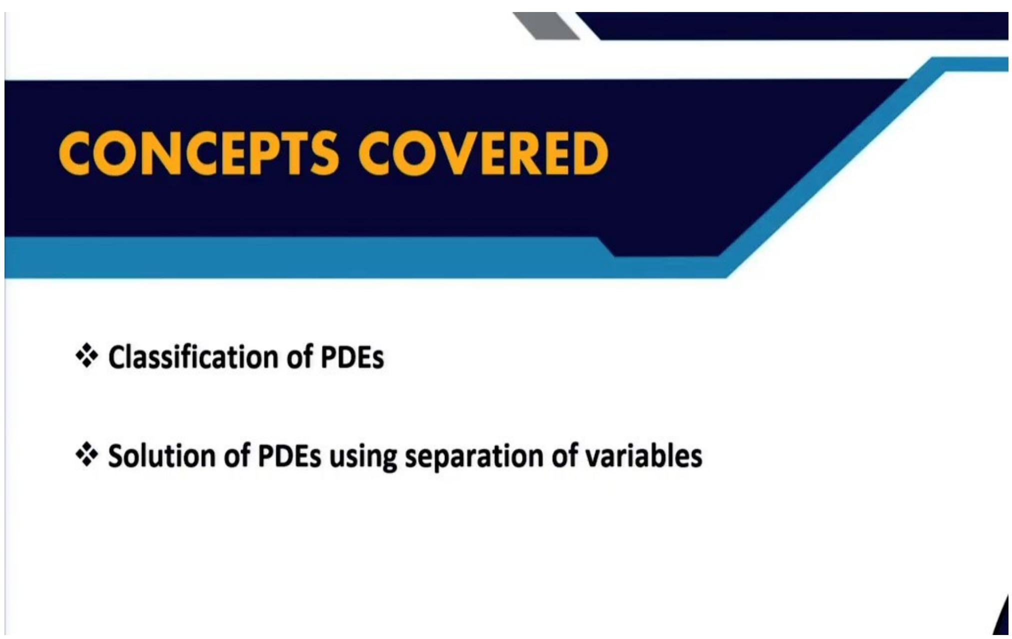
Mathematical Modelling and
Simulation of Chemical Engineering Process
Professor Doctor Sourav Mondal
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Lecture 07
Partial differential equations

Hello everyone, in this lecture, we are going to study about the different partial differential equations and their implications, how do we mathematically solve them, particularly the linear types? What are the different techniques? What are the different classifications essentially? Because these techniques are quite dependent on the type of the PDE is that we are looking forward to. Generally, we encountered PDE for any time dependent distributed system.

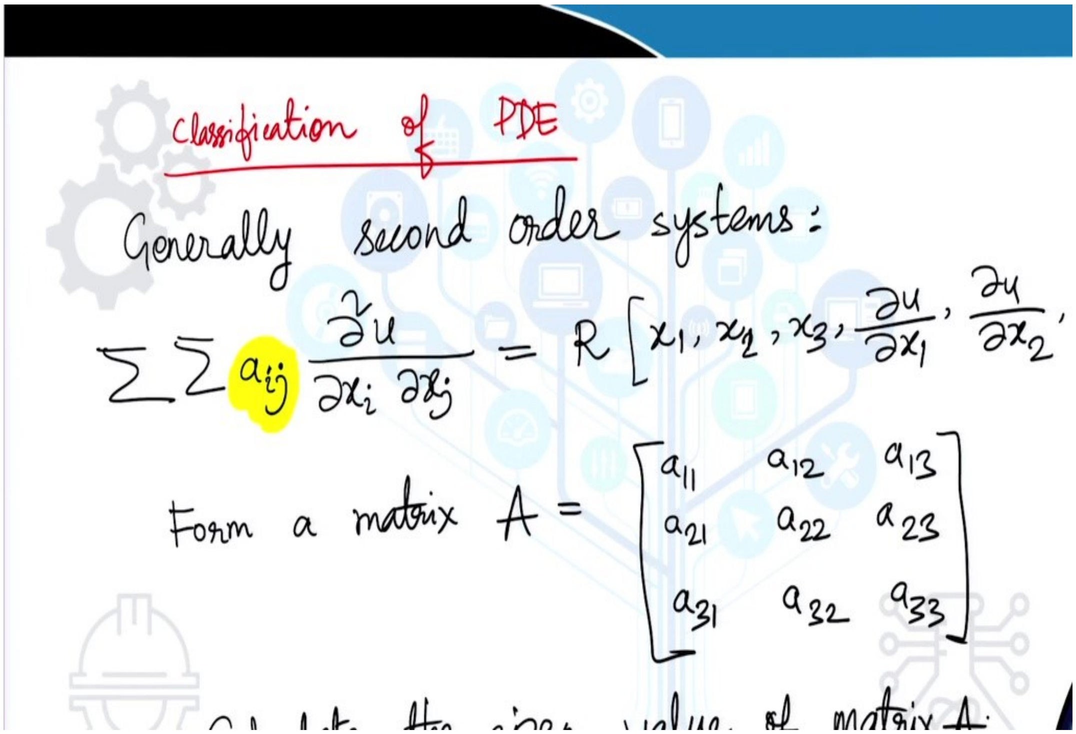
So, in a process, if there is a variation of a particular this, this variable along the space, then it is quite likely that you would encounter a PDE and whether it is 1 dimension in space or 2 or 3 dimensions that depends on, the dimensionality of the problem. But in general, if you have a time dependent spatially distributed variable, you are likely to end up in a scenario which involves the use of partial differential equations. So, partial differential equations or handling partial differential equations, is very prominent and quite common in chemical engineering processes.

(Refer Slide Time: 1:38)



So, with this let us look into the different classifications of the PDE, which is something we will be going through in this lecture and the possible solution techniques using separation of variables for different types of PDE's.

