CFD APPLICATIONS IN CHEMICAL PROCESSES

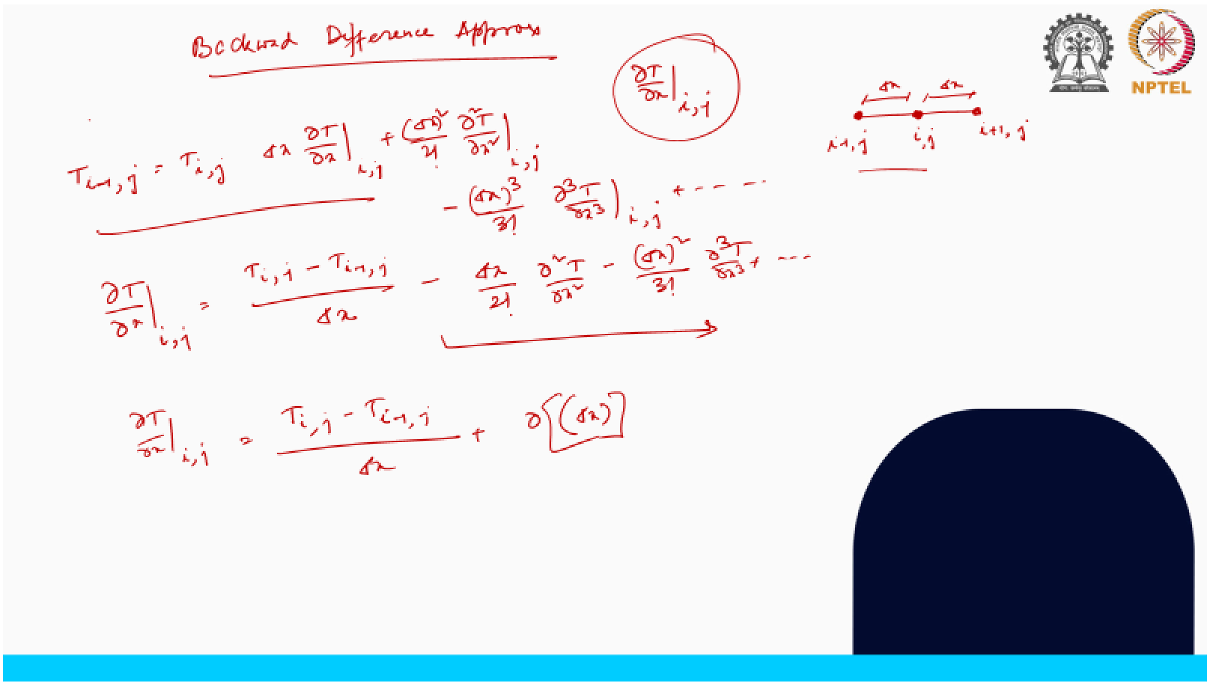
Prof. Arnab Atta
Department of Chemical Engineering
Indian Institute of Technology Kharagpur

Week-03

Lecture 11: Numerical Methods for CFD

Hello everyone, welcome back with another lecture on CFD applications in chemical processes. We were discussing some numerical methods in CFD and specifically in the last class we discussed about the, we were discussing about finite difference methods. So, in the finite difference method, as I have explained earlier, we can have two different approaches. One is the forward differencing scheme. We can have the forward differencing and we can have the backward differencing approach.

Now I have shown you this expression how we derived the forward differencing approximation for the del T by del X. Now for the backward I expected you that you would come up with this expression similar to that. If not, it is very simpler. Let me just show you how that can happen. backward difference approximation. So, there for the same or the similar points say equispaced.



$T_{i-1,j} = T_{i.j} - \Delta x \frac{\partial T}{\partial x}\Big] + \frac{(\Delta x)^2}{2!}\frac{\partial^2 T}{\partial x^2}(x = i)$-......

the higher order terms which I we are neglecting. Now, the point is again similar to our previous this is essentially equals to if we consider this part that becomes T ij minus T i minus 1j divided by delta x and this would be divided by the delta x all the other terms.

So, this will be and we are neglecting from here. So, essentially the thing that I showed last time that we are arriving plus all higher other term including the delta x. So, which means we can approximate this gradient based on either forward or the backward differencing scheme. Now, the other thing that can happen is that is that if we consider the central differencing scheme which means if you remember in the in this slide when I told you that when we consider this i minus 1 and i plus 1 connecting line that is more closer to the exact solution the slope of it is the more closer to the exact solution and the reason behind it.

