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Lecture 11
Numerical techniques of solving PDE - discretization

Hello everyone, welcome to the third week of this course on process mathematical modelling and simulation of chemical engineering process. In this week, we are mostly going to focus on the different numerical techniques associated with solving partial differential equations.

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In this class today, we are going to talk about the discretization and this forms the basis of the finite difference method of solving PDEs. Now, we are going to learn about the different basics of the discretization techniques, how to discretize the first and second order terms as well as framing the finite difference equation.

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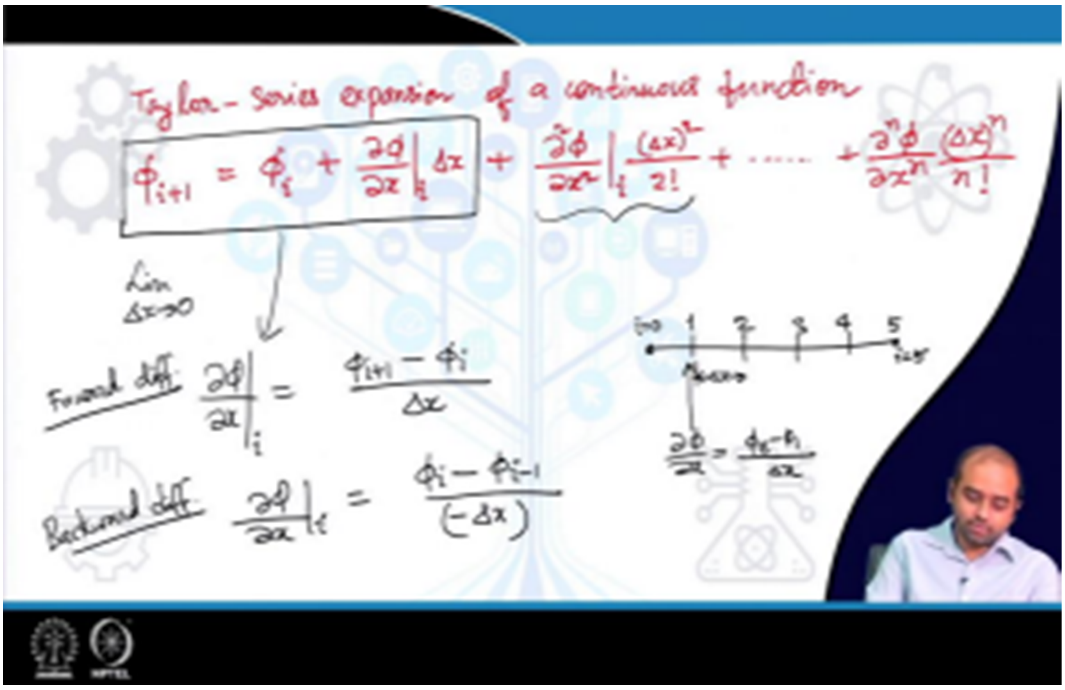

Now, in general how the genesis of the discretization or writing down the difference equation for any derivative component is based on the Taylor series expansion. So, we all know this Taylor series expansion for a single variable let me just write it down first for you. This is something all of you are used to, the Taylor series expansion that any continuous function can be written down as the infinite series of its derivative components.

And as we take the consecutive terms, we increase the order of the derivative components. Now, please note one very important aspect here, is that generally the discretization for any first order term or the first derivatives terms are restricted to the Taylor series expansion of this, up to the first term. If you have equations involving the second order components, the second order terms, then we go ahead up to the second order terms.

But there is one important point that needs to be noted here is that, when we try to discretize an equation and consider the derivatives based on the, one or two terms, we are essentially ignoring all the higher order terms of delta x, is not it? So, now, if so, this incurs some additional errors due to ignoring this higher order delta x term, and this is the primary reason why any computational scheme that you see, as you increase the size of the grid or if you make your mesh to be more coarse, the solution often becomes inaccurate.

On other words, if you refine your mesh or the resolution of your, this mesh size is reduced, of course, that increases the computational loads because the memory requirements etc. increases, then, essentially you have more accurate solution, is not it? So, how the finite difference works, actually is that you try to discretize or you try to form small segments of your space and over and based on these small segments you try to solve or discretize all the difference equations and that is generally done for all of the space segments.

