CFD APPLICATIONS IN CHEMICAL PROCESSES

Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Week-03

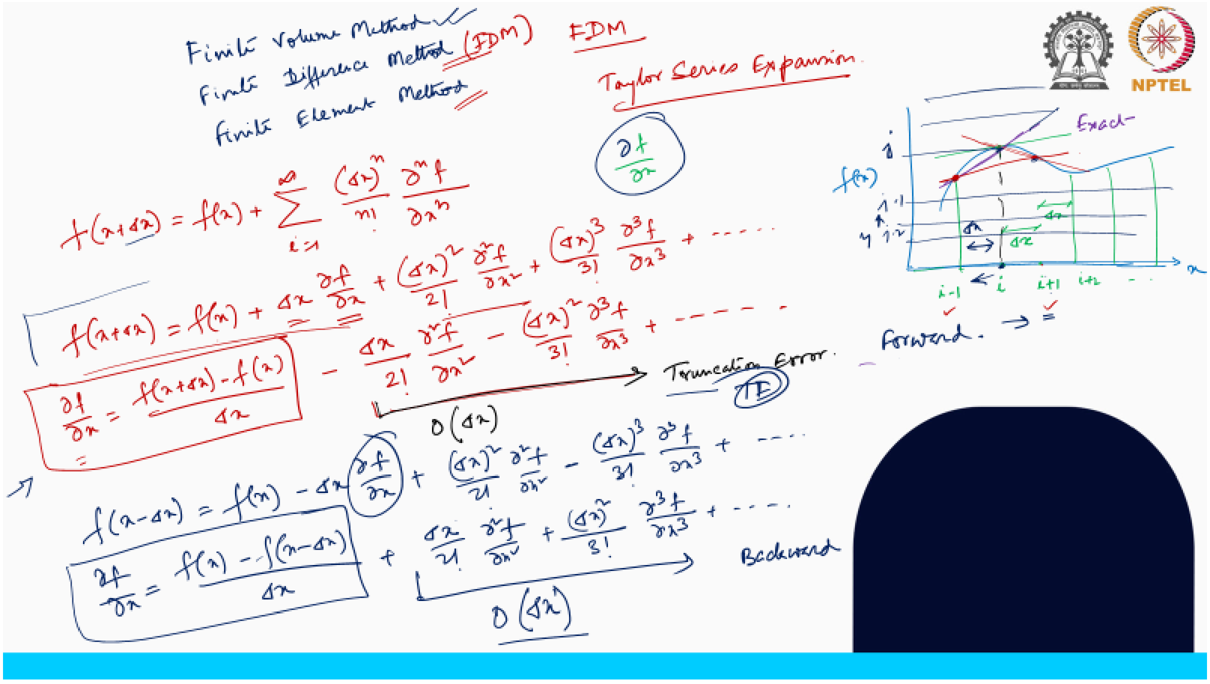
Lecture 11: Numerical Methods for CFD

Hello everyone, welcome back once again with another lecture in CFD applications in chemical processes. In the last class we discussed a bit about the finite volume method. We just introduced the finite volume method, but before going into the details of the finite volume method. Let us look into the other numerical methods that are popular specially the two other methods I will mention. There are several other methods in fact, say for example, to name those these names you have already heard in my lecture finite volume method.

finite difference method finite element method there is other methods are there, which we will not discuss here because several other special methods are available. For example, boundary element method, different more specialized methods are available. But we will mainly focus on these popular three methods that are used to discretize the partial differential equation or say to simplify the partial differential equations that we find in our governing equations to a set of algebraic equations and then we go for solving those set of algebraic equations now again as I told you in this course we will focus or we will go into the details of this finite volume method for which we had small introduction just an glance

Today we will see what is the finite difference method. This finite difference method is very popular. You may have come across already. So this is to brush up your memory that how it works. And we will also touch upon very briefly on the finite element method. Now the point is all these methods have their pros and cons. To start with finite difference method, it is the simplest to implement. People used it regularly until a few years ago.

But then these advanced methods come, that is the finite element and the finite volume method. And how those are different from the finite difference method, we will try to have a look at it in this class, in this lecture. so if we start looking into the finite difference method which is the FDM so finite difference method you have already seen as I told you in the heat conduction problem solution particularly in the unsteady state case so the point is that the for a domain we consider discrete points and by finite difference approximation we simplify the derivative terms and that comes from the Taylor series expansion. So the basics of finite difference method lies on the concept of Taylor series expansion.



So consider, say we have a function, we have a function like this. So if this is f and this is variation of x, And say we have to find at a particular location which is say at x = i. So, say at this location we have to find out the gradient of it. So, which means if we have to find out this thing. now to do that what is done is that we consider several points say for example to understand it at the first point in a simplest way we consider say these are the points which are δx spaced that means, equispaced and this point we consider as (i +1) and this is (i – 1).

