

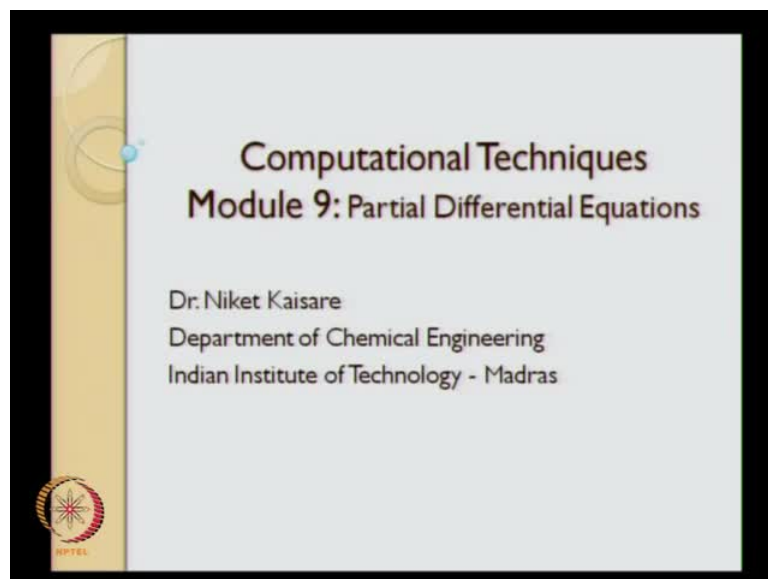
Computational Techniques
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Module No. # 09
Lecture No. # 01
Partial Differential Equations

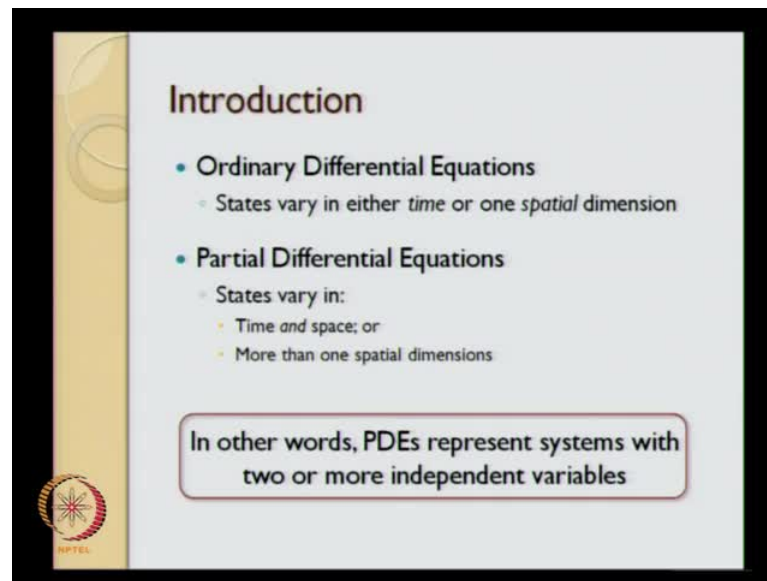
Hello and welcome to module 9 of the computational techniques lecture. We are finally reached the last module of our course. In this particular module, we are going to talk about partial differential equations and a couple of numerical methods to solve partial differential equations. What I am going to do is, describe what we mean by partial differential equations go over how partial differential equations arise in chemical engineering problem; and then talk about a few methods - couple of methods - to solve partial differential equations.

This is a very important and indeed a very vast field solution of partial differential equations; so, we are only going to give an introductory over view of the various things that are involved once when it comes to solving PDE's.

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The slide is titled "Introduction" and contains the following content:

- Ordinary Differential Equations
 - States vary in either *time* or one *spatial* dimension
- Partial Differential Equations
 - States vary in:
 - Time *and* space; or
 - More than one spatial dimensions

In other words, PDEs represent systems with two or more independent variables

The slide also features a logo in the bottom left corner with the text "NPTEL" below it.

So, let us look at what PDE's actual mean; so, this is the last module of this particular course. In the previous module, we covered ordinary differential equations; **the ordinary,** in the ordinary differential equations, the state variables change with respect to time or with respect to one spatial dimension only; for example, in the heat conduction problem the temperature varied along the length of the rod.

In the reactor problem, **the temperature,** the concentrations varied along the x direction, for example, if you have a reactor in which certain reactions are taking place, it is a batch reactor; and under those conditions the concentrations are going to vary with time and not with respect to space; so, **these, all these equations give rise to ordinary...** all these problems rather give rise to ordinary differential equations; and ordinary differential equations are written in the form of $\frac{dy}{dx}$ or $\frac{dy}{dt}$ equal to some function of (t, y).