Now, smaller the segments are, the lower is the error or the accurate is the solution because you can clearly see from the Taylor series expansion that often during discretization, we ignore the higher order terms. So, if delta x is small or it is continued to be smaller, then the errors associated with the higher order terms is less, but then this comes like how small is small ? So, if you compare two solutions, where in case in one case you have delta x larger than the other one, then in both the cases even though we ignore the higher order terms, the solution or the case where delta x is smaller will be more accurate, because the additional components contribute very less to the errors. So, as much as delta x is small, you approach, I mean these derivatives, so, these derivatives that we write is closer to the actual derivative, is not it? So, this is what the fundamental basis of the writing any different differentiation principle that you always consider that the limit to delta x tending to 0, is not it? Only in this case, we can say that, the derivative instead of writing the difference form after derivatives, it is actually the derivatives.

So, delta x theoretically cannot practically cannot go to 0, then you will have in infinite mesh, number of grids or number of mesh elements, for finite mesh number of elements, we can take delta x to be as small as possible, the smaller it is actually, the better is the resolution or the accuracy of your solution.

So, please understand this, that the solution accuracy improves on increasing the resolution of mesh, because you reduce the error in the Taylor series expansion of the discretized equation by truncating, the higher order terms, it is not because you get more information at the intermediate or the interval points in your space domain! That is not the correct idea. So, this error that you get in your solution or the final numerical solution is close to the actual answer this error actually is proportional to the delta x. Why? Because of the truncation of the higher terms in the Taylor series expansion. And this accuracy actually increases as you reduce this x, because again, the same logic the higher order terms which contribute to the errors in writing the derivative as a difference for.

So, from there we get this information that this higher order terms, if they are neglected or truncated, there will be some contribution that part, in the form of data and that will be minimised as delta x is small. So, I mean, from this what you get? you get d phi dx is equal to phi i plus 1 minus phi i by delta x.

So, in this this is the equation or this is the approximate version of the derivatives, of the first order derivatives in the form of difference of two quantities divided by delta x and please note here delta x is not close to 0 it is not in that limit. It is a finite quantity. So, this is from the Taylor series approximation ignoring the higher order terms you can reduce or you can convert a derivative into algebraic form.

This subtraction of two quantities and divided by delta x. So, this is the genesis that all derivative terms can be represented by some algebraic formulation and at the end, what you find is that the PDE or the ODE gets converted to an algebraic equation or a series of algebraic equation that needs to be solved at different space points. So, what is this phi i plus 1 and phi i?

So, if you have a space domain, let us say it is a one dimensional space like this, I consider this to be a rod and I discretized into equivalent intervals of delta x and this is, i is equal to 0, this is 1, this is 2, this is 3, this is 4, this is i is equal to 5. So, these are the individual indices that is what as written down as i, so, this phi i plus 1 and minus i minus 1, it means that the value so, if I want to calculate, so, this is a d phi dx at i, it means if we want to calculate what is the value of this derivative d phi dx here, I need to know the value of phi 2 minus phi 1 by delta x. So, this method of formulation is generally known as the forward difference, where you write down the difference based on the space point which is next to the current space point. Similarly, we can also write down the backward difference, where you write the derivative d phi dx, by the knowledge of the previous space point.

So, from the current space point and the previous one, the neighbouring previous one that is the backward difference. There is also something known as the central difference.

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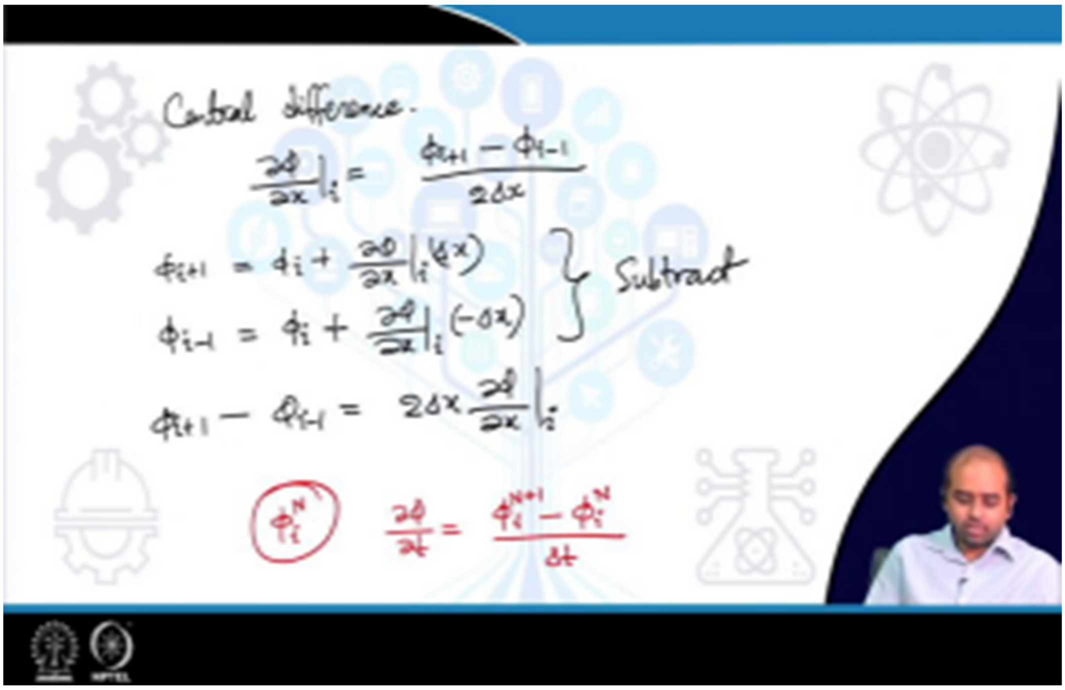