(Refer Slide Time: 1:55)

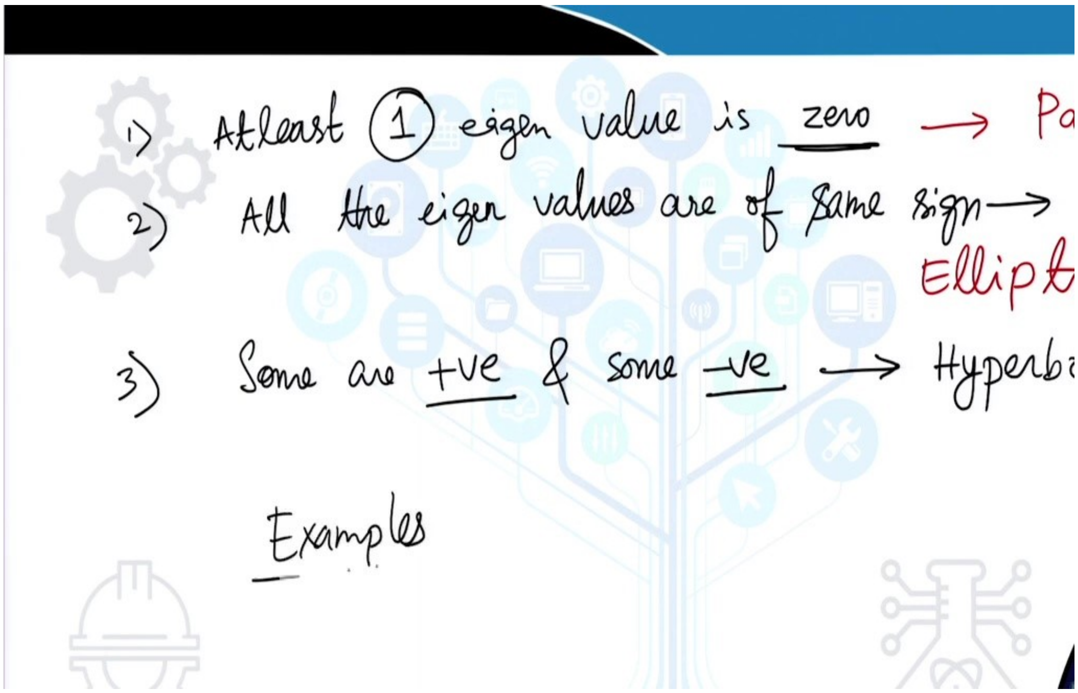


So, now, let us begin the classification the part of the PDE. So, generally write classification of PDE. So, generally these PDE's are second order systems. So, the highest order is 2 and the most generic framework of these PDE's can be written something like this and once we just write the equation you will realize that the generality is quite apparent here. So, these are all on the left-hand side we write all the second order terms on the hand side there could be functions of the dependent variable functions of the independent variable, it could have their first order terms it could have the dependent variable, also this is a generalized case.

For 3 dimensions in case if you have 1 or 2 dimensions and the different these independent variables would be less. Now, from here from this generic fashion of the PDE this coefficient, this coefficient before the second order term is actually the reason or actually tells you that how to determine the type of the PDE. So, when I say about the type I mean whether it is elliptic, parabolic or hyperbolic systems.

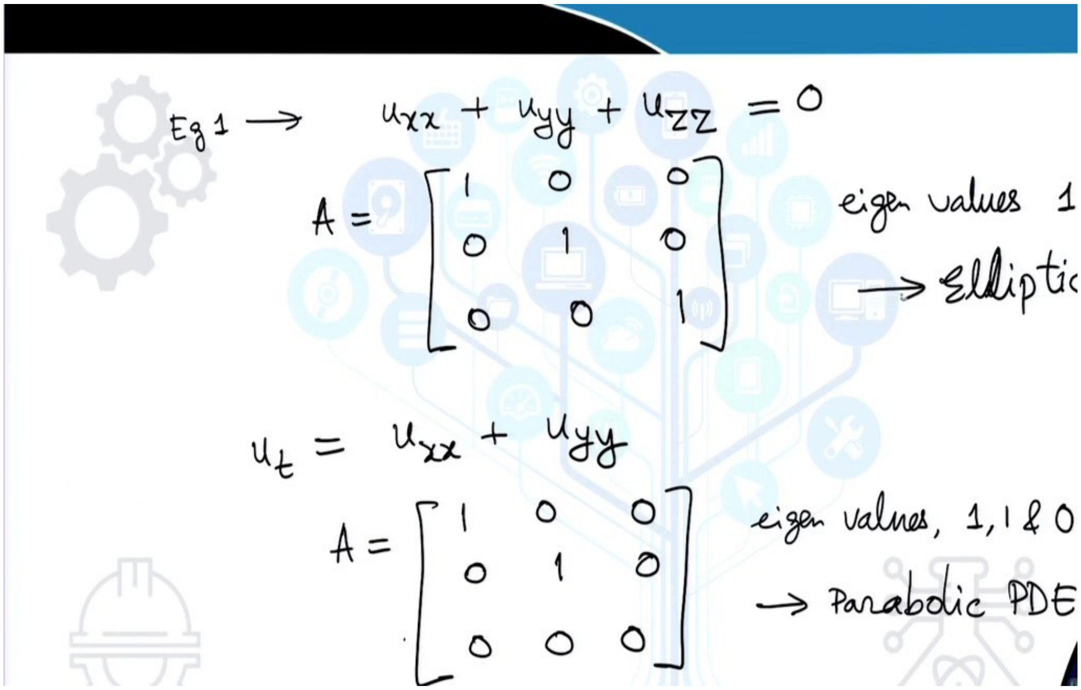
So, you need to form a matrix of these coefficients let us say for matrix sort of the coefficient matrix involving the terms of the second order quantities. Let us write this in this way. I hope the indices are quite self-explanatory to you. And then calculate the Eigen value of the matrix A of this coefficient matrix. So, based on the Eigen values there are possible classifications.

