Mathematical Modelling and Simulation of Chemical Engineering Process Professor Doctor Sourav Mondal
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Lecture 12
Stability of the Finite Different Schemes

Hello everyone, today we are going to learn about the different stability criteria, which is particularly essential for the explicit formulation of the finite difference schemes.

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Now, if you remember in the last class, we talked about the explicit formulation and why there is a need for this stability criteria. So now let us first talk about, so we are (going to) going to discuss about two stability criteria, and we'll see what is the condition that needs to be satisfied in each of these stability issues.

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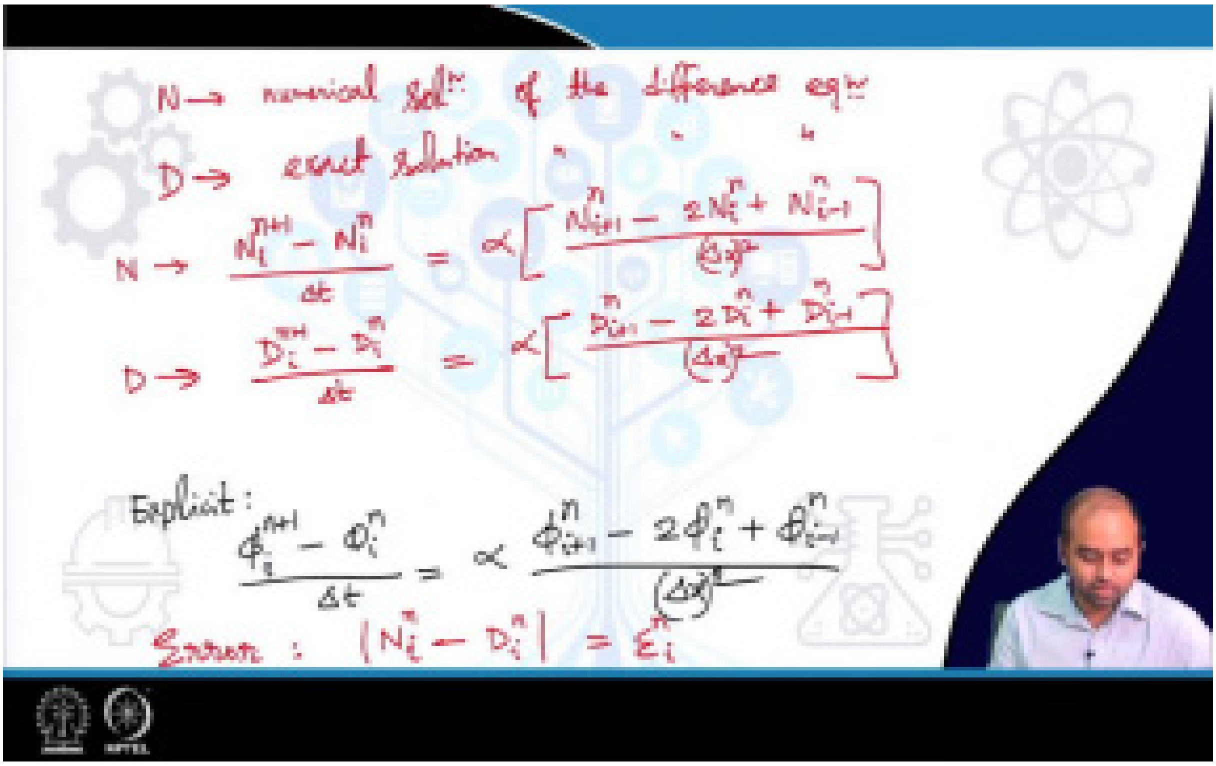

So, let us consider like capital N to be the numerical or the numerical solution of the difference equation. Numerical and also considered to be an approximate solution and let us call as D is the exact or the analytical solution to the problem. Now, (this) both this N and in the numerical solution and this D will be satisfying the discrete explicit formulation equation. So, let me just write down the explicit equation.

So, the explicit formulation equation for phi is phi i plus naught i plus 1 and plus 1 minus phi N phi i N from the last class if you recall, we wrote down forward in time and central in space isn't it? This was the equation. So, this is the explicit equation. So, both the numerical solution and the exact solution will satisfy this explicit scheme, is not it? So, in terms of the numerical solution, I can write something like this.

Similarly, D will also satisfy that is also a solution so, it will also satisfy this explicit formulation equation. Now, what is? How do we define an error? So, the error in a solution is nothing but the difference of this numerical solution minus the exact or the analytical solution. Let us denote the data as epsilon, is interest the absolute difference of the numerical solution with respect to the exact solution.

So, the numerical solution that we get from the discretized equation is always an approximate solution, I mean theoretically it may be close to the exact solution, but there is always some degree of error associated because of the truncation of the error terms in a Taylor series expansion. So, this difference of the numerical solution to the exact solution is what is known as the error. So, if both of these numerical solutions, I mean the numerical and the exact solution satisfy these explicit equations, the error will also satisfy this explicit equation, is not it?