So, in this particular case, our t or x becomes our independent variable, whereas the other quantities are the dependent variables. In case of partial differential equations, the states will vary either in time and in space or it will vary in more than one spatial dimensions, that means, it is going to vary in x and y directions or x and r radial directions so on and so forth.

In other words, technically what we say is, PDE's are used to represent systems which have two or more independent variables, time and space or more than one spatial dimensions.

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An Example

- A conducting rod
 - $\frac{d^2T}{dx^2} = \beta(T - T_a)$
 - $T(0) = \gamma$
 - $T(L) = \kappa$
- A conducting block
 - $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$
 - $T(0, y) = \gamma$
 - $T(L, y) = \kappa$
 - $T'(x, 0) = \lambda(T - T_a)$
 - $T'(x, d) = -\xi(T - T_a)$

So, these are these are the these are, this was one of the example that we took when we talk about ordinary differential equation, that was of a conducting rod, this end of the rod was kept at thirty degrees, the other end of the rod was kept at eighty degrees, and the rod overall was losing heat to the surroundings and we develop differential equations for that.

Now, instead of a rod, if this is going to be a block of brick or a block of metal or a block of wall, a rectangular piece, in which one end is kept at one temperature, the other end is kept at other temperature, and we have heat transfer taking place from these two ends; in that case, what we will end up getting is that, the temperature at any location is going to change with both x direction as well as with y direction; as a result we have two independent variables x and y; and dependent variable t is going to be expressed as with respect to the coordinate x coordinate as well as the y coordinate; so, t at any location in this particular rectangular block, we will try to find that using methods to solve partial differential equations.

Now, if you were to write the equations, this is the type of equation we had written in the previous module, $d^2 T / dx^2 = \beta (T - T_a)$, where T_a we had taken if you remember from last time as thirty degrees Celsius; and we required two conditions, the boundary conditions temperature was specified at either ends of the rod; and then we try to solve this particular problem and this resulted in numerical ways; two numerical ways to solve that problem, using shooting method and using the finite difference method, that is what we had covered in the ordinary differential equations module of this course.

Now, if we have, **you know**, temperature varying with both x and y , what we are going to get is a partial differential equation of this type; now, this is what is known as a Laplacian equation; so, temperature at any interior point in this particular block is going to depend on the temperature at all the four neighbors **in that** in that particular block; now, this gives rise to **in** equation of this form, $\nabla^2 T = 0$.

Now, if there is say an electrical heating or a reaction heating term, then we multiply this entire term by thermal conductivity and add that electrical heating kind of a term, **as a source term**, on to the right hand side; but again coming back to this original problem what we are going to have is, $d^2 T / dx^2 + d^2 T / dy^2 = 0$; x and y are the two independent variables; and **at** at this end that temperature is specified, that means, temperature at $x = 0$, is specified to be some value γ temperature at $x = l$ is specified at another value γ .

And what we do at these two ends is that, the flux is given, that means, the gradient in the temperature is **is** given to us; so, it is basically going to be thermal conductivity k multiplied by $d T / dy$ computed at $(x, 0)$ and computed at (x, d) , where d **is** is the distance in the y direction; those are given as the **heat** heat loss terms from that particular edge to the surroundings; so, that will essentially result in mixed boundary conditions.

So, here, at these two ends, we are going to have Dirichlet type boundary conditions; at these two ends, we have mixed boundary conditions **where** where both T as well as T' appear in the boundary condition; if any of this, so for example, if this particular wall is

going to be insulated, then we will have $\frac{d^2 T}{dy^2}$ at $(x, 0)$ is going to be equal to 0; under those condition we will have a Neumann boundary condition.

So, just the three types of boundary conditions that we spoke about in the previous module are also the kind of boundary conditions that would be applicable in partial differential equations as well; so, recapping what we have in case of partial differential equations is, the differential terms in more than one independent variable; and based on the order of the differential term in each of the independent variables, we will need that many number of initial or boundary conditions and in that particular domain.

For example, we have $\frac{d^2 T}{dx^2}$, which means we need two boundary conditions **in** at x ; likewise, we have $\frac{d^2 T}{dy^2}$, we will require two boundary conditions again at y ; this is one boundary condition at x equal to 0, other boundary condition at x equal to 1; likewise, this is one boundary condition at y equal to 0 and the other boundary condition at y equal to d .

So, this is the type of problems that, this is one example of a type of problem that we are going to encounter when we talk about partial differential equations.