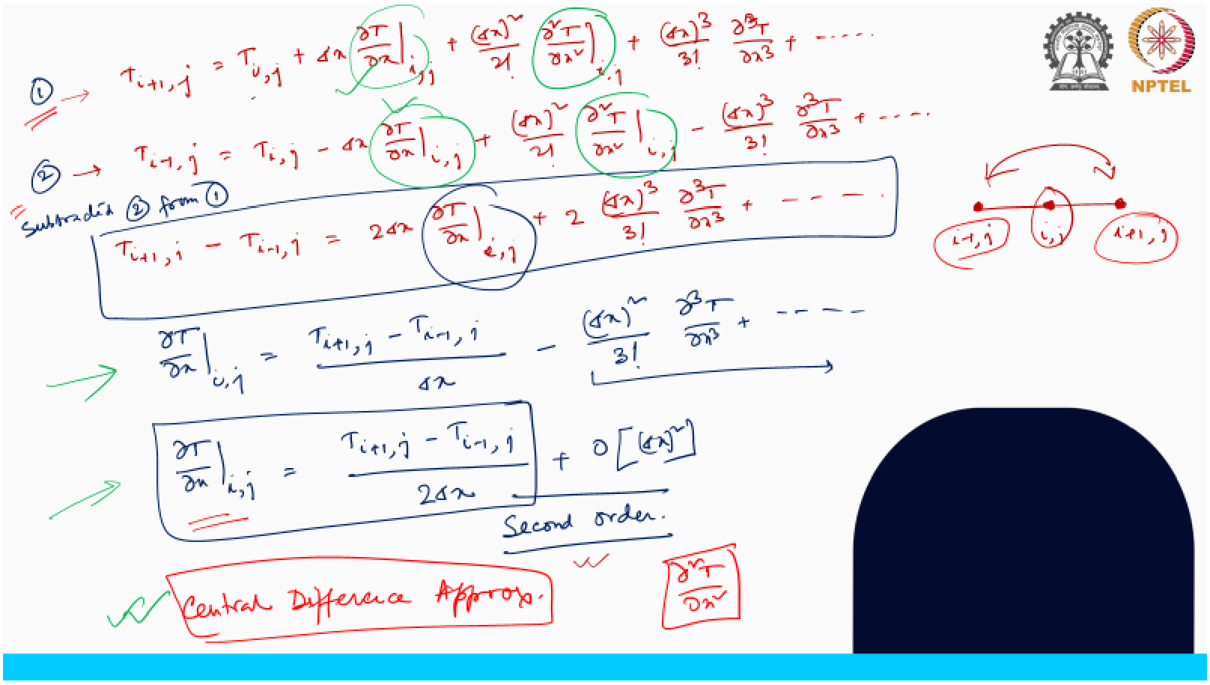
Why this is happening? Because what is happening here is that we had this expression this T i minus 1 j and in the forward we had this expression T i plus 1 j. Let us rewrite those two equations once again. So, T i plus 1 j is essentially T i j plus delta x at ij plus delta square factorial 2. This is the thing that we have seen earlier, factorial

plus the higher order terms and t minus 1 j was So, if we subtract the second one this second x equation from the first one what we get is that t i plus 1 j minus t minus 1 j is equals to 2 times delta x ij plus 2 times del x cube factorial 3 x cube plus so on. So, what we did? We have if we say this is equation 2 and this is equation 1, 2 from 1. Then we get these expressions because then this is eliminated, this first term vanishes, similarly the third term vanishes, similarly the fifth and so on, it would result in this form.

Now, from here from this expression if you look at this expression from here you can also find out another approximated form, but this one including i plus 1 and the i minus 1 jth point divided by 2 delta x. Now, since it has come on the left hand side this would be the negative sign factorial 3 plus the other terms which means. is essentially T i plus 1 j minus T i minus 1 j divided by 2 times delta x plus we are truncating now the term that is having del x square which means it is of the second order accurate. So, second order comes from that point onward we are truncating to approximate this derivative del t by del x around i j as this point. So, again do not forget the three points that we had.

