time: 14:48) of triangular depth. You can also have spectral methods and collocation methods and so many different ways of a solving these things. But in our CFD because we are dealing with a lots of coupled equations and when we are dealing with even more complicated phenomena like turbulent flow, turbulent reacting flows and all that, we have lot more number of equations of different complexity and non-linearity come into picture and in such a case people prefer to stick to finite difference and finite volume methods.

Finite, one would like to stick to finite difference methods, but finite volume methods of what can enables us to solve real world problems and that is where we make use of finite volume methods of fairly low order accuracy, and we make use of the might of the computers to reduce the error to within tolerable limits. With this kind of introduction let us just see what we mean by this finite difference method. So, the basis of finite difference approximation is the Taylor series expansion of a function at a particular point.

So, let us consider a function f of x, it is a continuous function and it is differentiable; that means, that you have continuous derivatives of up to order n what are the value of n is. And the idea of this Taylors series expansion is that the value of function at a neighboring point can be expressed in terms of a Taylor series involving the function f of x at x and that derivative all of which are defined at x. So, the value of the function f at location delta x which is close to the point x is expressed as the function value at x plus the first derivative evaluated at x which is why I put this in red color to emphasis the point that the derivative is evaluated at x, not at x plus delta x, not at similar in between it is evaluated at x times delta x plus.

Second derivative, again evaluated at x times delta x square by two factorial and plus so on plus the nth derivative of x evaluated at x times delta x raise power n divided by factorial n and so on. So, this is a series expansion and this series expansion would converge provided delta x is small and f is a differentiable and all these derivatives exist and they continues.

So, when you have these conditions satisfied then we have a converging series. So, what you mean by converging series is that although this can go to infinity after a certain number of these terms here you have the first term, second term, third term, fourth term like that. After set number of terms the successive term that follow that will become smaller and smaller in magnitude.

So, if you take the 10th term it is likely to be greater than the 11th term in terms of the magnitude and smaller than the 9th term, so that the 11th term is smaller than the 10th and 12th term is smaller than the 11th. So, successive numbers, successive terms and what we mean by term is that the nth derivative evaluated at x the numerical value of that times delta x raise power n divided by factorial n. The value of this whole term in magnitude becomes progressively smaller, so that it does not make that much difference if you add another 50 terms or another 100 terms the cumulative effect of those last after finite number of the forward terms, the first terms is going to be small. In such a case we say that the series is converging.

So, once you have a converging series you can say that a neglect instead of writing this up to infinite number of terms I can neglect the terms that are coming after n number of terms, and what is this n? This is a (Refer Time: 19:53) and it depends also on how small delta x is. If delta x is very small that is, if x plus delta x is pretty close to x then may be the third term itself is going to be very small and you can neglect from third term onwards or delta x is large then may be will take many more times before we can get into the converging thing and the contribution of the higher terms becoming smaller and smaller.

But, if you have a converging series then it is possible to write an approximation for the value of f at x plus delta x in terms of the value of f at x in the derivatives. And we would like to point out again here that all the derivatives are evaluated at x. So, that is this approximation this enables us to extrapolate from knowledge of the function and is derivative at x to the new value of the function at a neighboring point x plus delta x. So, this enables us to extrapolate using knowledge only of the function is derivatives at x. So, that is an important point to keep in mind.

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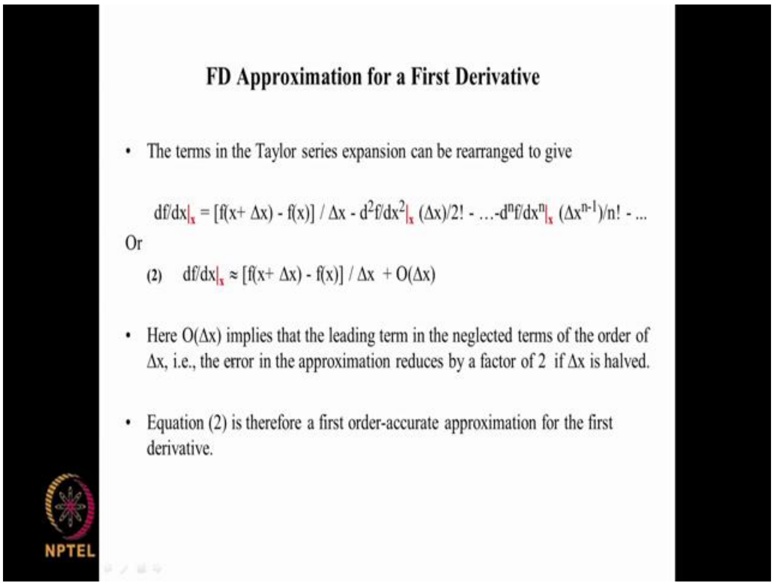