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Plug Flow Reactor

- **Steady State Model**
 - Model: $\left(\frac{F}{A}\right) \frac{dC_A}{dx} = -r(C_A)$
 - Initial Condition: $C_A|_{x=0} = C_0$
- **Unsteady Model**
 - Model: $\frac{\partial C_A}{\partial t} + \left(\frac{F}{A}\right) \frac{\partial C_A}{\partial x} = -r(C_A)$
 - Initial Conditions: $C_A|_{(t=0),x} = C_0$; $C_A|_{t,(x=0)} = C_{in}$

This particular equation is what is known as a second order linear partial differential equation and the type of this equation is what is known as elliptic equation; we will come to that in a few minutes from now. Let us go on to the second example; the next example

I am going to talk about is a plug flow reactor; we have consider the steady state model of a plug flow reactor in our ordinary differential equations course both in initial value problem as well as in boundary value problems; and boundary value problems we had modified this problem by using an axial dispersion term over here; in the initial value problem we had this kind of an expression.

In an initial value problem, an addition to this equation, we had the boundary conditions specified at x equal to 0; now, instead if we were to solve an unsteady module, a transient module for the plug flow reactor, we will result, that will result in partial differential equations, because the concentration c of a is going to vary both with time and space; this particular equation is a first order equation in both time and space.

As a result, we will have an initial value problem in time as well as an initial value problem in space. The initial conditions for this particular problem is, c_a at time t equal to 0 and for all the x is some initial value c_{naught} ; and the initial condition for x equal to 0 that the c_a is specified at all times at x equal to 0, that is entrance of the reactor as some concentration at the inlet.

So, subject to these two initial conditions, we are interested in solving this kind of a problem; so, that is the other example of sorry, that is another example of a partial differential equation; this is going to be depending on the rate of reaction term, it is either going to be a linear or a non-linear partial differential equation; and it is going to be a first order partial differential equation both time and space, because it is a first order partial differential equation in time, we require one initial condition in time, because it is first order differential equation in space we require only one condition in space as well.

Depending on whether r is a non-linear expression or a linear expression, this entire model PDE model is either going to be a linear model or a non-linear model; for example, if you have a zeroth order or a first order reaction, that is rate equal to $k c_a$ to the power one or $k c_a$ to the power 0; in either of these cases, we are going to have this equation as a linear partial differential equation.

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Typical PDEs of Interest

- First order PDEs

$$D\frac{\partial\phi}{\partial x} + E\frac{\partial\phi}{\partial y} + F\phi + G = 0$$
- Second order PDEs

$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial x\partial y} + C\frac{\partial^2\phi}{\partial y^2} + D\frac{\partial\phi}{\partial x} + E\frac{\partial\phi}{\partial y} + F\phi + G = 0$$

Linear if (A to G) are functions of x and y only
 Homogeneous if G = 0

So, let us summarize what are the types of PDE's that we are going to encounter; these are not unnecessarily the most general form of writing PDE's, but these are general enough for the types of problems that we are going to encounter in this particular course.

First, we have a first order PDE; phi is the dependent variable; phi is the variable that we are trying to solve these equations for we want to obtain phi as a function of x and y in this particular case; and this is the first order PDE in both x and y; as long as either d or e one of them at least are non-zero, we will have a differential equation; if one of them is 0, it is an going to be an ordinary differential equation and not a partial differential equation; at non-zero d and non-zero e are going to ensure that we have partial differential equation.

The second order PDE's on the other hand in the most general form would be written in this particular form, there is a d square phi by d x square term; there is a mixed derivative term; there is a second order derivative in y first order derivative terms; this is a term which does not involve derivative, but it involves only phi and this is going to be a constant term; in general f multiplied by phi plus g can be written as another function say h of phi in general, that is the other way of writing this equation.

