Introduction to CFD
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Module - 1
Lecture – 6
Methods for Approximate Solutions of PDEs

In this lecture, we would start discussing about the different methods for approximate solution of partial differential equations.

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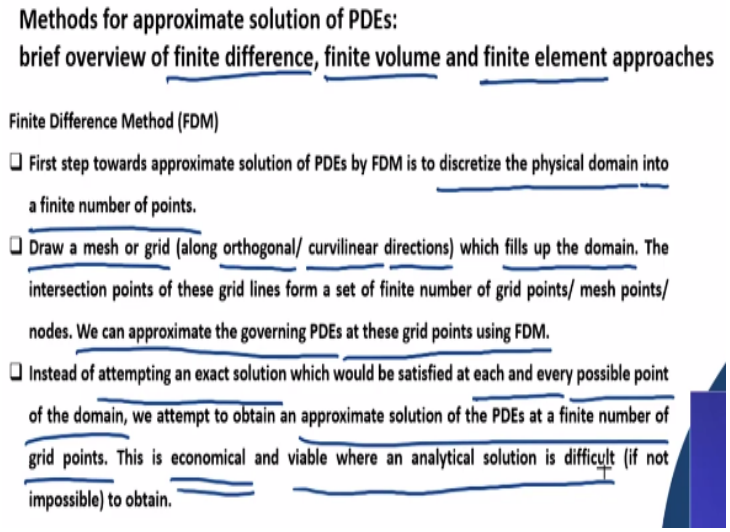

Over the next few lectures, we will discuss about the different methods of approximation which are quite popular and they include very important techniques like finite difference, finite volume and finite element techniques or approaches. To begin with, in this lecture we will discuss a bit of the finite difference method. In finite difference method we take a few steps to explain how the method actually works.

Here we discretize the physical domain into a finite number of points to begin with and then we approximate the derivatives of dependent variables at these points that we have defined. In order to generate the points, we draw a mesh or a grid. This mesh or grid covers the entire domain over which we are trying to obtain the approximate solution of the partial differential equation or system of partial differential equations.

These mesh or grid lines may or may not be orthogonal. So, when they are not orthogonal, we refer to them as curvilinear mesh or curvilinear grid. It is essential that the grid or the mesh covers the entire domain of interest. This filling up of the domain is a spatial activity. So, we have a certain region in space which we are trying to fill up and therefore we are discretizing, we are using some kind of mesh points to discretize it.

However, this concept also applies when we are trying to discretize time. So you can also split up a finite span of time into a large number of segments and then any specific point of time in that overall span of time would mean a certain grid point, but that grid point has a time meaning associated with it. Thus a grid point may carry meaning both in time as well as space combined.

So, the basic exercise over here is that we have a certain region in space or a certain region in time that we are discretizing into different point wise information that we are seeking and these points are essentially the grid points. Most often however, when we say mesh or grid, we mean its spatial implication. We can approximate the governing PDEs at the grid points using finite difference method.

And what we essentially do is we write down the governing partial differential equations where derivatives are approximated. There could be other methods of approximating partial differential equations, where we may be approximating integrals instead of derivatives. However, in finite difference method, we try to approximate derivatives. The important part over here is that we are not attempting an exact solution.

We would be satisfying the governing partial differential equation or equations only at a select few points rather than at each and every possible point of the domain. So, if we had an exact solution to the problem, it would mean that that exact solution would be valid at any point within the domain. This point could be quite arbitrary, but the moment I make that point specific, I can always get the solution of the equation at that specific point.

However, the moment I use an approximate approach, I may not have the solution available at each and every point of the domain. I will have them available only at the points which I have defined where this approximation exercise will be carried out. So I will have the solution available only at these so called grid points. This of course is going to be economical

and this is also the only viable approach where analytical solution of the partial differential equation is not available or may be difficult to obtain.

And then it depends on how many grid points we may end up defining for ourselves to solve the problem. If we have lesser number of points to handle, it will be more economical. If there are more points, obviously it makes the computation more costly.

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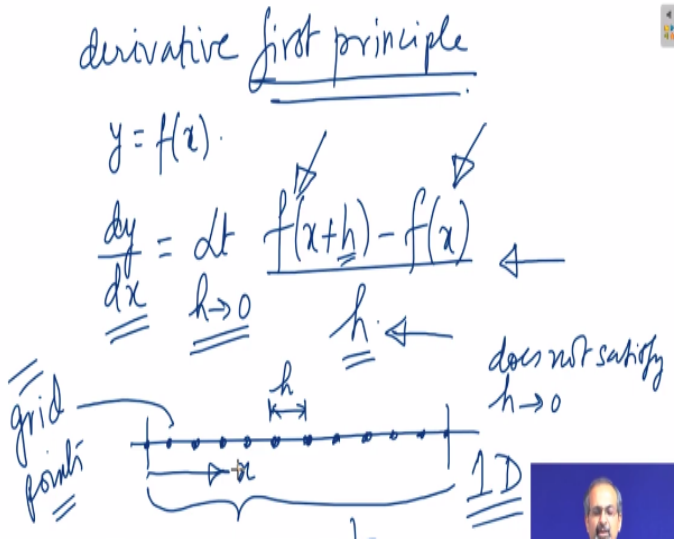