(Refer Slide Time: 4:38)



So, what are these? So, if at least the case 1 is at least, sorry, I do not know why, at least 1 eigen value is 0, if this is the case, then you are going to have a parabolic system. We will see some examples and it will be more clear, next situation is if all the Eigen values are of same sign, then you get elliptical or elliptic system. The third scenario is, if some are positive and some negative then you are going to land up with a hyperbolic system. So, these things are best learnt by an example.

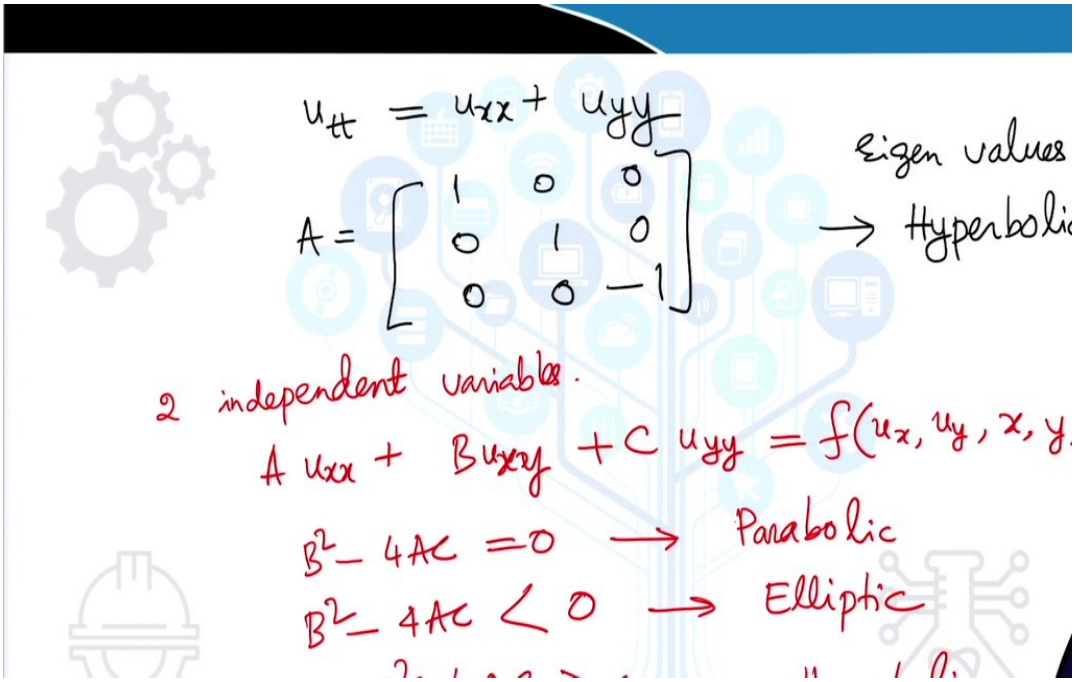
(Refer Slide Time: 6:13)



So, let us see some of the examples. Let us consider a scenario, example 1, something like a steady state multi-dimensional temperature field. So, u is the process variable you can think it to be a temperature or something like that. So, grad square T is equal to 0. So, in this case if you try to write down this coefficient matrix it's only the diagonal elements, as you can see do exist for the coefficient matrix and so, the coefficient matrix would look something like this identity matrix and in this case. You can clearly identify understand that the Eigen values are 1, 1 and 1.

So, this is a system as far the definition is an elliptic PDE. So, this is an elliptic PDE another example. So, this is a 2-dimensional time dependent distributed parameter system, and these are most commonly used types. So, this is the case here because for the case of time, there is no double derivative terms, there is no second-row terms the last row we have written down as 0, 0, 0. So, the Eigen values in this case are 1, 1 and 0. So, this is a parabolic PDE.

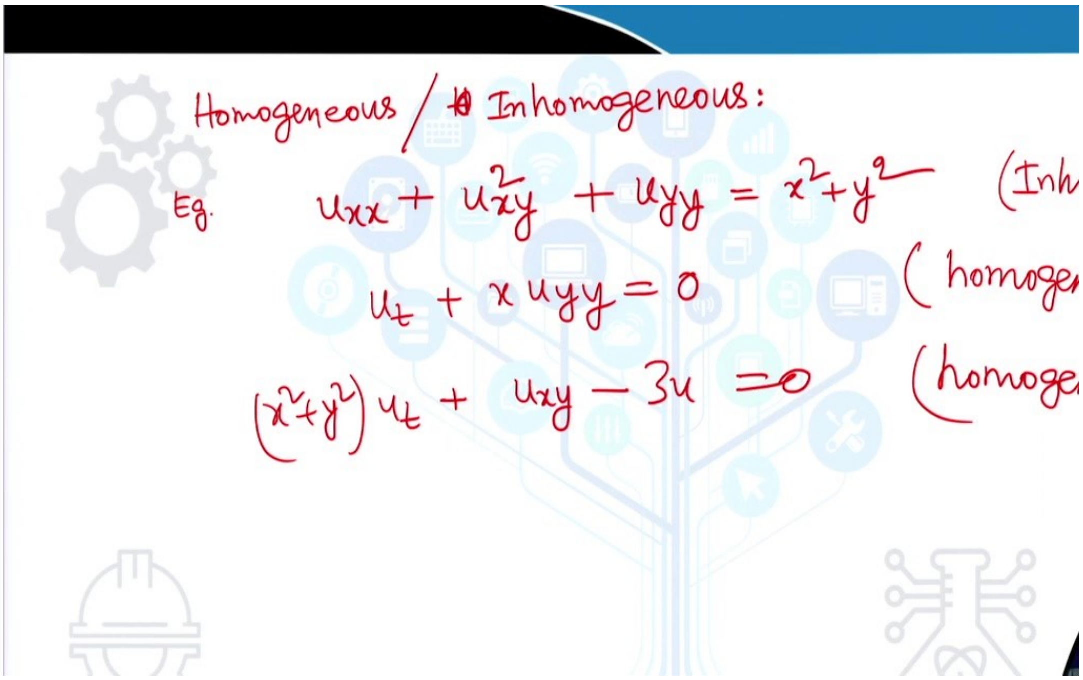
(Refer Slide Time: 8:08)