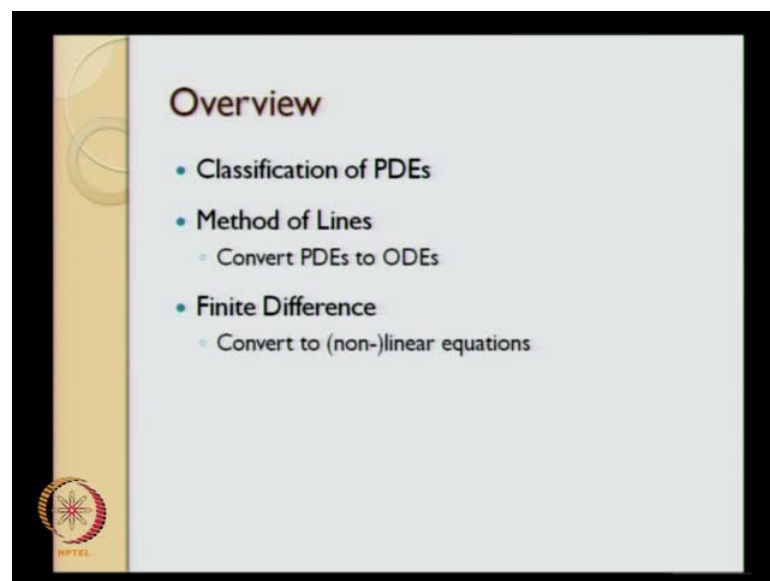
Now, if a b c d e f and g are functions of x and y only and they are not functions of phi or d phi by d x or d phi by d y so on and so forth; then this equation is called a linear partial differential equation; if a to g are functions of something other than just x and y or they are non-constant, under those conditions we are going to have this equation as a non-

linear partial differential equation; so, let us compare this with the two equations that we obtained in the previous two slides.

So, if we go to this conducting block, we we have a over here is equal to 1 and c over here is also equal to 1; so a is 1, c is 1, b d e f and g are all 0; as a result, that is going to be second order PDE in both x and y ; and it is the it is a linear PDE because a and c are both constants and other guys are 0.

In addition to being linear PDE, it is also a homogeneous PDE, because we do not have a constant term g in that particular expression; so, if g is 0, we are going to have homogeneous PDE, f a two g r either constant or functions of x and y only; under those conditions we are going to have linear PDE. And then further we are going to talk about classifications of PDE's based on the values of a b and c . We are going to have three different types of PDE's specifically; we will have what is known as elliptic PDE, parabolic PDE, and hyperbolic PDE's.

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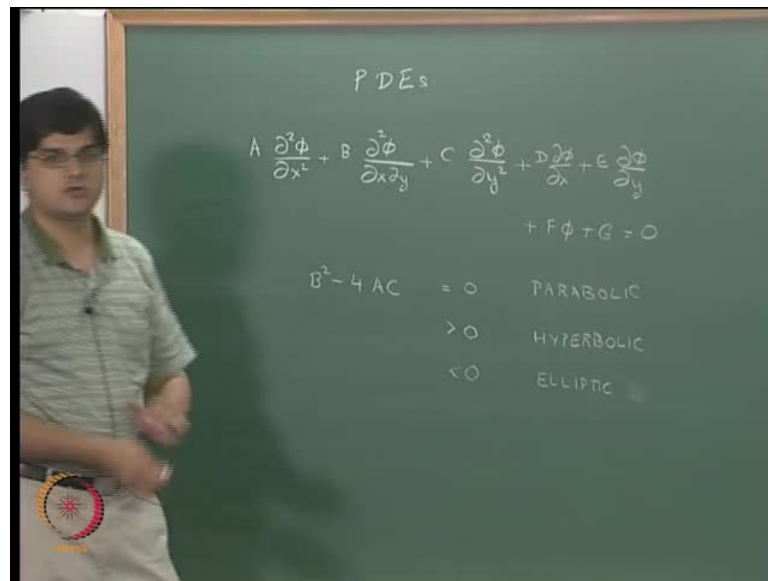


Now, elliptic parabolic and hyperbolic PDE's actually differ from each other in how solution evolves in that particular domain; we are going to indeed talk about that in a in a in a short while; and again it is not going to be very, it is going to necessarily be a very brief description of what what those things mean and especially what they mean when it in in context of solving using numerical techniques; we will we are going to cover that.

So, the overview of what we are going to do in this particular module - first we are going to talk about classification of PDE's, next we are going to use what is known as method of lines with convert PDE's to ODE's and then solve those ODE's using any of the ODE solution techniques. In case of method of lines, specifically, these are applicable to what are known as a parabolic and hyperbolic ODE's and they are applicable to first order ODE's. And then we are going to talk about finite difference techniques, where the oral PDE is converted to linear or non-linear set of equations; and then we use any of the non-linear solvers in order to solve this non-linear set of equations; so, that is going to be very brief overview of **what going** what we are going to talk in this particular module.

So, let us now go on to the black board and start talking about some of these things give us quick introduction to PDE's.