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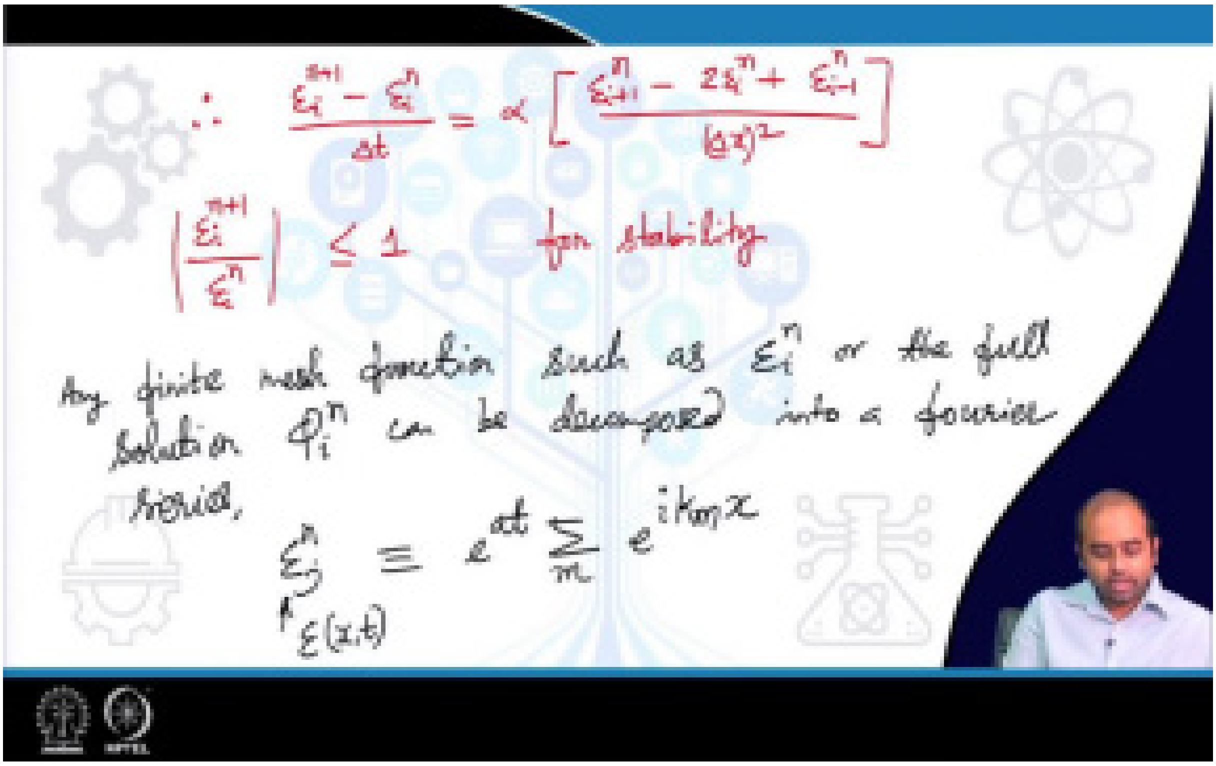

So, I can write this explicit equation in terms of the error also. Now, this error at the N plus 1 interval with respect to the error at the previous time scale, at previous time interval should always be less than 1 and this is something that based on which we say that the solution scheme is stable or it is converging.

So, these criteria should always needs to be satisfied for stability otherwise what would happen that the error will continue to grow with the time interval and that is not acceptable. So, you cannot have a solution where the error continue to rise as the time progresses. So, it has to continuously decrease or may remain constant. So, this ratio of the new error in the future time with respect to the past or the present time has to decrease or should not exceed or should not get increasing with respect to time.

So, this is the criteria for the stability. Now, let us look into the exact condition that needs to be satisfied for this stability case. So, any finite mesh function such as this error, any finite mesh function such as this error function or the full solution can be decomposed into a Fourier series. This is always possible. So, with this idea or with this inspiration, we generally write this error, I am changing the subscript from i to j which were of course, this is the error is that different space point and the time points, something like this.

So, where A is the amplitude of the different harmonics and km is the wave number of the different terms in the frequency domain after Fourier series. So, this is typical representation,, this is a typical representation of the error, and based on which we are going to write down this error or substitute this equation or any term in this series of the equation into that explicit equation.