Let us see another case or double derivative in time. So, the Eigen values are 1, 1 and minus 1 and as per the definition some are positive, some are negative. So, this is a hyperbolic system. So, these types of systems are generally not common in chemical engineering and this normally you had encounter in web mechanics or in quantum mechanics. So, in the case just to give you a short description or a short way or a quick way or say a quick shorthand on in the case of 2 independent variables like if you have 2 independent variables. The criteria for classification of the PDE can be slightly modified and it can be easier one, and this is something can also be proved from the general Eigen value theory also. If this is the case, now, if you calculate the quantity these are coefficients A, B and C to the corresponding second order and the first order, I mean corresponding all the first order terms if the criteria that B square minus 4 A C is equal to 0 then you are going to have a parabolic system, there is just a, different a shorter quick way to assess these systems, classify these systems if this is (sorry) less than equal to 0 this is elliptic.

So, let me not confuse you. And in the case of third case, which is B squared minus 4 A C to be greater than 0, it is hyperbolic. So, one thing that comes to the mind that why are we so worried about the classifications, why we care about them, the reason behind is that this techniques for solving different types of PDE is dependent on what category of PDE these are. And that is why their classifications are understanding or trying to identify them that in which category are they in it helps us to determine that what solution techniques should be applied or implemented what could be the possible challenges during this process.

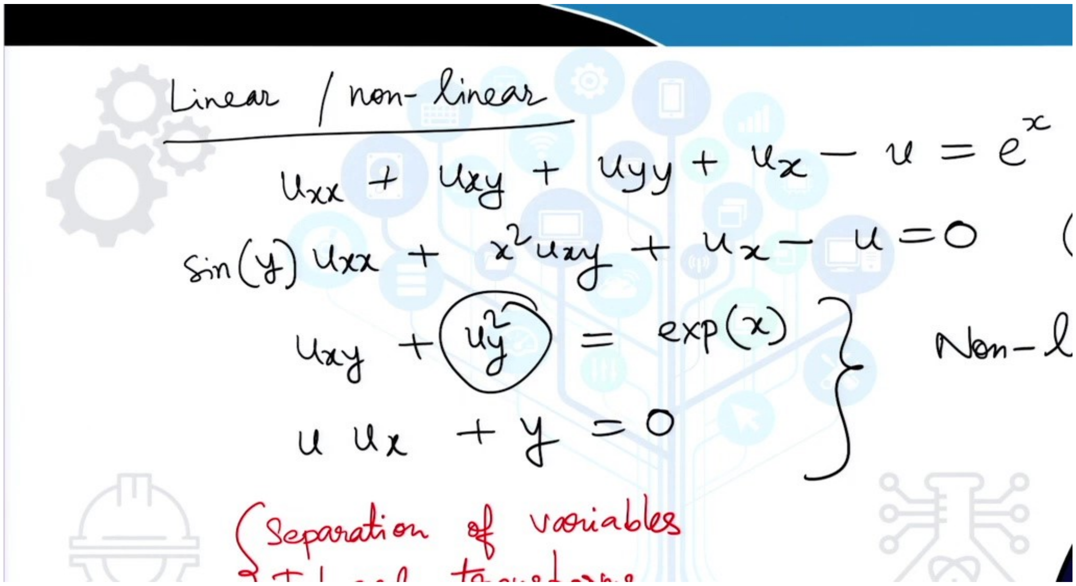
(Refer Slide Time: 11:07)



Next is the criteria for homogeneous or heterogeneous systems. This is something we call not heterogeneous but inhomogeneous. So, if all the terms in the PDE contains the dependent variable or its derivatives, if all the terms contain the dependent variable or its derivatives, we call that system to be as homogeneous else inhomogeneous. So, examples, possible examples, let us see something like this. So, whenever I write something in the subscript it determines the derivative with respect to that quantity.

So, you can clearly see that there are terms on the hand side which does not contain the dependent variable, so, this is an inhomogeneous system. So, for example, something like this… this is a homogeneous system, because all the terms contain the dependent variable other examples like this… this is also homogeneous.

(Refer Slide Time: 12:52)



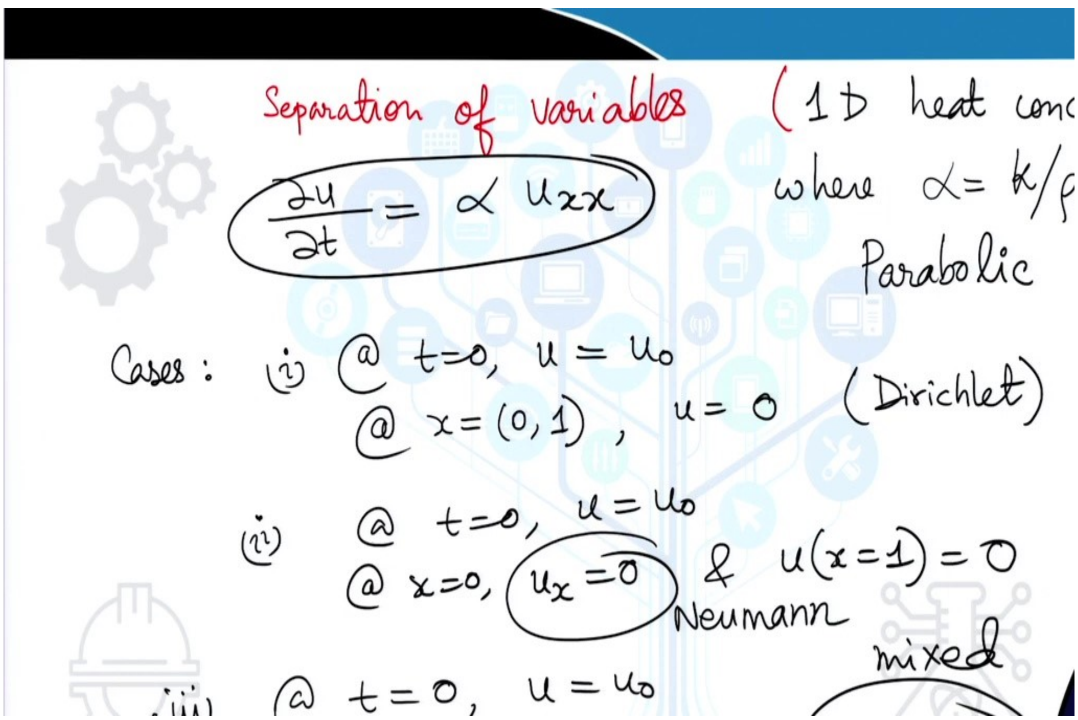
So, the next I mean other classification is the linear or the nonlinear versions. So, if the PDE if the order of the dependent variable in any of the term is 1 or 0 then it is a linear PDE. So, let us see some examples. So, let us say this one. So, we only consider the terms are the terms which have that dependent variable, it does not matter what about the independent variable we have. So, in this case you can clearly see that the terms which contains the dependent variable do not have order more than one. I mean the last time can be considered to be an order 0 term. So, this is a linear PDE. Another example could be sin something like this, again this use, if you see the order of the dependent variable is 1 or I mean there is no term without the dependent variable. So, this is again a linear PDE.