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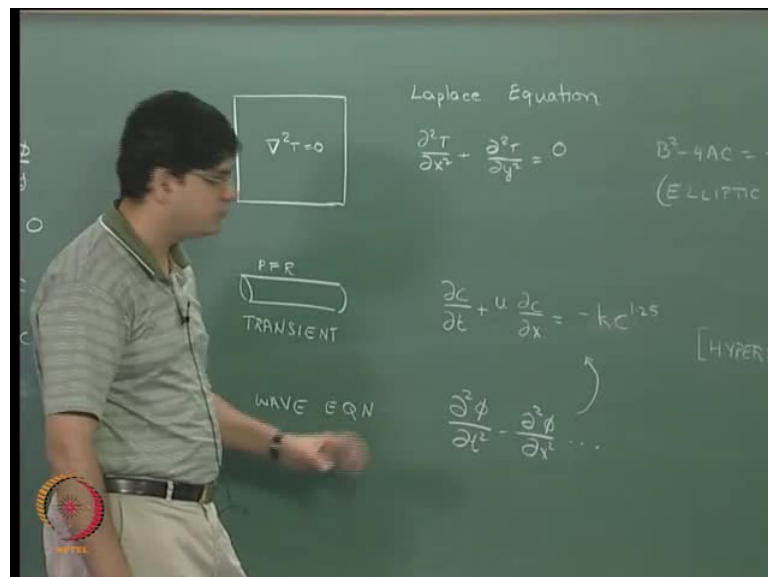
So, let us now continue talking about partial differential equations; what we said is, general second order PDE would be written in the form of a d square phi by dou x square plus b dou square phi by dou x dou y plus c dou square phi by dou y square plus d dou phi by dou x plus e dou phi by dou y plus f phi plus g equal to 0; that is going to be a general second order partial differential equation.

Now, this particular partial differential equation depending on the values of a b and c are classified into three types; and that classification is based on the value b square minus

four a c; if b square minus four a c happen to be equal to 0, we classify this as parabolic PDE's; so, an example of parabolic PDE **PDE** is going to a transient equation **of**, for example, if we have the axial dispersion model and we are going to do a transient equation of that, in that particular case we do not have a d square phi by d t type of equation; so, both b and c are going to be, for example, equal to zero; under those conditions this particular guy is going to be equal to 0, I will talk about that in a few minutes from now.

Now, if b square minus four a c, if that value is going to be greater than 0, then we are going to have hyperbolic equation; and if it is less than 0, we are going to have elliptic PDE's. So, **this**, these are what are known as the three classifications of second order PDE's in general. Now, **I** what I do not intent to happen is, just to memorize what parabolic, what hyperbolic, what elliptic are defined as; what I want to do **in this particular module**, in this particular lecture of this module is, talk about what do we actually mean when it comes to parabolic or hyperbolic or elliptic equations from point of view of solving these numerically; so, that is what is going to be more critical than just classifying them as parabolic hyperbolic or elliptic type of equations.

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Now, let us look at again the problem of that block of metal or block of brick or block of wall, where we are going to solve heat conduction problem; that particular heat conduction problem gives rise to an equation of the form del squared t equal to 0; this

particular equation is known as a Laplace equation; and what this amounts to in Cartesian coordinates is, $d^2 t \text{ by } d x^2 \text{ plus } d^2 t \text{ by } d y^2 \text{ equal to } 0$; now, if we **were to go and** use this particular definition, we have our a equal to 1, our c is going to be equal to 1, and b is 0.

So, 0 minus four $a c$ which is minus 4, minus 4 being less than 0 this is going to be an elliptic equation; the second example that we took was that of a plug flow reactor and we are going to develop transient or unsteady state model for this; and I am not going to **go into how to** - develop this model, but the type of model that we are going to end up with is going to be $d c \text{ dou } c \text{ by } d t \text{ plus } u \text{ or } f \text{ by } a$, u is a velocity of **by** a , a is also the volumetric flow rate divided by area of cross **cross** section, so that indeed is going to be a superficial velocity $d c \text{ by } d x \text{ equal to } -r \text{ of } c$; and the example that we had taken earlier, for $-r \text{ of } c$ is going to be was, $r \text{ of } c$ is going to be equal to k multiplied by c to the power one point two five.

So, if we can substitute this over here; so, we will have this as $k c$ to the power one point two five now, because this is c to the power one point two five, this is indeed a non-linear equation; this being a non-linear equation; what we have over here is a non-linear PDE; now, let us go and compare this to the general PDE that we have written over here; the general PDE that we have written now a b and c all of them are 0, so this is not a second order PDE.

So, in general, this particular PDE cannot really be classified **base as** whether it is parabolic, whether it is hyperbolic, or an elliptic PDE. So, in general, because a b and c are all 0, this is not a second order PDE, because it is not a second order PDE, it does not strictly fall into the classification of elliptic parabolic or hyperbolic equation.