In your first lessons in calculus when you learned to obtain the derivative from first principle, you took a function y = f(x) and then you tried to define dy/dx as a limiting operation.

$$\frac{dy}{dx} = \underset{h\to 0}{Lt} \frac{f(x+h) - f(x)}{h}$$

This is how you calculate the derivative and then the 'h' that you use here limits to 0, which means it is a very, very small distance, infinitesimal distance away from the point x, where we are trying to obtain the functional value.

Then subtracting it from the functional value at the point x and dividing it by that small distance to obtain the derivative. We are saying here in handling partial differential equations, we would approximate derivatives. Now how would we approximate them? If we were to use the above definition, then it would be exact, but that would be extremely costly. Very large number of points, almost infinitely large, would have to be used in order to accommodate such small distances like h.

So, in finite difference approach, instead of doing that, if we have a certain length over which we have to approximate a partial differential equation, we put in a discrete number of points. These finite number of grid points fill up that space and the distance between these points can still be named as 'h', but this 'h' certainly does not satisfy the condition that h tends to 0.

If it did, then these gaps would have to be made extremely small and then you would have to put in almost infinitely large number of points to fill up that finite length. That is what we essentially do when we calculate the derivative exactly. However, for finite accuracy computations, we approximate and therefore we cannot have that many number of points.

I was talking about grid points earlier. These are the points which we would call as grid points and here the domain is a one-dimensional domain. So, I am just concerned about one direction along which I lay the grid points to discretize a certain length L. You could happily accommodate grid points in multiple directions to cover up two-dimensional or three-dimensional spaces. Here, we are restricting it to one dimension to begin with.

Now, if we are not able to accommodate this kind of accuracy, which the limiting operation gives us, then what best can we do about it? So, that is basically the idea behind approximating the derivatives in a finite difference method.

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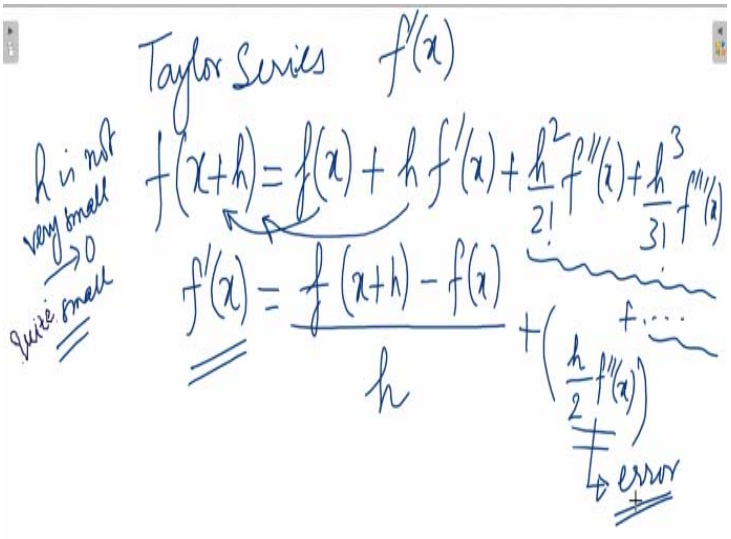

We will make use of Taylor series in order to answer this question that how best we can approximate the derivative. If I were to ask this question that can I write down an expression

for f(x + h) where h is not very small such that it tends to 0, but it is quite small, in fact as small as we can make it, without making the whole exercise too costly for us. The f(x + h) could be written as

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x)$$

and more terms to come because it is an infinite series after all.

From this equation, can I have an estimate of the derivative which I am looking for which is nothing but a $f'(x)$ and I am trying to compute the derivative at the point x mind it. For that, I need a small rearrangement to be done here. I can write it like this. What have I done over here? I have written an approximate expression for $f'(x)$ by transposing terms to the left hand side, dividing it by h so that I can have an expression for $f'(x)$.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \left(\frac{h}{2} f''(x)\right)$$

But then I am left with more terms here which also have to be divided by 'h' and then they all figure over here. So, if you look at what is left you can see that there will be terms, to begin with you will have a term like this

$$-\left(\frac{h}{2} f''(x)\right)$$

and there will be more terms coming later. So, what are these terms going to do? These are actually going to contribute to the kind of error that you are committing in order to approximate the derivative.