So, i j i plus 1 j and this is i minus 1 j. so now we are finding del t by del x for at the point i j including these two points these two neighboring points one in the forward directions the other one in the backward directions now you can relate with this expression or in this example that we are or we are connecting now because that relation if you look at it, it is again a simple straight line expression to find the gradient between the two points is connecting one forward point which is i plus 1, 1 is the i minus 1 and we received of expression which is of second order accurate. Now that means, since the delta x is supposed to be smaller and as much smaller as possible for the computational ability, it is becoming more accurate because as delta x is smaller you are basically truncating lesser important terms. If it is of first order accurate, then you are including some significant terms.

But in the second order accurate term, it is more accurate in terms of prediction accuracy than the first order approximations. And that is why this, now this strategy is called central difference approximation. So, we had backward forward and when we take two adjacent that means, i minus 1 and i plus 1 point we had the central differencing approach. So, what the point that we have now this is the first order derivative we have approximated Based on the similar thing now say instead of because as I told you even in the Navier-Stokes equation when you have to approximate or simplify that in terms of algebraic equation by the finite difference method you have to approximate this term or such term the second order derivatives.



Then Navier-Stokes equation is not with the t, it is with the u, the velocity profile. But the point is that such second order derivative and with respect to temperature here that terms becomes $\frac{\partial^2 T}{\partial x^2}$. This term also you have to approximate like this you have done for the first order case. And if that is the case then if you look at once again the equation 1 and equation 2 what we have done here we have subtracted the equation 2 from equation 1 to arrive at this expression. Now, all this is on the Taylor series expansion form and then truncating as per our requirement

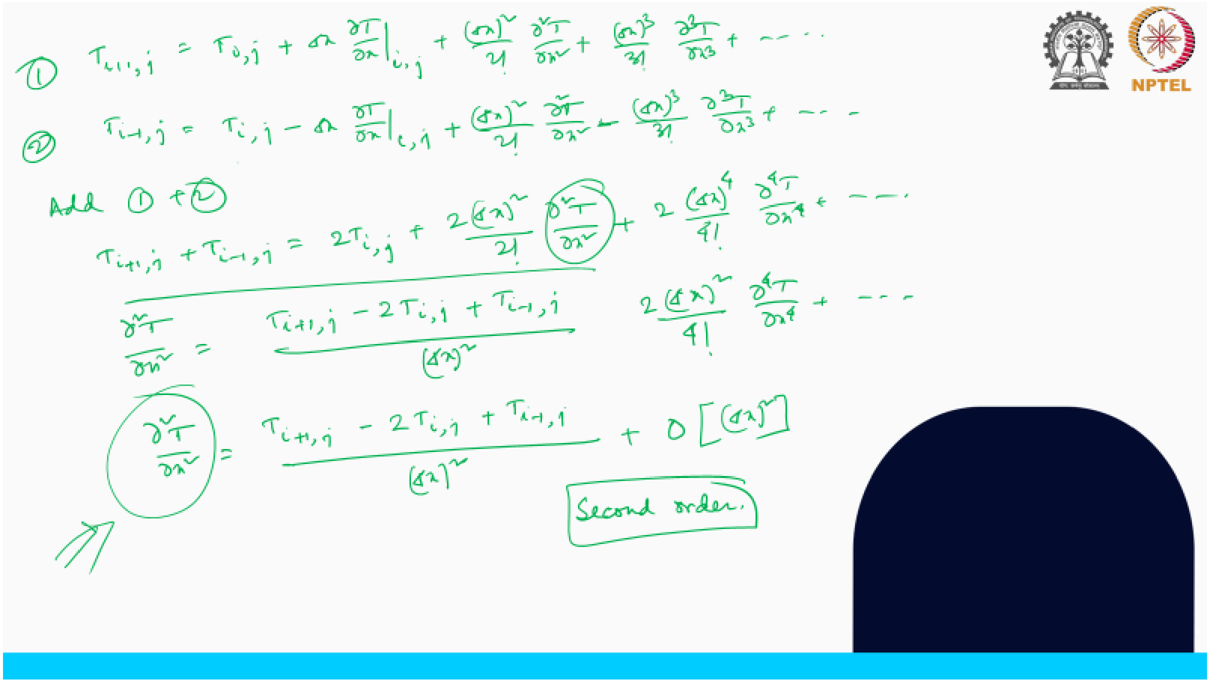
Now, if instead of subtracting if you add these two equation. So, what will happen if you add these two equation because what we are trying to eliminate or what we are trying to estimate here is the approximated form of this term by subtracting we actually eliminated this term. while arriving at or focusing at these terms. So, when these terms are important we subtract it or when we try to focus on it, but now what we are doing is that we are adding these two. So, now these terms this del x by del t by del x would now vanish.