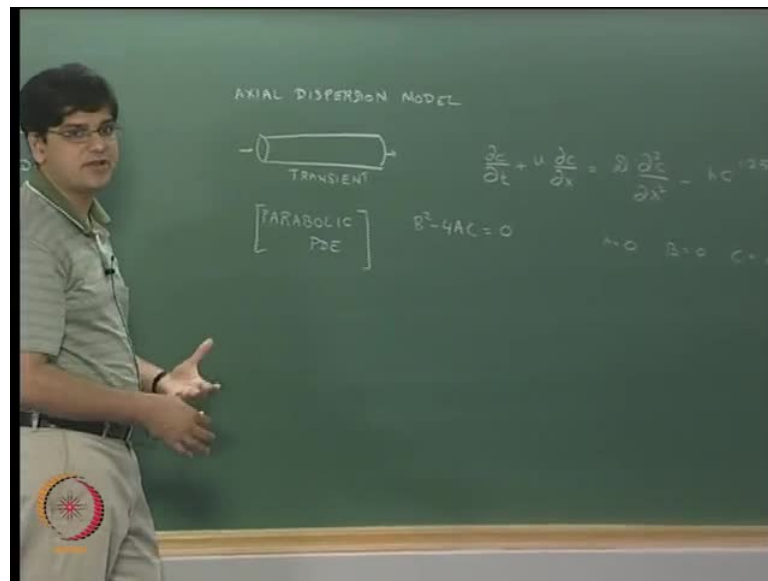
However, the way this particular PDE behaves, it has characteristics which resemble a hyperbolic equation; and therefore, where we are going to call this as hyperbolic PDE; and indeed in the next lecture of this module, I am going to talk about why or how exactly this particular equation comes to be called as a hyperbolic PDE; at this point of time, just take this particular definition as it is phase value; a more typical example of a hyperbolic PDE that you would have probably done in the **first** first year **of** of your engineering course perhaps **in** in the math course is a wave equation, wave equation will be an equation of the form $d^2 \phi \text{ by } d t^2 \text{ minus } d^2 \phi \text{ by } d x^2$.

So, that is what the wave equation **would** would be equal to whatever else terms that might be; now, in this particular equation, our a and c are, a is a positive number, c is a negative number, b is 0; as a result, b square minus 4 a c is going to be greater than 0; and this is going to be an example of hyperbolic equation.

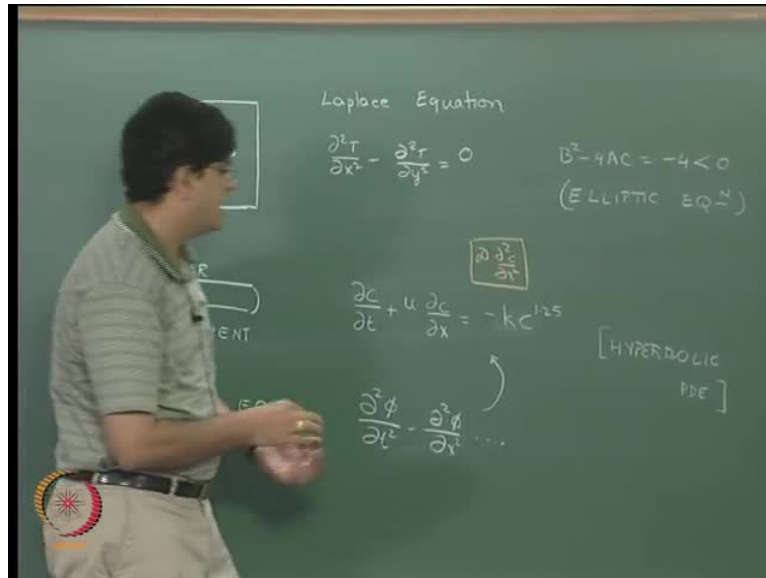
What I am going to do in the next lecture is, going to show how we can relate these two types of an equation, how we can go essentially from a wave equation and try to see how this type of a first order ODE has certain characteristic that resemble a wave equation; and so we will reserve that for the next lecture of this module.

And that will give us y, I am trying to call this as a hyperbolic PDE; and again why I am doing that is, it has certain results which we are going to use **when** when we discuss about how to use numerical techniques in order to solve the hyperbolic parabolic or elliptic partial differential equations.