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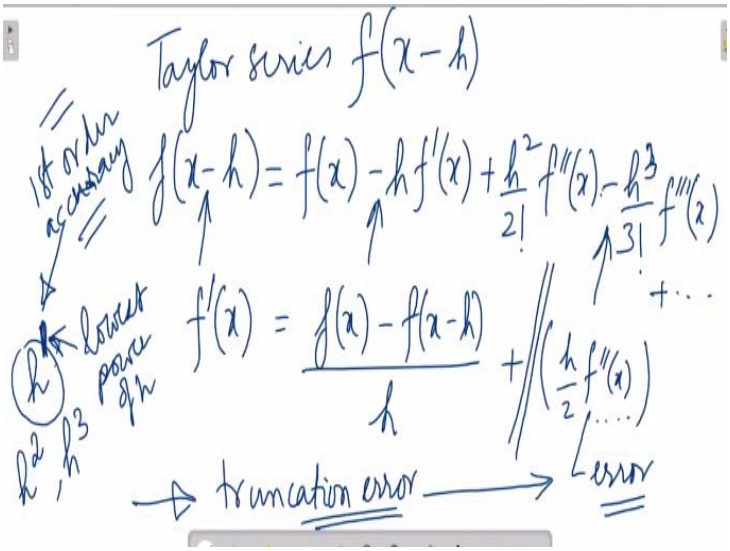

You could have used the Taylor series to find f(x – h) as well. Remember that here because you have a negative sign, there would be terms with alternate negative and positive signs in the Taylor series expansion.

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x)$$

So how do we approximate the derivative $f'(x)$ here using this Taylor series expansion? We could do it like this

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \left(\frac{h}{2} f''(x) \right)$$

and then again you will be left with some terms which look like this.

$$\frac{h}{2} f''(x)$$

These are the terms which will account for the error because we are not going to explicitly incorporate them in the approximate derivative expression. These terms will be left out from the expression of the derivative because we truncate the derivative expression here and therefore, because we truncate, we will call this as truncation error. As a consequence,

infinite number of terms are left out, which we cannot approximately represent or we would not like to represent to avoid complexity.

However, they would contribute to error and these terms account for the so called truncation error. We have to keep in mind that the first term in the enormous number of terms that are left out is the most important contributor to the error. Why is it? Because the first term contains the largest contribution in terms of the 'h', which is the small distance. The first term here has an index 1.

You can very easily figure out that the next term would have an index 2, the subsequent term an index 3 and so on. Now, 'h' is a small number. So, when you raise it to larger and larger powers, the value it will attain will become smaller and smaller. Therefore, the term with the lowest power of 'h' will contribute most to the errors. That is the whole idea behind identifying the first term in the series that you are leaving out as truncation error.

And that term will essentially decide the so called order of accuracy of the approximation that you are applying. Here, the index of the 'h' term happens to be 1 and therefore we have first order accuracy. If you had an index of h = 2, it would be second order accuracy. In general, our intention is always to look for approximations which have higher order of accuracy. The idea behind that is if you have higher order of accuracy, in general you are able to capture finer details of the function's variation with x.

Since you have y = f(x), it means that as x changes y will also change. Now, there could be regions where y changes very rapidly with small changes in x. Again, there could be regions where x variations even in large amounts do not create very large variations in y. A higher order scheme will end up capturing the very rapid variations of the function with small changes in x more accurately than the lower order accuracy schemes with the same set of grid points.

This is the primary motivation behind obtaining schemes with higher order accuracy to approximate a derivative. This is a very basic concept, which needs to be understood when we are discussing about the finite difference method.

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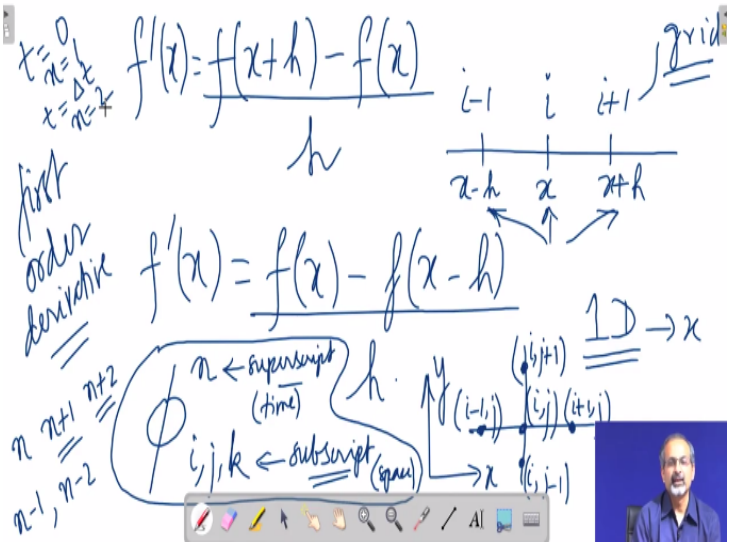


You may be wondering that the kind of approximation that we did would mean that you have different possible versions by means of which you can approximate the derivative. So, we already looked at two of them. This means that there could essentially be infinite number of ways by which you can obtain a particular derivative at a certain point in space and these are only two possible ways of doing it.