So, now you can derive this Taylor series expansion in this form. We have not made any approximation here, we just plot the df by dx on to one side and then put all the other terms, we have taken all the other terms on the other side so that you have the first derivative at x is expressed is given as f of x plus delta x minus f of x divide by delta x and minus dou square f by dou x square in this particular case you put as d - d square f by dx square at x times. It should have been delta x by two factorial, but since we are dividing by delta x here, one delta x cancels out and then you have delta x factorial two and similarly the nth term in this or n plus 1th term in this is nth derivative of f with respect to x evaluated at x delta x raise power n minus 1 divided by factorial n and so on.

So, now here we can say that we can look at this expression here as a possible approximation for the value of the derivative that is dou f by dou x can be roughly written as taking only the first term here that is f of x plus delta x minus f of x divide by delta x. And if you take only this part here you are only taking the essentially the first two terms in this. So, writing an approximation for this in terms of these two terms and we are neglecting all these things, it is a gross simplification. That if it would be OK, if delta x is small. It would be OK, if the higher order derivatives are very very small that is, if f varies smoothly then higher and higher order derivatives will have very small values and this value is going to be anyway small and is going to multiplied by this delta x raised power n here and delta x is small.

So, the contribution of this will decrease not only because you are raising the power of a small value and not only because you are in dividing by a factorial of an increasing number, it also because the derivative itself is a small value. So, in a smoothly varying functional space it is possible for us to make this gross kind of simplification and then neglect the contribution of all these things and then write an approximation like this.

If a fluid flow in many cases involving fluid flow and for example, temperature thermal diffusion type of problems we expect a smooth variation, in such a case it is not such a bad thing. So, to that extent although it is a gross simplification it is a feasible simplification, it is an admissible simplification provided that delta x is small and f varies smoothly with x. So, in such a case we can write this formula here as giving an expression approximate expression for dou f by dou x which is a derivative of f with respect to x and this is what we want to find an approximation for.

So, we can write it as f of x plus delta x minus f of x divide by delta x plus this thing here this is a technical jargon which says this terms or the order of delta x and lower and in a way higher order terms. So, what this means is that in this equation you have this term here, this term here, this term is there and from here onwards we are neglecting all these terms. We also have said that this is converging series and in a converging series the higher order terms here will be progressively smaller. So, the leading term, the term with the largest magnitude will be the first term which is neglected in theory provided delta x is small and f is smooth.

And this term, it depends linearly on delta x. So, that is why this is what we mean by an order of approximation here. So, this means that terms of the order of delta x are the terms which are being neglected here and because delta x is small this is going to be delta x square, we expect this one to be smaller than this. So, in that sense this is the leading term and the dependence of this term on delta x indicates the order of the approximation. So, we can say that this is a first order approximation for df by dx at x and expressed in terms of the value of f at x and the value of f at a small distance delta x.

So here, order of delta x implies the leading term in the neglected series of terms or the truncated series is of the order of delta x and it means that arrive in the approximation will become will reduce by a factor of 2 if you reduce delta x by a factor of 2. So, if delta x is halved then the approximation error in the approximation will reduce by a factor of 2. So, equation 2 here is therefore, a first order accurate approximation for the first derivative at x. So, the same idea can be expressed.

