CFD APPLICATIONS IN CHEMICAL PROCESSES
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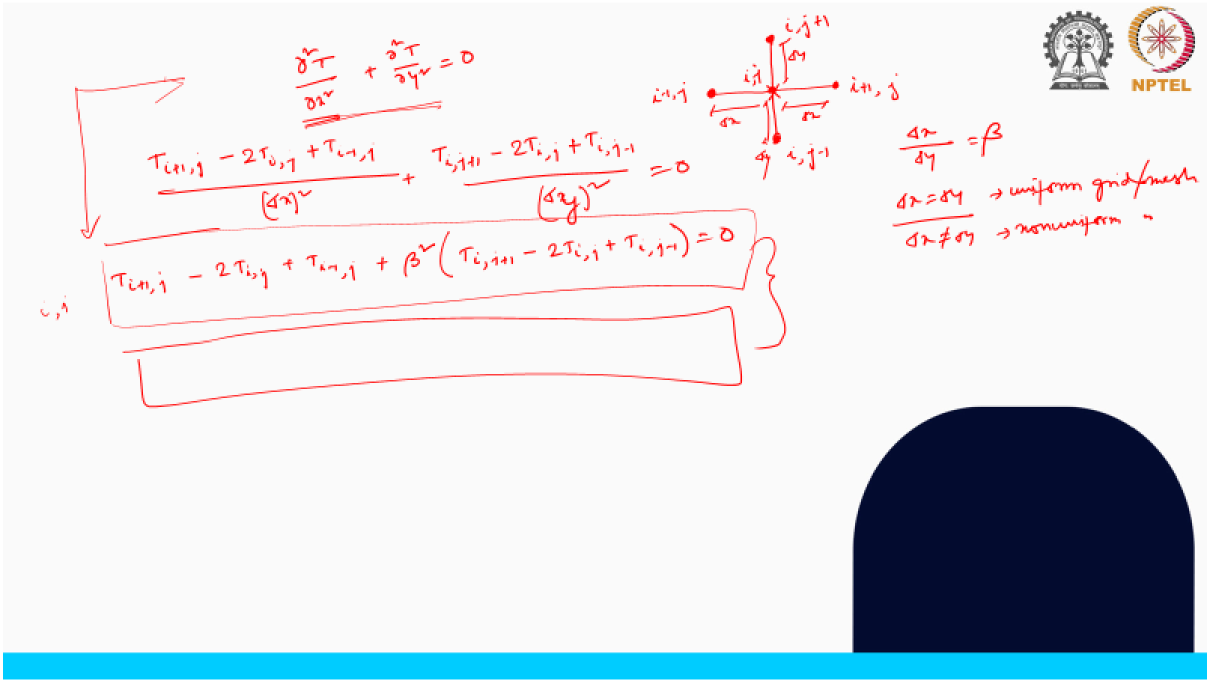
Week-03
Lecture 13: Numerical Methods for CFD

Hello everyone, welcome back once again with another lecture on CFD applications in chemical processes. In the previous lectures, I discussed the finite basics of finite difference method, one of the numerical methods that are used in computational fluid dynamics. Now we will continue discussing on the finite difference method because there are other couple of few things that I must mention because those are also relevant when we specifically will discuss the finite volume method in details. So, let us touch those things once again, but before I do that again let me show you the list of reference book that you may refer for whatever I have discussed till now. Earlier I showed this first three, this first three I showed you in the earlier lecture.