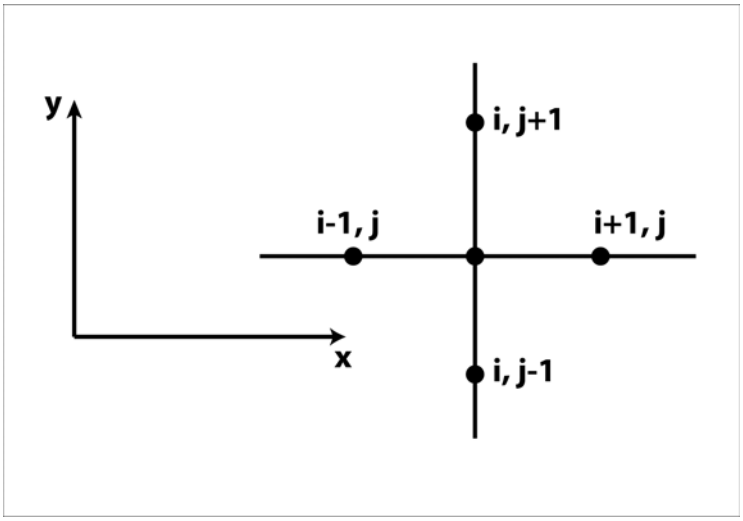
$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

Again, here we have obtained approximations of first order derivative. There could be higher order derivative approximations possible. Again, here we mean that this is essentially in an ordinary derivative sense. Very often you could also apply these principles to approximate partial derivatives. All those concepts could be developed gradually, but now the interesting point that needs to be understood is that we were talking about grid points.

While we have not identified them apart from the fact that we were at a point x and we have moved to two neighboring grid points (x-h) and (x+h) as we were approximating the derivative at the point x. So, in terms of distances or locations, these are the informations where those points are located, but usually when we try to indicate grid points, we use indices. For example, I have only one dimension to tackle over here that is the x direction.

I can use one index let us say ‘i’ to indicate a certain location. Its neighbor could then be called as (i+1) to the right, (i–1) to the left. This is the typical grid nomenclature which we follow, indicating points in space using a very simple way or simple nomenclature, a single letter i or j, and if it is a neighboring point, it could be (i+1), (i–1) when it is one-dimensional space. In two-dimensional space, you could have something like this.



So, when I am looking at it in (x,y) plane, I would say that a certain point would have two indices i, j and then if I move along the x axis to its neighbors, I write them as (i+1, j); (i–1, j) and when I am moving along the y axis, I would write them as (i, j+1); (i, j-1). Usually these are put in brackets. You can very well imagine that this can get extended to three-dimensional space, where you would need three indices to indicate the x, y and z directions.

This is the spatial part of the problem. You could also be talking about time as a possible direction and then you could be using indices to represent different time instants. Like I said that we are talking about space discretization, we can similarly talk about time or temporal discretization. So, a finite span of time can be discretized into different moments, where we are taking snapshots of certain events at different instants.

And those events could be given some indexing in terms of time. Very often, when we are talking about solving problems where both space and time are involved and the dependent variable could be something like ϕ, then the spatial representation of ϕ would be taken up by

using suffixes like i, j, k or rather subscript, I am sorry subscript would indicate spatial information and superscript to indicate time information.

$$\phi_{i,j,k}^{n}$$

This is a very common way of representing the information. So, you can figure out that you can have different instants of time, which are represented as n, (n+1), (n+2). These are yet to come, these are future events: (n+1), (n+2). You may have been computing for some time whereby you have accumulated time wise information and therefore you may already be having information about (n-1), (n-2) and so on.

When we start computations for example at t = 0 and proceed, we start from initial conditions and then we try to look at how the dependent variables' variations come up with time and space. In that case, t = 0 may be marked as n = 1 (initial time step) and then when we move to the next time instant, which is a small time away, then that could become n = 2 and so on. So, like we can march in space, we can also march in time.

And in many problems of fluid mechanics, these marchings would have to be taken up simultaneously. We will discuss more about the finite difference scheme in our later lectures. Thank you.