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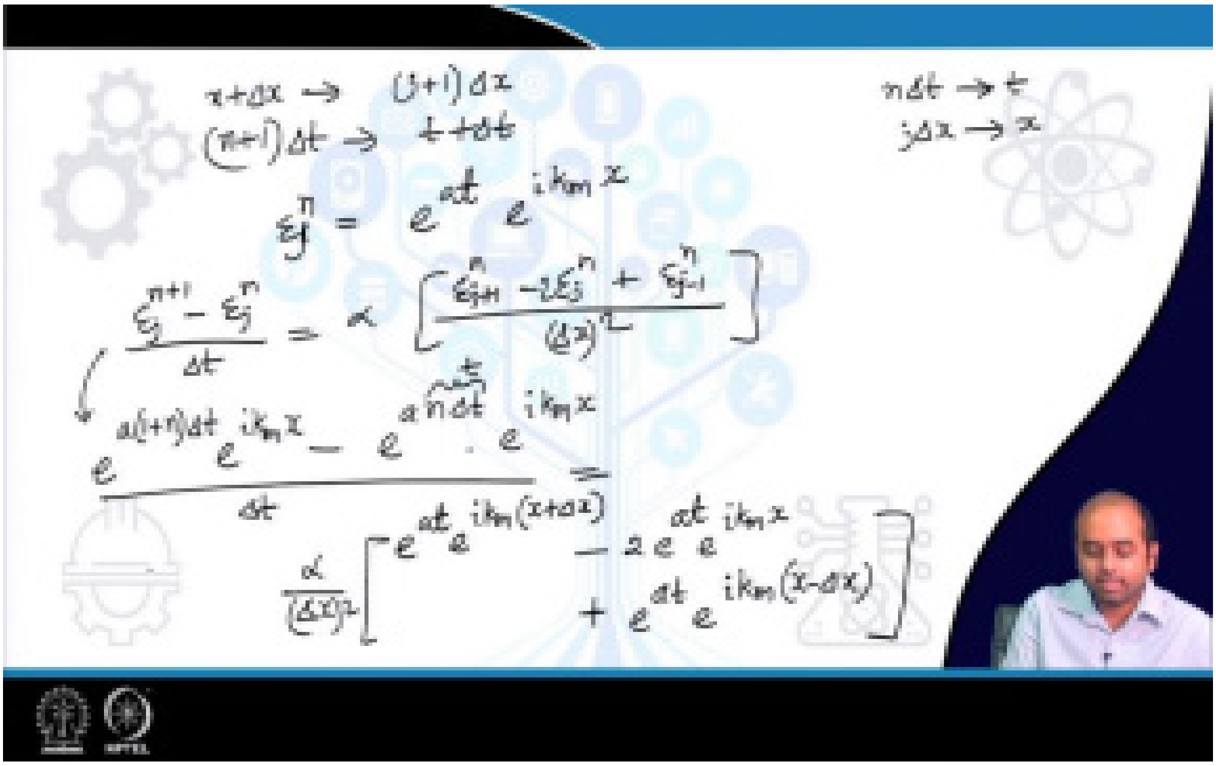

So, before we move ahead, just let me also highlight that here we consider that the time intervals are constant and the space intervals are also constant. So, what does it mean? So, x plus delta x can also be represented as j plus 1 delta x. Similarly, N plus 1 delta t is nothing but t plus delta t. So, that is something that we inherently consider here. So, anytime in this series epsilon like j is nothing but I mean if you consider the single any single term in this series, it is something like this.

So, or any term based on any term on this series, I can write that this error from the explicit equation is also satisfied by these terms that how we write down the error. So, pardon me I am rewriting that equation once again just for the sake of completeness to the problem, and the subscript j is replaced from i because we do not get confused with the complex i here. So, this is we are rewriting as in terms of e to the power.

So, this is the first term and this is the second term. So, please note N delta t is nothing but our t, is not it? So, N delta t is nothing but t. Similarly, j delta x can also be represented as x divided by delta t and the right-hand side, I am just writing below, alpha by delta x square. So, it is e to the power at e to the power ikm x plus delta x 2e to the poor at and plus e to the power ikm x minus delta x that has the j minus 1 term.

So, I divide both sides by e to the power at and e to the power ikm x.

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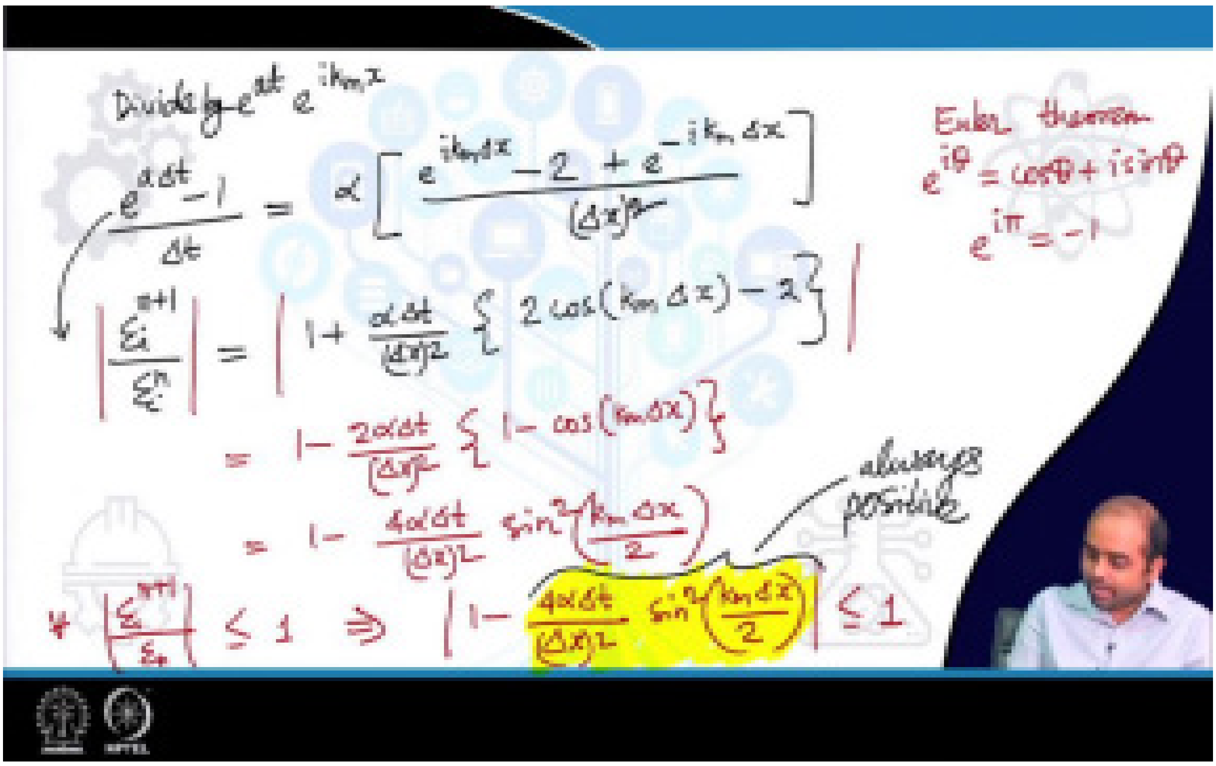