Terms like this brings in non-linearity to the system. So, these are nonlinear equations. So, Navier stokes equation, Navier stokes equation with the convection term or with the inertial term that is genuinely what you see in the left-hand side those are the nonlinear terms. So, the full Navier stokes equation with the inertial terms is a nonlinear system. Again, Naiver stokes equation without the inertial terms, only the viscous terms is a linear system. Same goes for species transport and your heat transfer equations that without the convective term, generally these systems are linear.

Please note that all analytical techniques can only be used for the solution of linear PDE. It could be homogeneous, it could be in homogeneous but at least a system has to be linear. This is a very, very important criteria for solution of analytical techniques. Only under very special circumstances in 1 or 2 cases nonlinear equations can be solved, but in general it is the linear equations that can be solved analytically. For nonlinear equations, we have to resort to numerical techniques. Possibly in the next I am lecture, you will be discussing about the different numerical techniques for solving mostly nonlinear types equations or even linear equations, but in general analytical equation solutions are only possible for linear systems.

So, there are different techniques for solution of the (I mean the) different analytical techniques for the solution of PDE's are I mean this is the most popular type, separation of variables or combination of variables also it is sometimes referred to in many books, then you have the integral transforms. So, there are other techniques also for solution of PDE, but at least in this course, we will just have a discussion on these 2 techniques mostly for other types of techniques you can always refer to any book on partial differential equations.

(Refer Slide Time: 16:54)

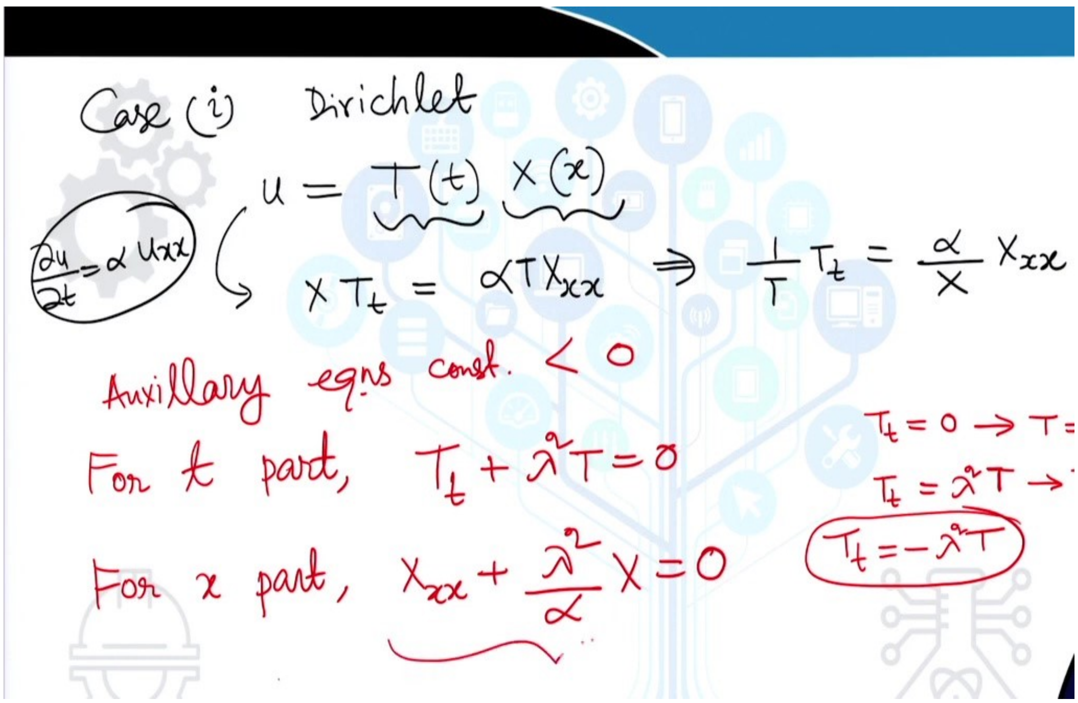


So, let us first start with the separation of variable techniques for our 1-dimension heat conduction problem. For 1D heat conduction time dependent heat conduction problem. So, how does the in the Cartesian system you can write this equation as. So, where alpha is equal to k by rho Cp. So, this is a parabolic equation I think by now all of you have understood or realized this and linear also.

So, there could be different possible cases, and we need to investigate at least all of them. The one is at t is equal to 0 these are defined or classified I mean the different types that I am talking about are the different possible scenarios that I am talking about, mostly from the boundary conditions.