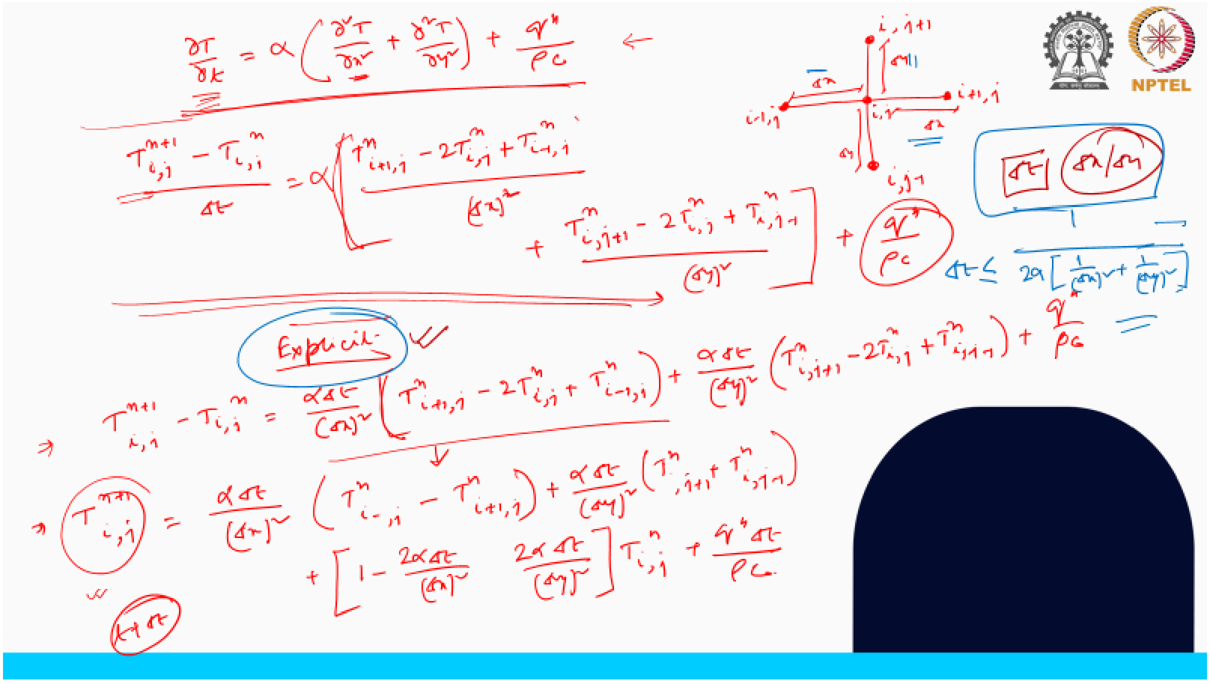
But this is also very important specifically when we will discuss in future about the multiphase flow modeling turbulence and the other aspects of this course. So now going back to the finite difference method. So, in the last lecture where the point I stopped was the steady state heat conduction equation. So, if you remember that the steady state heat conduction equation that we approximated this steady state heat conduction equation for the points or we consider for the sake of simplicity equispaced points.



So, delta x these are delta y this point is i j. So, it becomes i plus 1 j it is i minus 1 j this is i j minus 1 and this is i j plus 1. So, for this now the points these points we typically call nodes in So for these nodes and what we are trying to approximate the second order derivative for ij. So, on the point so, around the point i j by the central differencing scheme we have approximated already and we have seen its form.

So, what I can write here again this are from the last lecture is that T i plus 1 j minus 2 times T i j plus T i minus 1 j. divided by delta x square plus T i j plus 1 minus 2 times t i j plus t i j minus 1 divided by delta y square which is equals to 0. So, basically then we wrote plus considering delta x and delta y taking this as the ratio of beta. So, it would be 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. So, what we mentioned last time is that for the uniform grid this delta x is equals to delta y is the uniform mesh, if it is not then it is non-uniform meshing or grid.

and accordingly, the formulation follows. So, for every point i j, i j means the point of attention or on the nodal point where you are approximating this function or this expression. So, similarly throughout the domain in all nodal points you have to approximate this function.



So, for all nodal points you will get a similar expression which you can see that from a partial differential equation we come to similar a set of algebraic equation for every ij. As the ij increases we get similar say similar expressions similar set of equations. So, these set of equations then we have to solve.

Now, this is the case where we what we discussed for the steady state case where it is not time dependent. Now, for the time dependent say conduction unsteady state heat conduction equation that is having say a form like this, where alpha is the thermal diffusivity sorry this is say plus there is a source term. So, there is considering a uniform volumetric source term is there or the heat generation term or the heat sink term is there in the unsteady state case.

So, this is a typical expression for such scenario when we have the two dimensional unsteady state heat conduction equation. So, here also the similar thing the nodal points again if we draw that. So, this is point ij. So, it is i plus 1 j this is i j minus 1 i j plus 1 this is i minus 1 j. So, now coming to discretization of this function of this expression what we will do there are two different formulation that can happen. One is that Now, we can see that here we have a time dependent term. So, this time dependent term has to also be discretized.

Now, typically what we do is that we consider that n is the say current time step ok. So, if you go marching on the time step. So, n plus 1 would be the say the next time So, similarly the time you march with in the with time. So, for each and every time step this expression has to be evaluated that is the additional complexity that comes with the unsteady state case.

In the case of steady state that we have seen here there is no such time dependency. So, we solve for a particular time, but here with time we also will merge will merge. So, that means, we have two in two different time step or two different time we will have two different temperature profile that is the reason this form is there and we look for unsteady state say temperature profile in a heat rod when we consider such example. Now with time we march means if we at particular time t is n then it goes in time say n plus 1 n plus 2 like this.

So, that means, this first term what we can write is that T n plus 1 at a point i j minus T n divided by the delta T, a small time step increment delta T. that is happening from n to n plus 1 for a particular nodal point ij ok. So, now this part we have seen earlier how we can do that for a particular nodal point. So, inside this what I can write Say the first term that we have already seen we assume that we are approximating this term for a time step in which the values were known.