So, what we get on the left-hand side is e power a delta t minus 1 by delta t the right-hand side becomes, please note that this i here is the complex number. So, this left-hand side, e to the power a delta t minus 1 this quantity and e to the bar a delta t, e to the bar a delta t can also be written down as e to the N plus 1 by epsilon i n, is not it?
And right-hand side becomes 1 plus alpha delta t by delta x whole square and we also use this Euler theorem and if we just use the Euler theorem that e to the power i theta is going to equals to cos theta plus i sine theta we get something like this. So, the Euler theorem can be used for the conversion of the polar trigonometric functions. This is something all of you have already studied in high school, is not it?

And from here you know that e to the power i pi is called minus 1. And I can, since this is has to be a absolute function, so, this also becomes absolute function and just doing some rearrangements, I can write 1 minus 2 alpha delta t by delta x as whole square into 1 minus cos k m delta x and this can also be written down 1 minus 4 alpha delta t by delta x whole square.

So, I can use this sine square k delta x by 2. So, 1 minus cos x can also be known as 2 sine square or something like that x by 2, is not it? So, what is the idea here? so, for this quantity to be less than equal to 1 implies that this 1 minus 4 alpha delta t by delta x whole square sine square km delta x by 2, this also has to be less than 1. Now, when that is possible? That is something we have to investigate.

Now, please note here that this part in, so let me use the highlighter, so, this part here is always positive. Alpha, delta, t delta, x sine square all these terms are always positive, it is not possible to have any negative term. So, all these terms these are always positive. So, what does this mean?
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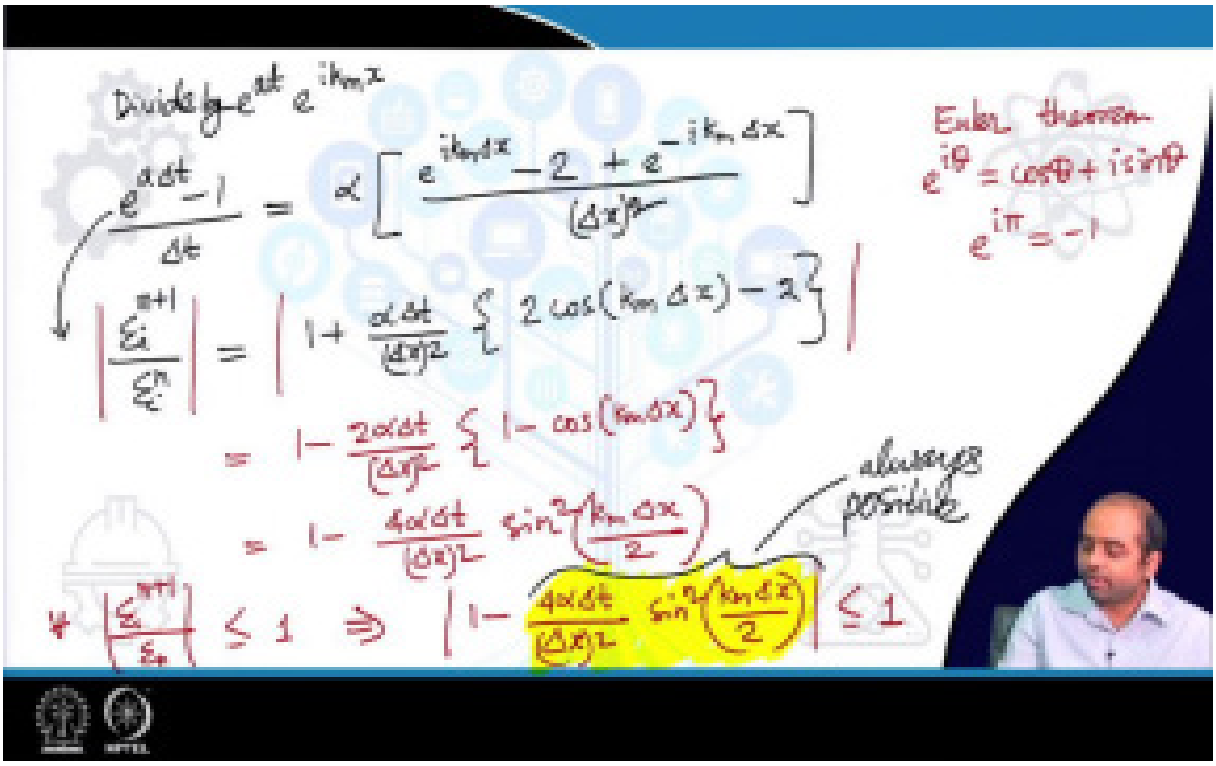