So, if you have this sort of Dirichlet type conditions on both the boundaries that is like case 1. Case 2 is you have Neumann conditions in one of the boundaries. So, this is another type, so, here you have the Neumann condition and the third case is the mixed type, x is equal to 1, let us say it is something like this. So, this is the mixed type and these types of conditions generally arise when we have a convective boundary condition. So, the conductive heat transfer is equated to the convective heat transport at the wall to the surroundings.

(Refer Slide Time: 19:36)



Now, let us look into the case 1 systems where we have Dirichlet boundary conditions. So, this is the Dirichlet case. So, now we assume, or we consider this is the first step in the separation of variable technique that this dependent variable is a solution of two linearly independent function and one of this function is dependent to time and another function is dependent to the space and then we start working on this, you try to incorporate this you into the main equation and work out the remaining part from this.

So, this is assumptions, I leave it to you to find out that under what conditions these assumptions hold true and when we cannot have this sort of assumption and that is the point where separation of variables cannot be used. So, with this let us go ahead and here we are trying to use the main equation which is this.

So, if you try to use this u substituted here you are likely to get something like this. So, from here you take the variables on both sides of the equation. So, it will look something like this. Now, if you see the left-hand side and the hand side of this equation, the left hand side contains term related to only functions of time and the hand side contains term related to only functions of space and these terms may only equal when they are constant is not it.

That is only possible that you can equate a function which is appears to be a function of time and the hand side it is a function of space whatever and these 2 are equal. How does it possible? it is only possible when they are constant is not it each one of them is constant or these terms actually represents a constant quantity. Now, the question comes that what should be the value of this constant? can it be 0? can it be I mean of course, we are assuming it to be a real number can it be negative can it be positive what it is? Now, please note couple of things.

So, there could be these 3 possibilities it could be 0 it could be positive quantity, it could be a negative quantity, why I am intentionally writing this something lambda square because a square of particular quantity will always be a positive. So, it is like forcing it to be positive and forcing it to be negative cases. So, if this constant is equal to 0, what does this immediately imply? So, if I set this criteria for 0, if the constant is equal to 0, it means this T(t) is equal to 0 or immediate implication is T is constant. So, this is a steady state scenario the constant is equal to 0 there is no time variation, is not it or the time temporal part does not vary with time.

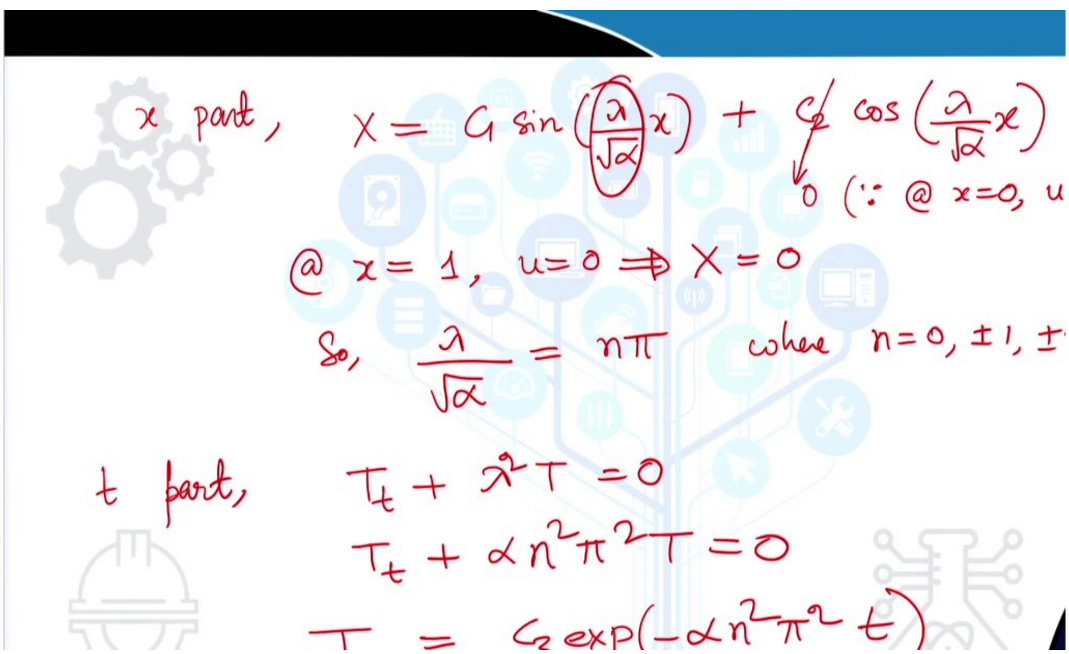
So, there is no dynamics to the problem. If this is positive, so, this is like (lambda square) lambda squared T, then you are going to have this solution in terms of exponential increase, isn't? it clearly this tells you that this is going to increase exponentially with respect to time and at a finite I mean, there will be a possibility that it will as time goes on the temperature value is going to increase it is becoming like unbounded, that is not the case. It will always have a steady state value which is cannot be in finite.

So, this possibility is also not I mean then T becomes unbounded. So, this also does not look to be a possible scenario, the other likely scenario that you can understand is this the minus quantity and this you can clearly understand it will give you an exponential decay form, and that becomes that tells you that T is like become a reaches a finite value at infinite time. So, this is the most likely scenario, and this is the correct choice of the constant. So, let us frame the auxillary equations with this lambda squared this to be ah sorry not lambda squared this constant to be negative.

So, in this case, we are going to have for the time part, for the time part T(t) plus lambda square T is equal to 0 isn't, this is the case for the time part and this immediately tells you that you are going to have a sort of exponential form, but at least this is the auxillary equations this is the ODE now and for the space part for the x part you are going to have… So, these 2 auxillary equations are themselves two ODEs.