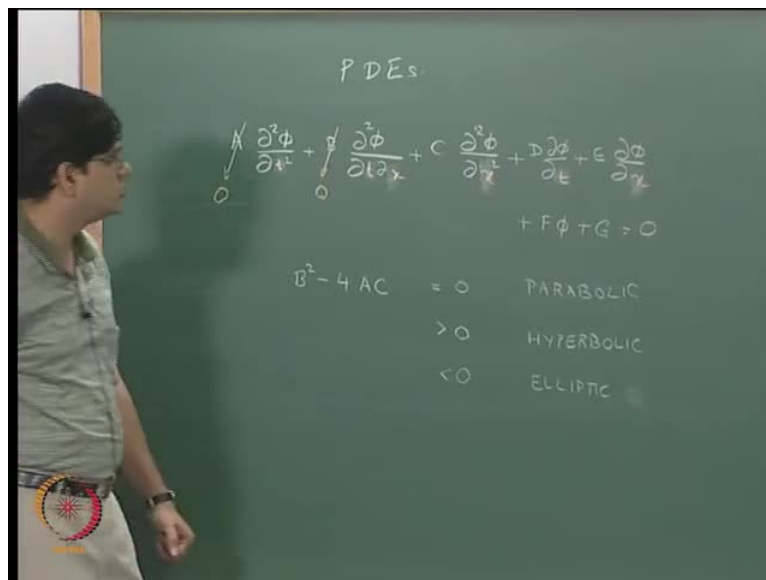
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And the third example would be say a plug flow reactor with axial dispersion, so we have an axial dispersion, axial dispersion model, so we have this reactor, and we want to get a transient model for it. And the model in this particular case is going to resemble the model that we have over here, the only difference is we are going to have a mass diffusion term added at this location.

So, the mass diffusion term that we are going to add at that location is going to look like diffusivity multiplied by $\frac{\partial^2 c}{\partial x^2}$; so, this is the kind of term that we are going to add at this particular location; and so, when we do that, the equation that we

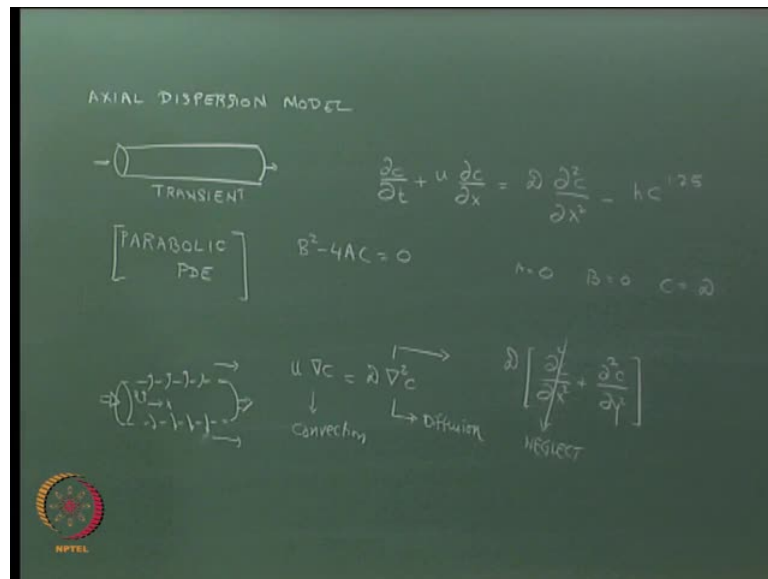
are going to get is going to be of the type $\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x}$ is going to be equal to diffusivity or dispersion coefficient multiplied by $\frac{\partial^2 c}{\partial x^2}$ minus $k c$ to the power one point two five or in general it is going to be minus plus negative $r a$ or minus negative $r a$ **sorry**.

So, that is going to be our final equation. Now, if we compare this with $\frac{\partial^2 \phi}{\partial t^2} + b \frac{\partial^2 c}{\partial t \partial x} + c \frac{\partial^2 t}{\partial x^2}$; in that case, we will have a equal to 0, b equal to 0, and c equal to either we can call it c equal to d the diffusive the dispersion coefficient or diffusivity d or c equal to minus d whichever way you want it; what we are doing over here is, compare that to the general equation that we had written over here; in this particular case, what we are going to do in the general equation is just modify this in this particular way.

And if we are going to compare this with this equation, this a is 0, because there is no $\frac{\partial^2 \phi}{\partial t^2}$ term; this b is going to be equal to 0, because there is no $\frac{\partial^2 \phi}{\partial t \partial x}$ term; and then this c is going to be equal to either the diffusivity or the dispersion coefficient that we have represent as represented with the symbol d . So, under this particular condition, we again calculate $b^2 - 4ac$ and because b is 0 and a is 0, $b^2 - 4ac$ is 0.