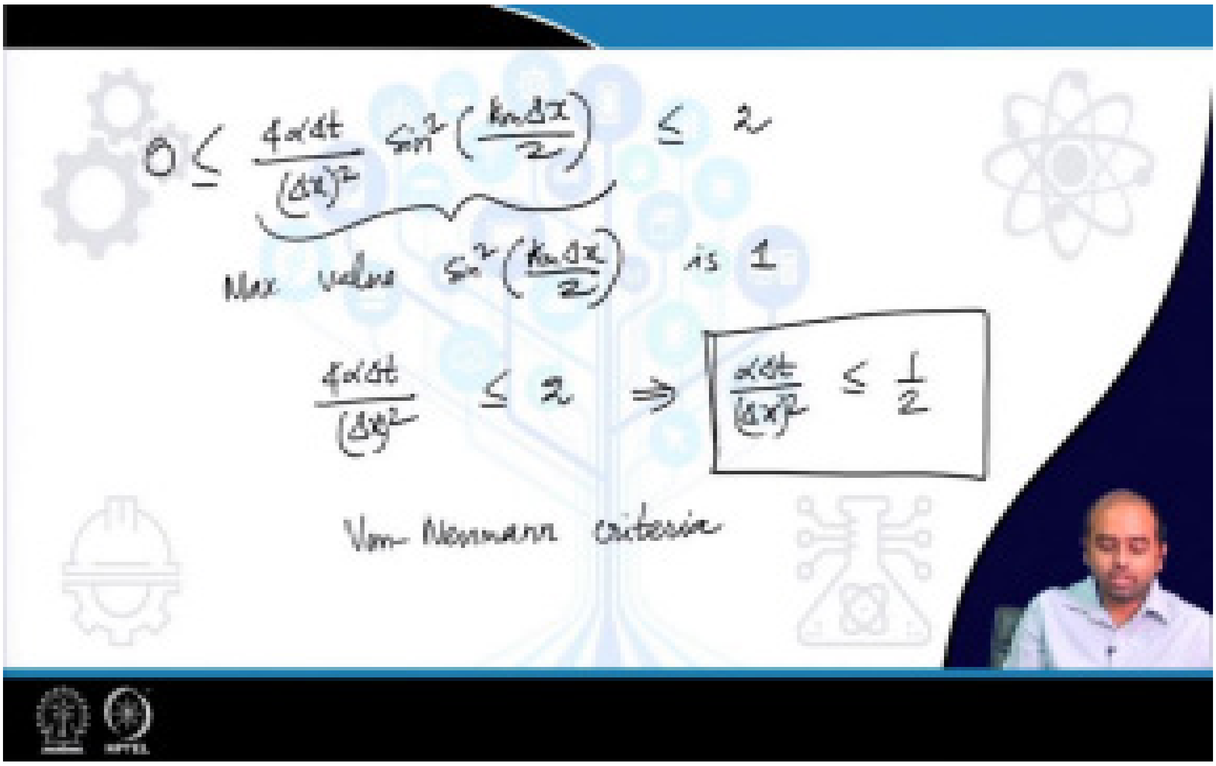

That for alpha delta t delta x whole square sine square. So, this is always positive, so, it is always greater than 0 that is part is clear. Now, from the previous case to satisfy that this component 4 alpha delta t, this part, if it is not only positive, other thing is that it is also within I mean the value of this component has to be less than 2 otherwise this equation cannot be satisfied, is not it is?

This whole alpha delta t delta x square sine square this entire component, has to be less than equal to 2, because this is within this modulus. So, this left-hand value can be plus minus 1 within the modulus. So, it will still be less than 1. So, these components will be less than 2. So, the limit of this quantity is positive but less than 2. Now, please note that the sine square term so, the maximum value of this sine square term, is 1.

So, at the maximum value if we are able to satisfy this equation, then it will always be satisfied that is the necessary condition or let us say the sufficient condition. So, what does this tells you that for alpha delta t considering the maximum value of sine square that is 1 has to be less than 2 and then only this is I mean inequality will be satisfied and this simply implies that alpha delta t by delta x s whole square should be less than half.

So, what does this tell you, alpha is the sort of thermal diffusivity and delta t is the time interval and delta x is the space interval. So, this ratio of delta t by delta x whole square if only if it is less than half then only this parabolic equation or any sort of this diffusive equations would be stable or the solutions or the errors would not be growing in time using the explicit formulation of the finite difference scheme.