Usually for such problem you will be given with a initial value. that at t is equals to 0 the temperatures were this or at t is equals to some second the temperature of the rod was this and then you are asked to calculate the temperature profile at t is a certain value when there is a constant amount of heat generation or volumetric heat generation or there is a heat sink or two different boundary condition at the end and at the beginning. So, the time step at which you know ok. So, that that is the old time step because we will march in time.

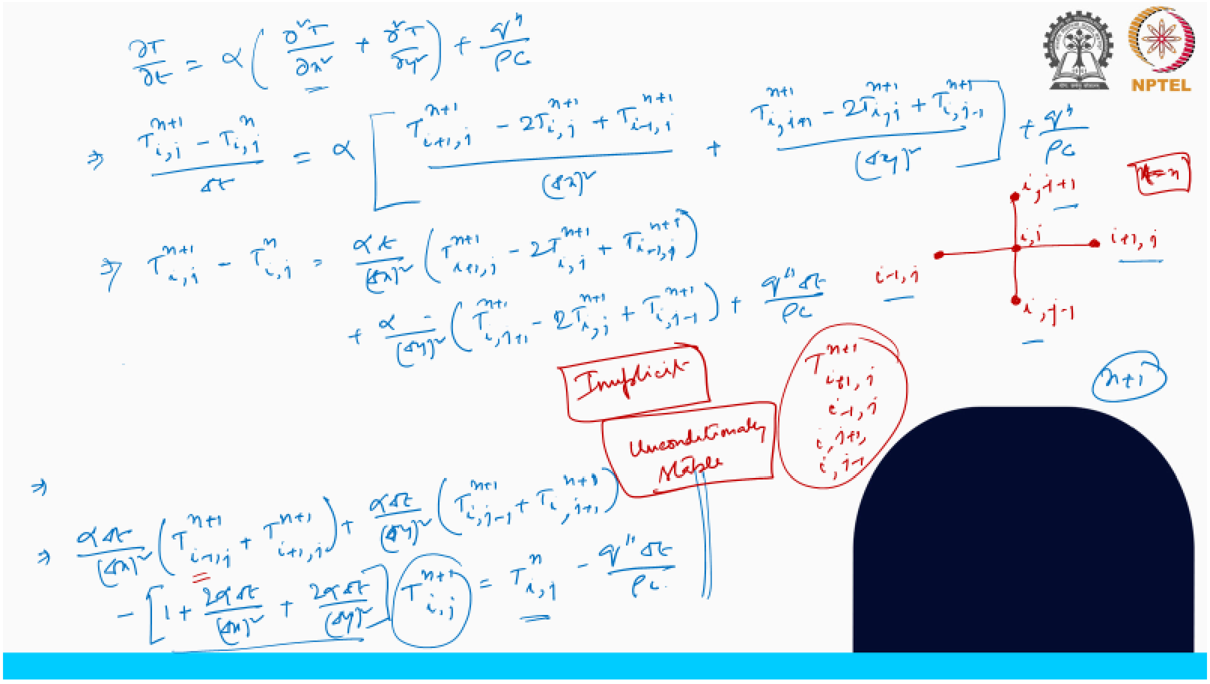
So, that is why what we can approximate this function as again it has to be discretized in the spatial coordinate ok. So, which means at i plus 1 j 2 times t ij plus T i minus 1 j exactly like we have done earlier, but the point is that these temperatures are at the nth time step or say where you knew the values. Similarly, For this part again if you for the time being do not consider this n what you can write exactly like this we had done it earlier ij minus 1 divided by delta y square. Now these are at the time step where the values were given.

So, what happens or known or given or known? So, what happens if you see this expression and then there is this constant term is there. So, what you see here is that here in this expression or in this equation only one term is unknown to you. that is the temperature of the i and jth point or the nodal point at n plus 1 time step or that is say with the increment of delta T from where the temperature you are aware of. So, which means now if you segregate the variable and try to find out that what is the expression for this term.

You would see on the left hand side only one unknown term would exist and on the right hand side all the terms that the values you are given or known. Such kind of formulation so that means in this case you can calculate this unknown term without depending on the other nodal point values or the other time step values. So, in this case that means you can go by iterative method to find out this unknown term easily and that is explicitly that explicitly you can solve this term or this equation and that is why such kind of formulation is called the explicit formulation. So, if I try to refine this expression would be something like. So, n plus 1 T ij minus T ij n is equals to alpha delta T by

del x square and then I will have say T n i plus 1 j minus 2 times T n i j plus T n i minus 1 j plus again alpha delta T del y square And we have a term, this phrase would come inside or this whole thing would be there, j plus 1, 2ij plus tij minus 1 plus this source term would remain there, rho c. So, further you rearrange this to know Tij in plus this whole term would be or this whole thing would come as it is here and again if you try to separate it. that what will happen ah for say the T specifically ah say if you try to. So, this is the T here. So, further arrangement of rearrangement of this would

look like say alpha delta t divided by delta x square multiplied by t i minus 1 j plus n i plus 1 j plus alpha delta t y square tn ij plus 1 plus tn ij minus 1. And then what you will have is that 1 minus 2 alpha delta t del x square 2 alpha delta t del y square. This is of t i j at nth time step plus q w delta t by rho c. So all the terms, so this is just the rearrangement of this expression.