So, similarly this is (i + 2) and so on. Now, the point is If we have to find the gradient at this point, what we usually do? We draw a tangent on it. That would give us say

the exact value of this. So, for a simple function we can get this $^{\partial f}/_{\partial x}$

and we can find out the exact value of this gradient. Now, by finite difference method as we are approximating this derivative to a set of to a equation that is in the form of algebraic equation.

Now, while doing so as the term says that this is the approximation and that brings in the error in modeling which we have to minimize in order to close the gap between the exact solution and the numerical predictions or the numerical estimation. Now, the point is if we consider say one point at the left of point i which is (i – 1) and if we try to approximate this curve or this function. How we do that? We can connect these two by say this line like this ok. So, using a point on its left side, I can find an approximate value of this gradient.

Similarly, if we use a point on the right side, then the approximation goes like connecting these two points something like this. So, both of these neither close enough to the exact solution. It is not capturing the exact value. But the point here is that if you make this δx very small enough then it goes closer to the exact estimation or the exact value. Your numerical estimation goes closer to the exact value. The third way that can happen

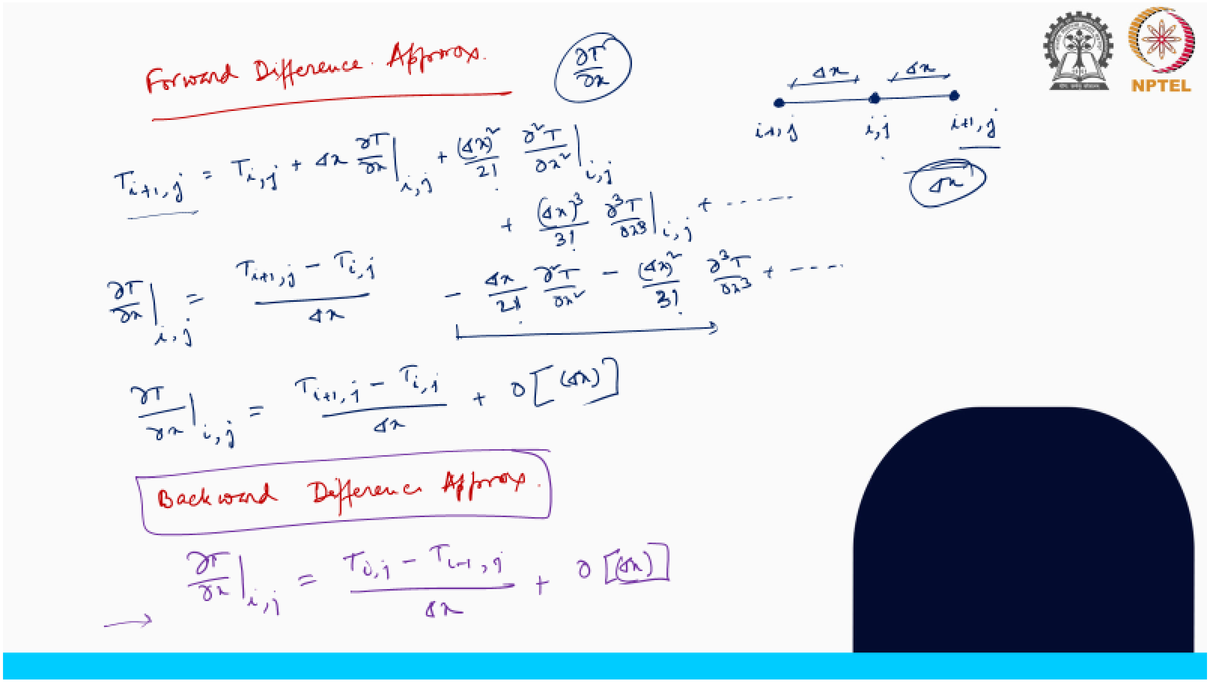
is that if you consider these two points that instead of one left and the point or in the other case one right point and the concerned point which is point i if we consider one point left and one point right that means (i – 1) and (i + 1). these two point if i connect it actually gives a similar value or more closer value to the exact solution. Now why this happens? We will see by this Taylor series expansion. That what is the science behind or why this is happening that now I have the similar slope that is with the exact tangent to that or the exact value due to the tangent at that point. So when we expand a function across or around the point say this point I which is $f(x + \Delta x)$ by Taylor series expansion this is essentially (i = 1) to say infinity. The thing becomes is that δx to the power n factorial n. Which means if I now explain this, this is the more compact form, what will happen is that f of x plus delta x factorial 2 factorial 3 plus the higher order terms. And by approximations or by understanding this gradient which is in the limit of del x tends to 0 if we do that then what happens is that now if you look at this expression and if you try to find out that the gradient on the right hand side what you have is that

This term that we have already written I can write from here because I have taken this term on the left hand side ok. So, the first term minus second term divided by Δx here that I have gotten to understand this value of del f by delta x. minus because the sign has changed it has come on the left hand side. This term is getting divided by Δx. So what we have here is again minus factorial three and the term on the higher order term.