This criteria has to be satisfied. So, what does this bring into the constraint is that the choice of the delta t and the delta x would be such that these criteria, this stability criteria is satisfied. So, this is known as the Von Neumann stability criteria which is generally applicable for any diffusive systems, whether it is heat transfer, momentum or mass transfer. This criteria needs to be satisfied for explicit type of formulations.

Now, let us move to the new case when we have only convection to be presenting the problem.

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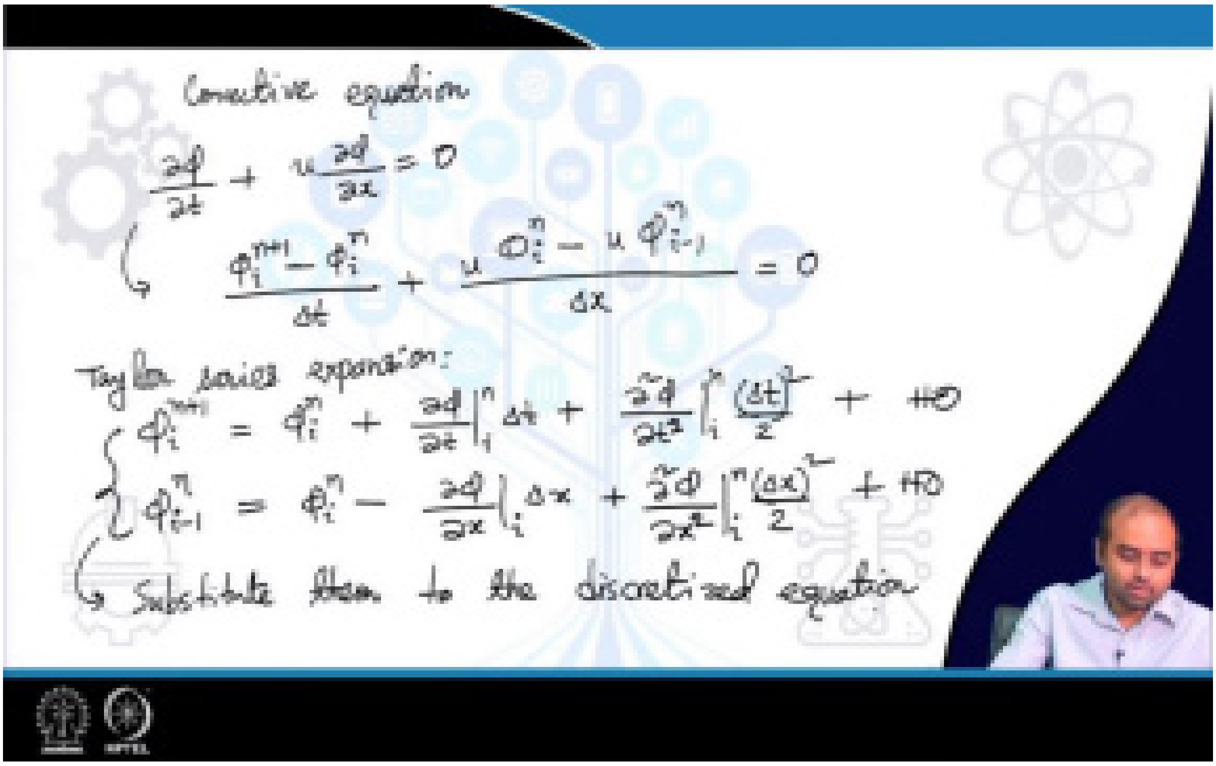

So, let us look into the convective equation. So, consider inviscid transport of our scalar flux variable phi and the equation or the convective equation would be something just like this. So, this is like the inviscid transport of a scalar flux phi. So, from the Taylor series expansion if I try to write down the discretized equation, I can write phi i N plus 1 minus phi. So, this is the forward difference in time and also, we do forward also we do the forward difference in space. So, this is the discretized equation. Now, let us use the Taylor series expansion and look into the case here. So, please note that there are no second or third terms here in the original equation. So, in the Taylor series expansion, let us see if I consider the terms up to the second order quantities, next would be the higher order terms.

So, I can easily write down that my phi in my plus 1 minus N minus 1 pi delta t looks like with the addition of the second component I mean with the addition of the I mean, bringing in the second term so, instead of just saying right away discretizing the first order derivatives I can rewrite that equation that what is the additional error that I get in that discretized equation by discrete by considering the Taylor series only up to the first term.

So, that error we are going to quantify considering the addition of the second order terms and of course, higher order terms it will further make it more complex. So, at least if I, ignoring so, in this case we are ignoring the second order terms while writing the discretized equation. So, what if I try to invoke or incorporate the second order terms into the discretized equation to see how the original equation is modified or what extra artificial components are added because of this discretization and ignoring the second order term to say the least?

So, I can also write down the Taylor series expansion for the space part. So, now, these two equations if I substitute them back to the discretized equation. So, if I substitute them to the discretized equation, of course, I will be getting my original equation plus some additional terms.