because we are adding equation 1 and an equation 2 ok. So, what will happen if we add these 2 terms? So, if I once again quickly write those and add So, the point what will happen is that T we had T i plus 1 j is equals to T i j plus delta x del x. So, let me quickly write those once again factorial 3. T i minus 1 j is T i j minus delta x. So, this was my equation 2, this was my equation

So, if I now add these two, what will happen is that T i plus 1 j plus T i minus 1 j is plus 2 times to the power 4 by factorial 4 by T x 4 etcetera. So, now our focus is to approximate this or find approximation for this value and that becomes T i plus 1 j minus once we take it on the left hand side and try to isolate it T i minus 1 j and rearranging this divided by delta x square. If we rearrange this part

And, then what is left is that 2 times this x to the power delta x to the power 4 would be divided by delta x square. So, this term will be like this plus the other terms which means is t i plus 1 j plus 2 t i j plus t 1 minus i 1 minus i minus 1 j divided by delta x square plus we are truncating essentially the second order terms. So, this is also once again as the second order accurate central differencing approximation or the central difference approximation or we can say central differencing scheme for the second order derivative. So, I hope this is clear that how we are approximating it

and to apply this thing now to say a steady state heat conduction equation. So, what we have done here, we have seen what is the forward difference approximation, what is backward difference approximation, what is central difference approximation for the first order derivative, for the second order derivative, ok. Because this till this second order derivative we have any governing equation that we can find while solving this CFD problems.



So, we will restrict our discussion till this point on the approximation and if we see that how it is now applied for say steady state

heat conduction equation. So, for steady state heat conduction equation the governing equation is equals to 0. So, how the points or the nodal points that we have discussed that would be, but because now we have two dimensions. So, for the sake of simplicity let us consider that this is delta x equispaced this is delta y consider uniform grid which means delta x is equals to delta y. if that does not happen then we have non-uniform grid and our development of this process becomes a bit slightly difficult.

although it is a very simple problem you can find its analytical solution to compare with this finite difference approximation result. But the one of the drawbacks of the finite difference method is that it is sometimes difficult it is it is difficult when there is non-uniform grid it becomes complex to implement but still it is fairly easy to implement than the other methods the problem becomes when we have irregular shaped bodies or irregular shaped computational domain this computational domain what that is we have discussed earlier so for the irregular shaped bodies and irregular shaped geometries there it becomes difficult to fit these equispaced or even non-equispaced cells or the meshes that we like one of the example is that we will see for this example that in this case what we have is that say this is i j plus 1 this point is i j minus 1, this is i j, this is i plus 1 j, this is i minus 1 j. So, in case it is non-uniform, then we define usually aspect ratio, grid aspect ratio by some term.