So, let us also write that one. Central difference. So, and so, central differences d phi dx at i. So, if you do not take the current space point, but you take the neighbouring one ahead and one previous space point divided by twice of the grid space and how do you get this relation? If you just take the difference of the two. So, let us say I have phi i plus 1 is equal to phi i plus del phi del x. So, this is I am trying to write in the forward direction and if I try to write in the backward direction with respect to the current space position i so, I will be getting d phi dx minus delta x. So, you if you subtract these two equations. So, you will be getting phi i plus 1 minus phi i minus 1 is equal to two delta x d phi dx. So, this is how you get the central difference scheme.

For each of these schemes whether you go for forward difference whether you go for backward difference or central difference has their own advantage and limitations at different context. So, if you generally for PDE or solving transport problems we generally consider the forward different schemes. So, if you have the fast order time, if it is in time domain, then we generally write down for different schemes.

Because time always marches ahead. So, in the case of space, we generally take central differences, that is the idea. So, now, if the variable phi, if this variable phi depends on both space and time it is important to choose their index very properly. So, if I write something like phi i and then N which means, i is the index of the different space points and N is that time interval point. So, if I am supposed to write d phi dt, I would be writing something like forward difference in time, always that is the idea. So, I will not change the space indices, I will be using the time indices to represent the discretized equation. So, this is just, way of writing the equations and so, that we are careful with the subscript or superscript or whatever the indices that we represent here and not get confused with the derivatives of the time part or the derivatives with the space part.

So, if you are dealing with the space part, you change the indices of i if you are dealing with the time part you change the index capital N which is in the superscript. So, this capital N is not like the power form, it is just a representation of the index in the time part. So, it is not phi to the power N, not like that. You can alternatively write as i comma N also you can write at the in the subscript form, it is just a way of writing.

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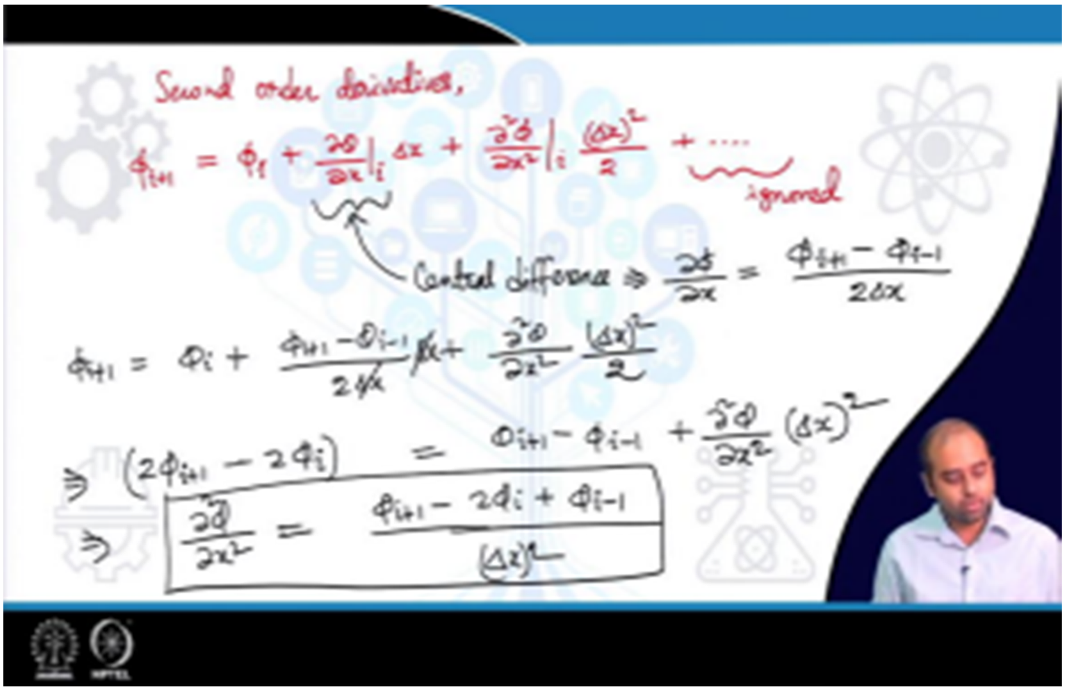