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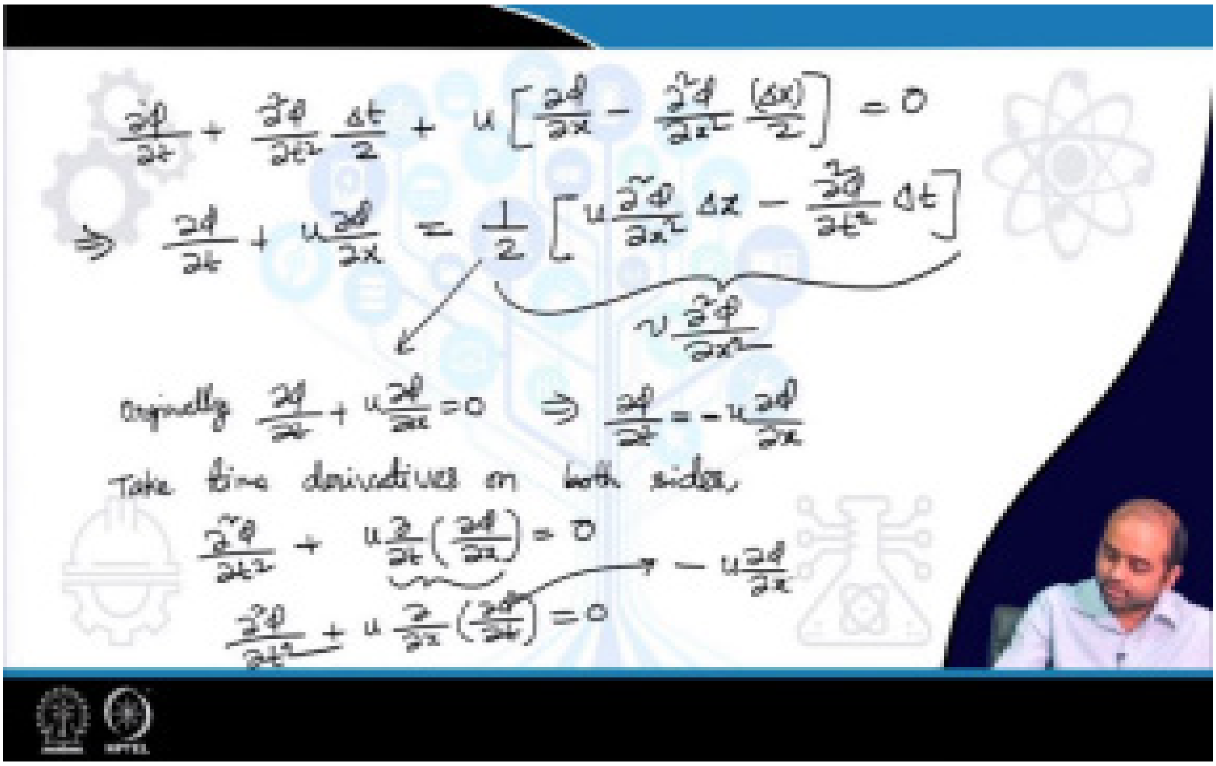

So, what are those? So, if I discretize them back I will be getting something like this and I can just rearrange the above equation. So, this is the part of the original equation and then I am getting and on the right-hand side instead of 0, I am getting this additional term or the second order terms which got introduced because of the discretized version of the original equation and considering the Taylor expansion up to the second order term instead of just the first order term.

So, these are everything on the right-hand side, somebody can say to be something like this and

I will talk about how this is possible. So, at least you can realise here that there are some second-order terms are coming in the right-hand side because of the discretized version, I mean trying to represent the discretized version in the form of the finite difference scheme.

So, if I put back the original trying to recover the original equation from the discretized equation, I see that there are additional terms, which is mostly of second order in nature that is appearing and these terms are generally known as the artificial diffusion or the numerical diffusion to these inviscid problems and this is very common, when we generally encounter try to solve high mach number of flows or extremely high in inviscid flows, where the viscous components are negligible.

In that case, trying to solve the numerical equation it is often important to tune these numerical diffusions, because this numerical diffusion should be kept minimal as possible, but this also comes inevitably along with the problem or along with the discretized equation in the as a source of some error due to the ignoring the due to the the removal of the second order terms in the Taylor expansion to write down the discretized version of the first order terms.

So, how this I mean, we can just do a simple, the manipulation of the terms. So, originally you have this equation and this is true always, d phi dt plus u d phi dx is equal to 0 and this is true always. So, from here I can write d phi dt is equal to u d phi dx, minus of this. So, if I do the time derivatives, take time derivatives on both sides, you get d2 phi dt square plus u del del t of d phi dx is equal to 0 and again d phi dx can also be written down and this we can represent as del del x of d phi dt. This can always be written down and now, d phi dt, d phi dt can also be substituted as minus u d phi d the x.