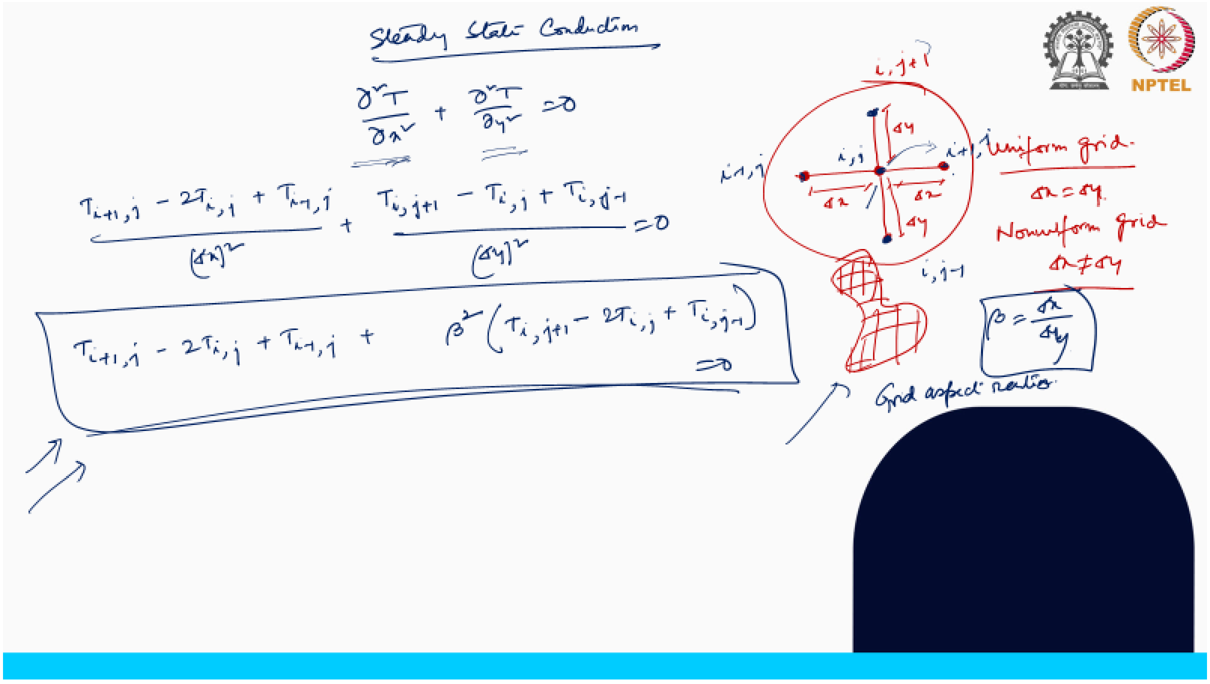
say we can define we will not define alpha because here in conduction that alpha stands for the thermal diffusivity. Let us say we call this as the beta which is the grid aspect ratio, but for the uniform grid delta is equals to delta y ok. So, now, based on our previous understanding what we require is the approximation of this term or the and the approximated form of these two terms del 2 x del 2 t by del x 2 and del 2 t by del y 2. So, what we can write here? We can write

if we consider our previous form that is T i plus 1 j minus 2 T i j plus T i minus 1 j divided by delta x square. So, we will write it here. T i plus 1 j minus 2 times T i j plus T i minus 1 j divided by delta x square. Similarly, for the second term this is del 2 T by del y 2 here what we can write in the analogous form It is now in j plus 1 t i j plus t i j minus 1.

So, j i plus 1th point j i minus 1th point divided by delta y square is equals to 0. which means T i plus 1 j to T i j plus T i minus 1 j plus delta x by delta y square which is I can write as beta square because we have defined that as the aspect ratio. So, we can write beta square multiplied by T i j plus 1 minus 2 times T i j plus T i j minus 1 is equals to 0. Now, this expression you can see this is the algebraic expression for i j.

which is I say the point of attention or the point of focus. On this point we approximated this second derivative touch. Now, the point is once you go from ij point, if now your i plus 1 j point becomes your point of attention or there you have to again approximate these expressions. In that case, when your attention focuses from this point to here, this point becomes i and jth point and this one becomes then your i minus 1 j. And, similarly you will find a set of expressions like this for all the nodal points.

Nodal point means these points that we have highlighted that i j i plus 1 j i minus 1 j i j plus 1 i j minus 1 these are the nodal points. So, in these nodal points what we have These expressions, a set of these expressions for those many points you have in the domain. So once you have this set of algebraic equation, you can then go for solving it by some appropriate method. We will not discuss those solution methods here.



Because those you can find it in any classical mathematics books, mathematics books, advanced mathematics and all. Because those are now setting how to solve a set of algebraic equation. It can be solved directly, it can be solved iteratively. Now those methods to name a few is that say for example Gauss-Seidel method, Gauss-Jordan method etc. Several methods are there and those we consider at this point say those are say trivial process.

But our aim in this course is to understand this algorithm that how this set of these equations that we can derive or we achieve. Because once we have this set of equations, we have some standard solver in MATLAB, in several other cases that we can solve a set of algebraic equations. Now here also in finite difference method in the next class we will touch upon the fact that what is implicit and explicit formulation. Because that these things these terminologies are also relevant in the standpoint of finite volume method. because this is the development in terms of chronology you can think of that the finite difference was there and then people find out difficulty in having this kind of irregular shaped body as the computational domain to be considered by finite difference method it becomes very complicated in such cases if you have uniform grid sizes

regular shaped body where you can fit that body with this grids of finite difference then it is the easiest method to implement and get the result. But also as I told you there for the unsteady state cases there is implicit and explicit formulation. In the next class we will take up that. So, for now Thank you for your attention and hope to see you with the next lecture. Thanks.