So, you sort off, transform this PDE into 2 auxiliary ODEs and solution to these individual auxillary ODE satisfying the boundary conditions will give you the total solution or their product of these 2 individual functions will give you the total solution. So, first let us look into the x part. So, the x part equation as you can clearly understand from here, we will have solutions.

(Refer Slide Time: 26:07)

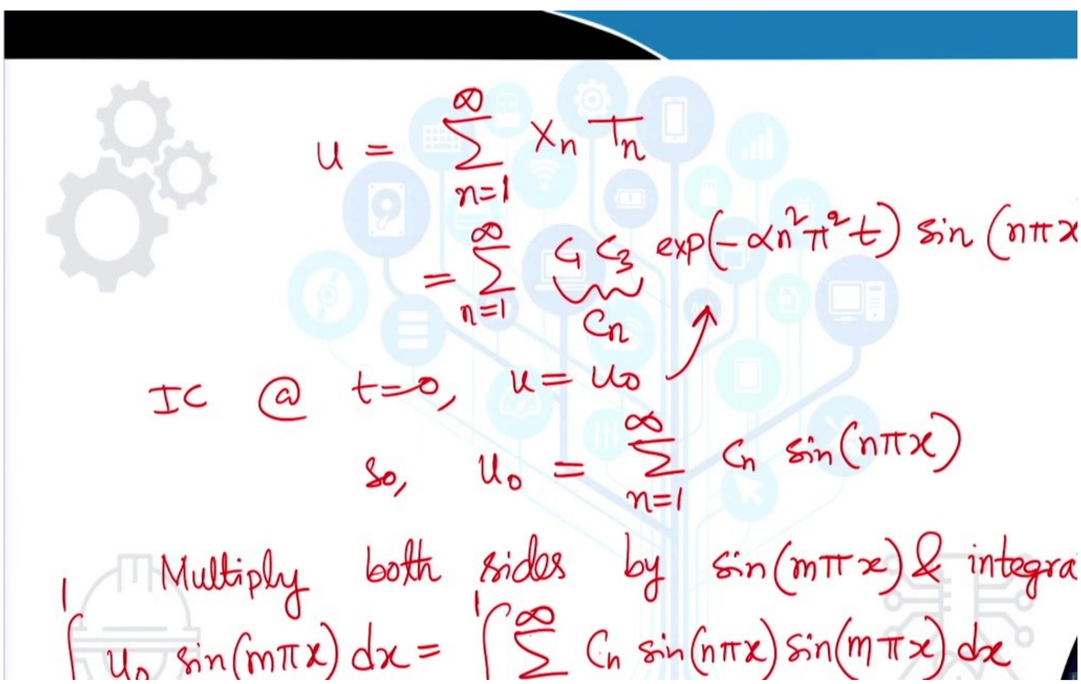


So, for the x part or the space part from that equation so, you can clearly understand that the solution to x is sin and cosine functions. So, it is going to look something like this. Now, that from the boundary condition at x is equal to 0 this u is equal to 0. So, if we and this is the space part, so, I can easily say that the x is equal to 0 time for the time component is not equal to 0. And in this case, we can easily set that the space part will be equal to 0. So, this tells you that it is only possible that if x is equal to 0, unless and until C is not equal to 0, it is not possible to have this solution.

So, C has to be equal to 0 because at x is equal to 0, u or capital X is equal to 0. So, this suggests that you are having only one constant C. So, at x so, we applied other boundary condition at x is equal to 1, u is equal to 0 which implies capital X is equal to 0. So, this means, that (this means that) if the x is equal to 1 if the capital X is 0 clearly C1 is not equal to 0. So, you will end up with the condition that this lambda by this quantity this should be equal to integer multiples of pi where n could be 0 plus minus 1 plus minus 2 or any, any positive or negative integer quantities, and from the time part we get this, we already have our lambda here.

So, from there we will substitute, I have just invoked added additional constant thus identified instead of T as Tn because for different values of n you can expect to have different functions of these. So, these are different linearly independent functions and finally, we have to add them up to get a final solution. So, the final solution let me talk about this first.

(Refer Slide Time: 28:57)



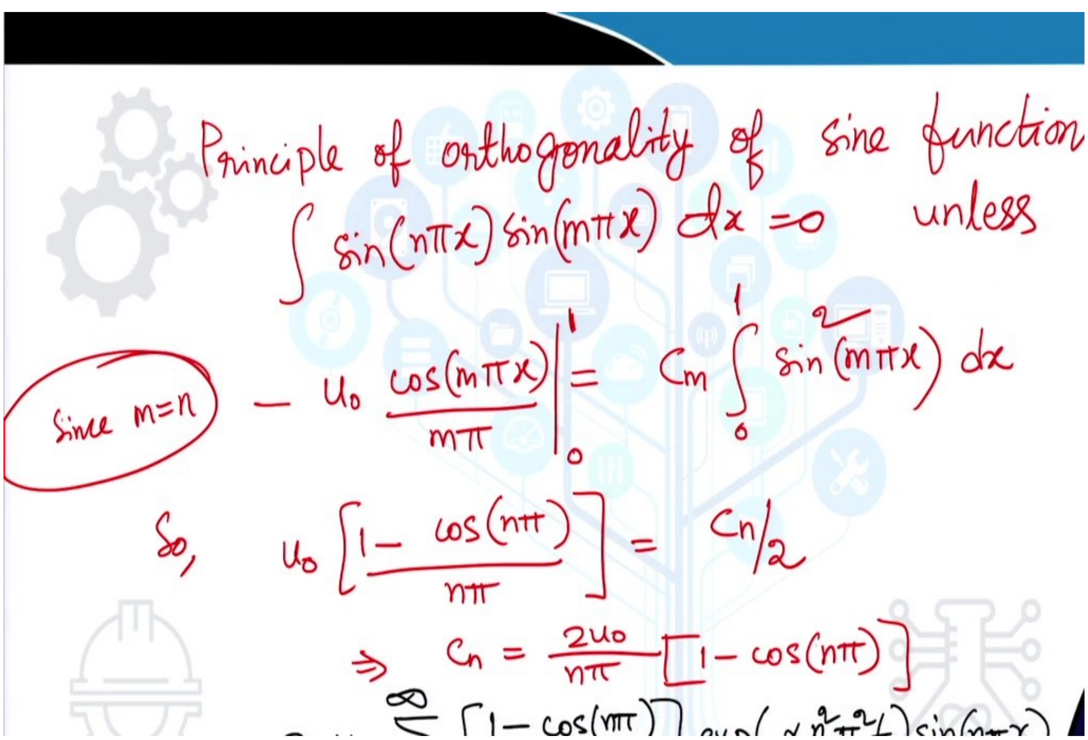
So, the final solution is the linear superposition of all the possible Eigen solutions. So, this u is equal to Xn and Tn, n is equal to 1 to infinity. So, this means, you are going to have C1, C3, first this exponential part let us say we clubbed them this together and write this as Cn because these constants can also be functions of n.