Now, what about second order derivative terms? So, far we have discussing only with first order derivatives. So, generally from the Taylor series expansion you can write, I am writing only the space, considering only space variables. So, since if we are to consider the second order derivatives, we need to write the Taylor series up to the second order term and remaining terms are ignored, plus higher order terms, which are ignored. So, of course, this brings in error, but we sacrifice that part to write the variable in terms of some finite quantities. So, now in this equation if you substitute this first order term, this component, from central difference so, from the central difference you have d phi dx, as phi i plus 1 minus phi i minus 1 by 2 delta x, when you substitute this component here.

So, what do you get by i plus 1 plus 1 minus y i minus 1 by 2 delta x that is d2 phi. So, if you do the algebra, you will be getting 2 phi I plus 1 minus 2 phi i, is not it? Multiplied with delta x. Sorry there is also delta x here, so, delta x, delta x gets cancelled out and you will be having something like this. So, you can easily work out what does the second order term look like. This is phi i plus 1 minus 2 phi plus phi i minus 1... So, this is the discretized form of the second order term again following the central difference. I hope all of you are getting it. So, let us see if I am supposed to write down heat equation.

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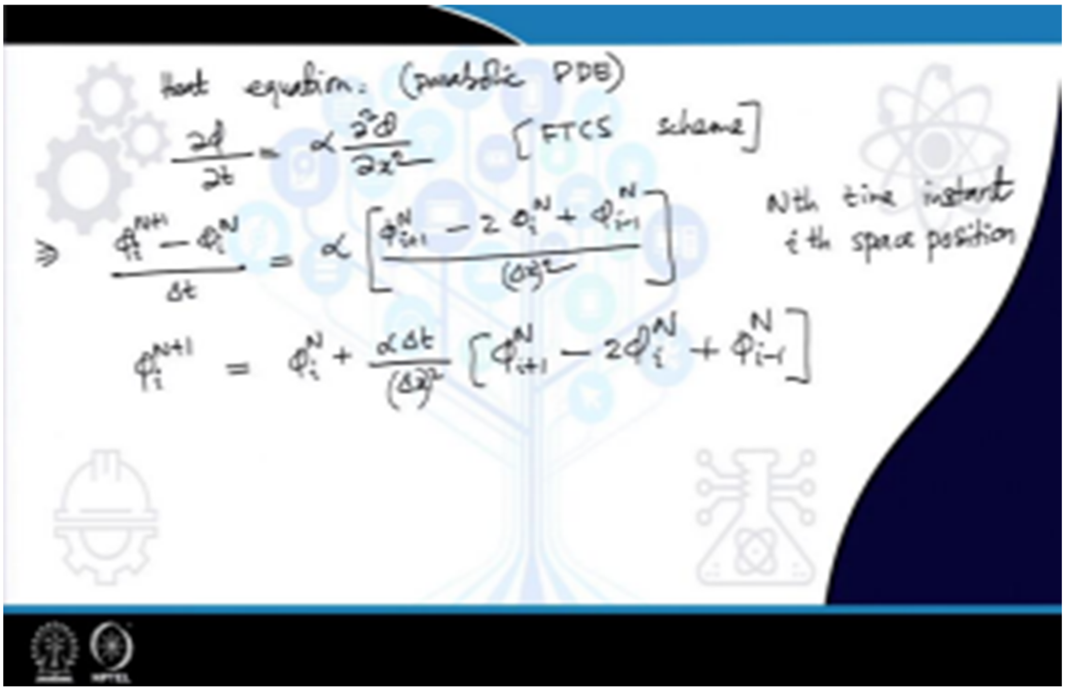

Let us say, so, I am supposed to write down the heat equation which is nothing but a parabolic PDE. So, the left-hand side I will do a forward difference and the right-hand side I will do a central difference. Which is known as, this is known as if FTCS forward in time and central in space. So, let us try to write, I bring down the subscript as well as the superscript to distinguish between the space and time part.