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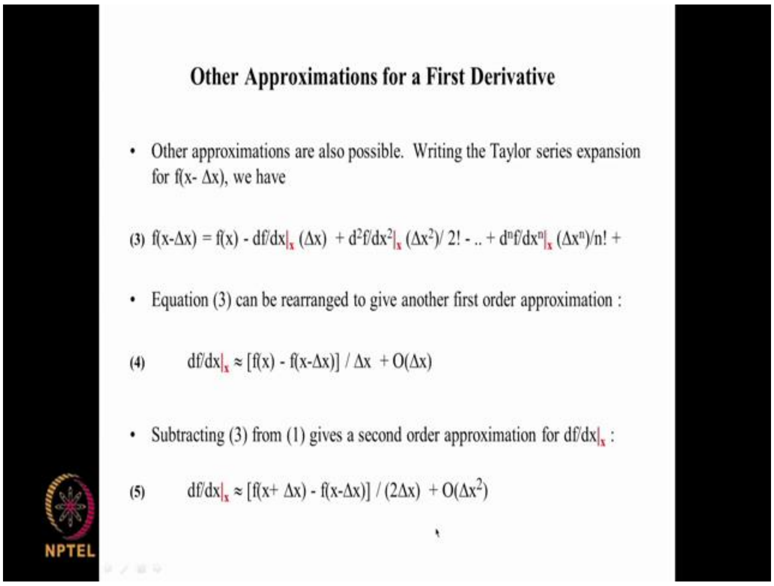

We can also go back to the equations and then write other approximations for example, writing the Taylor series expansion for f at x minus delta x. So, that is to the left of it instead going forward in the x direction it going backward in the x direction, you can write f of x minus delta x as f of x minus df by dx again at x time delta x plus d square f by d x square at x delta x square by 2 like that. So, this thing here has to multiply by minus 1 raise power n here. So, it is not always plus it is alternating as minus plus minus plus minus plus like that and that depends on whether this delta x to the power n here when it is square, it is even power then it is plus odd power it is negative. So, multiply this by minus 1 to the power n. So, that will give us the sign of this particular term here.

So, in this case because delta x is negative here it is going to be a alternating like this and we can do just like what we have done, we can bring this to the left hand side and take this to the right hand side. And then we can write df by dx at x is equal to f of x minus f of x minus delta x divide by delta x this is here and then all these other terms will be d square f by d x square times delta x square by delta x. So, you have delta x by factorial 2 and all that here.

So, again the leading term in this approximation is again of the order of delta x, is this term greater than the other term or it is exactly the same in magnitude, in this particular case it is going to be added and in the other case it is subtracted. And it is same thing because we are looking at the functional second derivative at x which is the same in both cases and delta x also the same. So, in that sense the same error is being introduced here it is being added here and subtracted there. So, in terms of the error it is same thing whether it is this or that, but if the delta x is different than; obviously, the error value will be different.

So, this is different approximation involving f of x and f of x minus delta x. So, if you know the value of f at x minus delta x then you can use this to evaluate their derivative and if you know the value of f at x plus delta x and x then we can make use of this. So, both are possible and we can also derive other approximation. So, you have this approximation here given by equation 3 for f of x minus delta x, and you have equation 1 which is f of x plus delta x and if you subtract equation 3 from equation 1 then what we get is f of x plus delta x this f of x will cancel out, the second derivative term will cancel out and this becomes plus 2 df by dx and so on and that will give us a different approximation.

So, df by dx again at x is given roughly as f of x plus delta x minus f of x minus delta x by 2 delta x plus terms of the order of delta x square, because the leading term here that this term will cancel out and you have d 3 f by dx 3 at x times the delta x cube by factorial 3 divide by delta x, divide by this 2 delta x here. So, that gives us delta x square.

So, the leading term in this particular case is delta x square, that means that this approximation is such that if you reduce delta x by a factor of 2, if you halve delta x then the error will reduce by the factor of 4. That means that this approximation 5 given by equation 5 is better than this approximation, because you can reduce the error faster with the second order accurate approximation as compared to the first order accurate approximation. So, we can derive many such approximations.

In the next lecture, we will put these things together and we will see what they mean and then we will move on to further applications of this. We will look at how to derive an approximation for a first derivative or any derivative of any given accuracy.