So, here what we have done is that we have taken This first three term into the consideration to find out the value of del pi by del x. And here what we have x plus delta x minus fx divided by 2 and the other term that we see. So if we approximate this gradient by this value or this term only then we are neglecting all the terms starting from here. and that introduces our truncation error. Because we are truncating any term starting from Δx ok.

So, in this case we say with this approximation that del pi del f by del x is equals to this term has an accuracy in the order of delta x which is the first order accuracy. So, as your delta x values increases your truncation error increases if you make a small this points or difference between these the gap of this particular width delta x smaller and smaller, your truncation error reduces and you go nearer to the exact solution or goes closer to the exact solution. Similarly, if we expand or if we write this function by Taylor series expansion.

This also shows such expression. here we will have minus just replace this delta x by minus delta x and you have this similar expression like this and here by doing so which means we are coming a point so with this expression that we have done here x plus delta x if it is our point of concern around which we are finding the gradient So, x plus delta x means the i plus 1th point. So, function of x plus delta x means basically the fx at i plus 1th point. if the similar expansion we do, but taking a point on the left hand side which is f x minus delta x this is also delta x, but on the left hand side.



So, we are considering x minus delta x then the truncation then the expansion is in the this form. And now again if we will focus on this term So, then it becomes fx minus f of x minus delta x divided by the delta x plus factorial So, here again we have a similar expression, but on the backward side of the point of concern. So, in future again we will discuss when we will discuss the finite volume method such discretization.

Again, discretization means the approximation of the differential term to the algebraic expression. This is, we have done taking a forward point from the i plus 1, from the i towards i plus 1. So, this kind of discretization we call as the forward differencing or the forward discretization. and this is the backward because we have gone on the left hand side towards i minus 1 and this fx minus delta x is essentially the fx at x is equals to i minus 1. So, now once you have this

So these are basically the approximation of connecting the backward point and the point of concern this line. This one is the forward one is the connecting line between the i plus 1 and the point i which is this line. And as I told you if the delta x is not sufficiently small we will see that such kind of measured deviation from the exact solution for del x by del x which is the actual gradient at point i. And this also from here since we are truncating this also introduces this truncation error Due to the Taylor series expansion. Omission of the higher order term.

We are omitting starting from the delta x. So this also has the accuracy. The model prediction accuracy will have the first order accuracy. We are omitting from delta x values onwards. So, if you have understood this then comes that what will happen if I take i plus 1 and the i minus 1 point and connect this and find that this is. far better than the corresponding forward or only backward the standalone values and this when that happens we call that as the central differencing scheme we will come to that but before that if we try to have this say instead of f now we try to relate that with some variable

to practical variable to understand that how it is implemented in the problem. Say for example, the temperature. If we have to find out the temperature or the temperature gradient del t by del x at a point i j. So, this is the i. Similarly, if you start connecting this lines or if you draw such lines where in the y direction and this points is say this point as you as we mentioned is the jth point. So, all this becomes j minus 1 j minus 2 and above these are the j plus 1. j plus 2 etcetera.

So, based on these coordinates we actually designate that this is say the i j point. Now, the first order forward differencing. So, now, since the first the reason order we are mentioning is that due to the truncation error. the amount of error introduced due to truncating the Taylor series expansion and from where we are truncating this. So, this backward and forward differencing scheme or the differencing approximate here the approximations that we have made are the first order approximations.

So, now if we try to say find out that what is happening for a real case say a practical variable if I consider that say 3 points equispaced points to understand it better that I have this point as ij this is i plus 1 j and this is i minus 1 So, this distance is essentially delta x a one dimensional case. So, here we try to find out what is this delta x by delta del t by del x. So, based on our previous understanding or previous derivation that we have seen if we consider forward difference approximation

then what we can write is that T i plus 1 j essentially is T i j plus delta x at i j plus the higher order terms. You have seen mostly we are our governing equations even in Navier Stokes equation the terms are going up to the day 2 x by the second order derivative terms del x square. So based on the Taylor series expansion for the forward difference approximation we can write t i plus 1 j as this expression and then again if we try to find out what would be my approximated value. yeah the higher order terms which means

T i plus 1 j minus T i j divided by delta x plus I am truncating all the values starting with the first order terms. So, my approximation by forward difference approximation scheme for the delta T by del x is I is T i plus 1 j minus T i j divided by the delta x. Similarly, if you do this for the backward difference approximation, you would land up So, if you do this for the backward difference approximation, you will land up with the approximated form, which is t ij minus t i minus 1j divided by delta x plus this form. So, one by the forward difference the other by the backward difference. I hope at least the forward difference approximation is clear to you based on this previous Taylor series expansion on the forward and the backward case.

Try to do this for the backward difference approximation again since this is brushing up your old memory. This you have already done in maybe couple of places. I hope you will be able to reach to this expression. If not we will start our next lecture from here. So with this thank you for your attention. We will see you with the next lecture. Thank you.