Time part is given by the subscript capital N and the space part is given by the i or the subscript formation. So, the time is given by the superscript, capital N and the space is given by a subscript i. So, please note that on the left-hand side when I write the time derivatives, I took the space component as the i th point and now, on the right-hand side when I try to write the discretized form of this spatial derivatives, I will take the time, I mean the time component as the N th time.

So, all are in N th time instant at different point i th to write down the space derivatives. To write down the time derivatives, I will be taking the N plus 1 time interval and N th time interval at the i th space point. So, this is the N th time instance and i th space position. So, if I am supposed to write, so, the i N plus 1, I can write something like this. So, please note here that if I know the knowledge of phi or this variable, the scalar variable phi at different space point in the N th time instant I can evaluate what is the value of that quantity or that scalar variable at N plus 1 time instant.

Please note on the right-hand side of this equation every all the information is known. So, because at the N th time instant to find out the value at N th time. So, let us say go back to the original starting point. So, for the first-time interval, I will need the information from the N th initial condition that is how I will be starting off at the first time then I move to the second time.

So, to calculate the second time instant or a second interval, whatever that could be, I would be needing the information from the first time instant and all the space points, because this i will be across all the grid points. So, that is how if I know the solutions and initial condition is valid for all the space points. So, from there, I can find out that what would be my next time interval, the solution of the next time interval provided I will be knowing the value of this variable, this dependent variable this scalar quantity phi at all the space points in the previous time instant. And that is how I am going to estimate phi i N plus 1. So, this phi i and this N plus 1 I can easily calculate for all the space points. Now, when I go for N plus 2, I already know what is for N plus 2 I will be needing the information for from N plus 1, is not it?

And now, I already know what is my information present at N plus 1 from the previous equation and this this equation that I mean that is written down here for N plus 1, this is for all i th locations I can calculate it out right and this is this is something known as the explicit formulation.

What do you mean? What essentially this explicit formulation tells you that if you know the previous time instant you can calculate the current time instant or if you know the present time instant you can calculate the future time instant explicitly in a single equation. So, this single equation on the right-hand side everything is at the past (time), at the N th time and we want to calculate it for N plus 1.

So, that is the reason why this is an explicit equation, it seems to all everything on the right-hand side is known and that is just equated to the quantity at the future time instant. So, the future times can be easily updated with the knowledge of the previous time step or the time interval or the time instant and this is true for all the space locations.

If I want to calculate for i plus 1 or i minus 1, N th, N plus 1 time, I will only need the information at the previous time which is known to me. Until and unless I know all the information at the previous time I cannot move ahead, this is what the explicit scheme tells you and essentially at the previous time instant, each space points can be evaluated based on its historical information.

So, now it becomes, I mean everything becomes known on the right-hand side because all we are calculating at the N the time to find out what would be its value at N plus 1 time. So, this is the explicit formulation and this is how we march forward in time with the knowledge of the past. So, this is something is very vital and explicit schemes are actually quite popular because it has very minimal computational loads.

So, because to find out the solution at these particular space points, you will only need all the past information. You need not to know anything at the present time of its neighbouring information everything that is known is required is from the past. So, if you just showed the solution of the previous time instant that is sufficient enough to calculate the present time for all the time instants.
So, this is known as the explicit time this formulation. And also, please note one more thing here that you will see that this partial differential equation is so, nicely converted to the algebra equation straight away. Only thing is that you have to solve this algebraic equation at different space points and at different time intervals right but essentially this directly convert these partial differential equations into an algebraic equation and this algebraic equation as you can see is also an explicit form.

So, just using sort of a formula direct formula. So, use this formula to calculate the values at the different space points as well as the different time points. So, this has to be noted down. The second thing is that these explicit schemes all have certain stability criteria, why? Is because, as you continue to move march forward in time, it is very essential to ensure that the solution does not diverge or the solution does not blow out like what should be the time step or the interval time with which you should calculate the next time?

And it should also necessarily imply that during this time progress, are you missing any vital information? is it sufficient to capture that temporal change of that variable? for which temporal as well as the spatial change or the spatial gradient that is correctly captured, for which there is a stability criteria that needs to be satisfied for all explicit formulation schemes because they are not stable by default and there are certain criteria which needs to be satisfied based on which you should be able to select whether the time interval or the space intervals are sufficient or properly resolved or not.

So, in the next class, we are going to talk about some of these stability criteria, which is very vital for the, this explicit formulation schemes. I hope you liked today's class and understood the basics of the discretization schemes and the genesis of all finite difference and finite-volume numerical techniques. Thank you.