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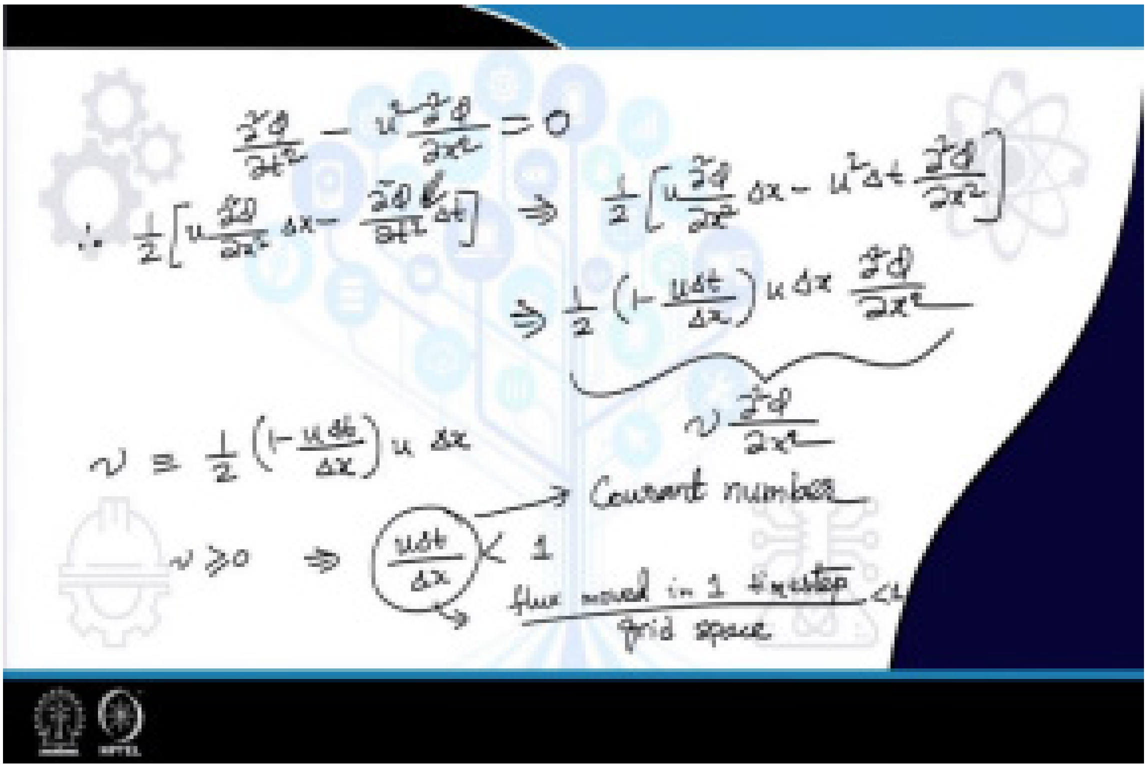

So, what we get? So, from here we get d2 dt square minus u square d2 phi d x square like this, is not it? So, this whatever this numerical diffusion component that we have that is half of, it can be represented as. So, I am just representing this equation into this part, is not it? And this implies that is nothing but half of 1 minus u delta t, delta x, u delta x, delta phi, delta x square. Now, please note here that this parameter I mean this entire thing can be considered as like nu d2 phi dx square, is not it?

It is similar to diffusion in space. So, this nu is half of 1 minus u delta t delta x u delta x. So, this is like this numerical diffusion coefficient which is introduced by this discretization and it is responsible for the numerical or the artificial diffusion and of course, this helps in stabilising of the problem, but one thing we must be careful here that this cannot be negative.

Diffusion cannot be negative, is not it?

So, this numerical diffusion that we are whatever we are adding this nu has to be positive always which means that u delta t by delta x has to be less than 1 and what does this tell you? u delta t by delta x it is nothing but I mean this is nothing but the flux or the transport, convective transport that is made in or the flux that is transported in one time step divided by the grid spacing.

This has to be less than 1, is not it? So, that is the, that tells you that how would you like to make a choice of your delta t and delta x and this this this factor is generally known as the Courant number. So, essentially the Courant number should be below 1 for when we have high advection or high convection present in your system. This is also known as a CFL stability criteria. So, whatever, this u delta t by delta x has to be less than 1.

I mean u is as you can think of this to be as a certain convective transport scalar, convective flux scalar or velocity scale whatever and this also helps determine our choose to what should be your delta t based on your grid resolution to the problem. And these criteria also needs to be satisfied when you have high advection or convection-dominated cases, high Peclet number in your system or high Reynolds number also in your system. And this is very essential for the stability.

So, this Courant number is less than 1 for one-dimensional space problems, if you have two or three-dimensional space problems, this needs to be either you can satisfy this to be this needs to be satisfied like for two dimension it is less than half and for three dimensions less than one third. So, the largest value of this Courant number should be satisfying this maximum value for this stability to happen.
So, I hope all of you have realised or understood the different stability criteria present for explicit finite difference scheme and these needs to be satisfied or kept in mind while trying to do the framework for numerical solution using finite difference or essentially explicit finite difference schemes.

In the next class, we will see how we can use this approach method of lines or this finite difference to solve using explicit method, a simple problem as well as in the upcoming classes we will also see how, what do we mean by the implicit schemes of finite difference and what is the distinction between these two strategies and these two. I hope all of you liked today's class, see you again in next class.