And what will happen is that you clearly segregate the unknown from the known term. So on the right hand side, all the values and the properties, if it is given to you or will be given to you, you can easily find out what will be the temperature of the i and jth point So, this i at jth point at a next time step or at a time step which is t is equals to t plus delta t, t plus delta t at this time step. So, this is called the explicit formulation.

Now the same expression or the same equation if I further consider that.

the same expression I have now again what I can do this similarly what we have done earlier is that t i j at next time step and a previous time step or the time step at which I know the value. Now, the first term the difference comes in here that i plus 1 j 2 times i j plus t i minus 1 j divided by delta square. This is what we have delta x square. This is what we have seen for the steady state case or say for the simply by the central differencing scheme without considering the time dependency. Now, here what we can think of or what can be done also is that all these temperatures are at the next time step or at the next time step value.

So, similarly So what is done here that it is considered that we have discretized or approximated this partial derivative term in the time step where nothing was given or where in which time step we have to calculate it. So if you look at it here, we will have more than one unknown parameter. of the variables. So, here what we have now if you would write it in the form of say if you try to write it in the form of t i j at a time step of t n plus 1 where you have to find it.

So, just like this that t i j at t at the n plus 1 th what will happen is that it will have an equation which in the only one expression or with that simple formulation you cannot solve it in a standalone manner. It is dependent on the other nodal points as well because here if you remember that if you remember this nodal point. So, this was i j i plus 1 j i minus 1 j i j plus 1 and i j minus 1.

So, here what happens that at the beginning or with the initial condition that means when n is T is equals to n where this is my say initial condition temperatures say at each and every nodal points were known to me. And that is why we could solve the previous formulation which is the explicit formulation independently without waiting for the other expression. But here you see that this expression T n plus 1 i j contains the terms where at the i plus 1 and j, so at these locations or all its neighbor points, the value were unknown at that time step, n plus 1th time step.

Because at the n plus 1th time step, we do not know what are the temperatures of each and every point. And those are appearing on the right hand side. So, let me quickly write this formulation then you would further understand. So, T n plus 1 ij minus T n ij similar to our previous sorry. what we have the first term first phrase is the whole term is there so 1j at the end plus

so if you now try to write only in terms of T in plus 1 IJ is equals to something on the whatever the terms that appears on the right hand side what you will find just the rearrangement of this is that we will have T n plus 1 i minus 1 j plus T n plus 1 i plus 1 j plus alpha delta Y square I G minus 1 T I G plus 1 minus T n plus 1 ij is equals to T n ij minus rho c. So, the coefficient of this has been identified and if you see the all other terms only except this one all others are unknown.

So, this equation cannot be solved in a standalone manner and such formulation. So, that means for this to solve you will need the expressions for these parameters also that i say n plus 1th time step i plus 1 j i minus 1 j j plus 1 i j plus 1 and i j minus 1. So, all these expressions you would be requiring to solve for a single point or the single node. This formulation is called the implicit formulation.

Now, which one we should choose? Principally, this implicit formulation is unconditionally stable during the simulation. that if you formulate in this way you solve the whole set of expressions you get a stable solution. But in the previous case this explicit formulation requires judicious choice between the delta t and delta x or delta y and that dictates the stability of the formulation. So, it requires a stability criteria.

For this particular case, the stability requirement for this is that the delta T has to be less than equals to 2 alpha 1 by delta x square plus 1 by delta y square. This criteria has to be satisfied regarding the choice of your delta t or the time step increment and the mesh size or the grid size that means this delta x and delta y choice. So explicit simulation or such formulation requires judicious choice of delta t and delta x that means the time step increment and the grid size or the mesh size but the implicit solution is unconditionally stable. If it is not the case for explicit formulation it will give some weird values or in the predictions if that have the stability criteria is not maintained.

We will see that while solving or while implementing finite volume method because the similar analogy or the similar principle is applied there as well. This finite difference method is as I told you earlier is the simplest to implement, but for the unsteady state case when you apply it you have to be careful whether it is an explicit formulation or it is implicit formulation. So, I will stop here today. We will continue this discussion in the next class as well where we will have a brief look at the finite element method as well. So, thank you for your attention. We will see you with the next lecture.