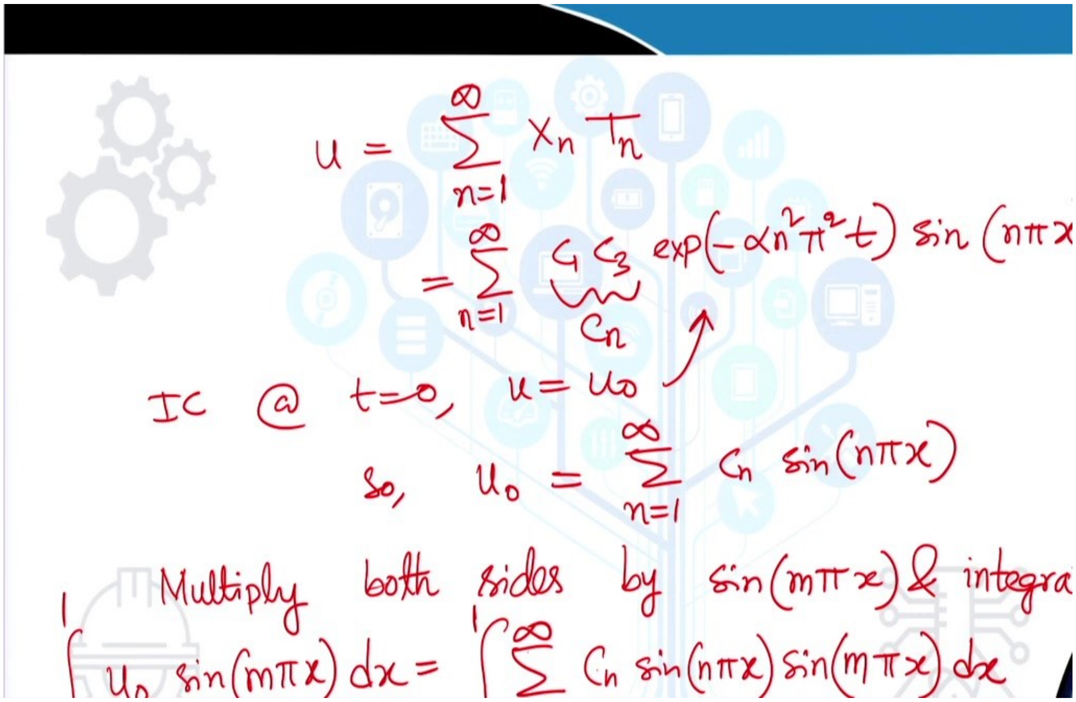
Now, it is time to use the initial condition which tells you at t is equal to 0, u is equal to u naught. So, if I use this condition here, this tells me that all the exponential part will go away. So, U0 left hand side is equal to summation of Cn sin n pi x, n is equal to 1 to infinity.

Now, if you multiply both sides, if you multiply both sides, so, now, how to proceed from here, how to find out your Cn? So, for that we will try to use the principle of orthogonality of the trigonometric functions. So, let us say I multiply on both sides. So, you multiply on both sides by sin m pi x, where m is not equal to let us say we say this later on is equal to x. So, we write the integration and we integrate on both sides. So, sin m pi x dx integration and then you have the summation Cn sin and n pi x sin m pi x dx 1 to infinity and this is integration so, we multiply and then integrate.

So, clearly you can see that the right hand side unless m and n are equal this will be 0 that is what the principle of orthogonality. So, the principle of orthogonality tells you that if you have two sin functions or two trigonometric functions until and unless this m and n values are equal this will be 0 the product will be 0.

(Refer Slide Time: 31:48)





So, principle of orthogonality tells you sin functions tells you that sin n pi x, unless m is equal to n. So, unless m and n are equal, this integration does not exist. So, from the summations term here, all the terms except the case when m and n are equal will go away. So, this now summation sin will not I mean summation will not exist because all the quantities will be equal to 0 except for one case. So, this brings us to the condition that I can easily integrate, let me write the hand side let us say m and n are equal.

So, I can write that to be as m, so, this is sin m pi x and both these two are equal to the square dx this is the hand side and the left-hand side I can easily integrate it out. So, I will be getting u naught cos m pi x. So, please note the m and n are same and only in that case only we can evaluate this system. So, 0 to 1 it is possible because m and n are equal. So, what we get. So, we just do the steps here. So, I can interchange always my n and m this will become Cn by 2 and this gives you your C is equal to 2 u naught n pi.

So, you can clearly see that this constant is also a function of n. So, the final solution, the final solution turns out to be we just replace this n here, Cn here, and this looks something like this. So, this is a linear superposition of all the different functions for possible values of n. So, n can take any values from 1 to infinity. So, I hope all of you have got an understanding of the solution of PDE's by partial differential technique, considering the boundary conditions are deliberate in nature.

So, in the next lecture we are going to talk about, again, the same technique but for different boundary conditions, because there you will end up with a slightly different set of auxillary equations and solutions. I hope you liked this lecture. Thank you.