And this is then an example of a **parabolic** parabolic PDE; so, these are the most general type of PDE situations that we are going to encounter in chemical engineering problem; now, it could be a flow problem; it could be a heat transfer problem; it could be a mass transfer problem; it could be a reaction problem or combination of all these types of problems.

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But these are typically the type of PDE's that we are going to encounter; another set of example **where** which we can take is, let us say, we have a membrane reactor **where**, so what we can do is we can take a membrane and then fold it around **in** in form of a cylindrical tube and you can have water passing through the tube; this is indeed what you have in your RO filters, reverse osmosis filter, the eureka Forbes, or the Kent water purifier; when they talk about RO filters, that is what indeed they have; what is done in those type of filters is, you have this unclean water **that** that is actually going to pass through **this particular** this particular module and indeed depending on; so, in general, in a membrane reactor, what happens is, the certain species, for example, the dissolved salts in in the liquid water they are going to essentially diffuse out of this particular system, or in other type of **other type of** problems what is going to happen is, that the water diffuses out of that system and a more concentrated salt solution remains in the system.

So, either ways what is happening is, one of this species is diffusing out of this system and the other species is going to be going to flow through that system; **this** these two fluids we are then finally going to collect; now, if we were to do the modeling for **this** this system within the reactor, if within **sorry within** the membrane module what we are going to have is, the concentration of that is species, that is diffusing out the concentration of that species will vary along both the x direction as well as it will vary along the r direction.

So, what we are going to have in that particular case is that, **we will** we will have the equation in the form of $u \nabla c$ is going to be equal to diffusivity multiplied by $\nabla^2 c$

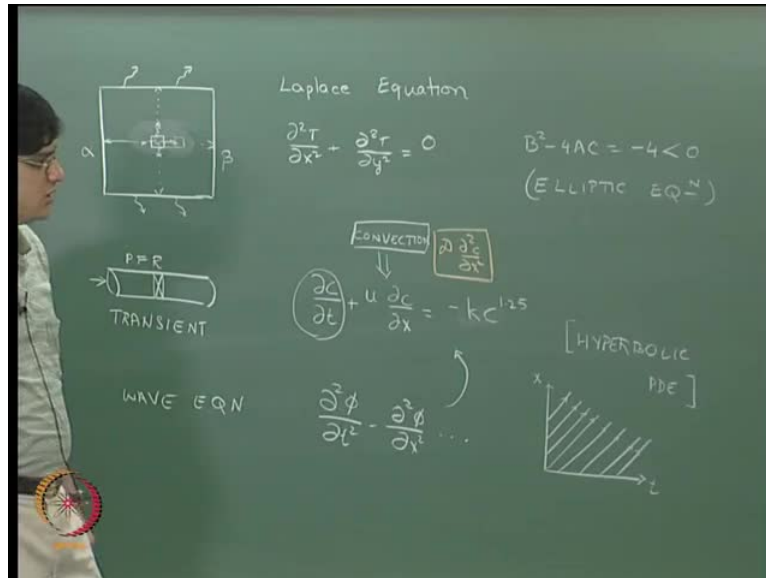
c , where this is the convection term and this is going to be the diffusion term. And this $\nabla^2 c$, $\nabla^2 c$ is going to expand as $\nabla^2 c$ by ∇x^2 plus $\nabla^2 c$ by ∇y^2 in cartesian coordinates or $\nabla^2 c$ by ∇y^2 plus $1/r \nabla c$ by ∇r multiplied by $r \nabla r c$ by ∇r .

So, that is the kind of expression that we are going to get; so, if we expand this particular expression, this expression will expand and give a term kind of similar to this particular term; so, when we have when we need to solve this type of an equation, we will end up with an elliptic set of an equation; and if we are going to neglect $\nabla^2 c$, so this term what I mean is going to expand as ∇ multiplied by, let us just look at the cartesian coordinates for simplicity, $\nabla^2 c$ by ∇x^2 plus $\nabla^2 c$ by ∇y^2 .

And if we are going to solve this particular equation for this system, what we are going to get is, we are going to get an elliptic equation; some times what we do is, we neglect this term and we neglect this term, because this term is less important than the $u \nabla c$ by ∇x term; it is lesser less important than the convection term; and under those conditions what we will get is, we will get a parabolic set of equations, because when this term is neglected, we will have our c as non-zero, but our a and b are going to be equal to 0.

So, depending on our assumptions for the system, we will either end up with an elliptic PDE or we will end up with a parabolic PDE; so, we will just stick with these three examples for parabolic, hyperbolic, and elliptic PDE's.

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Let us start with an elliptic PDE; in an elliptic PDE, **what** how we end up getting this PDE essentially is, if we were going to do an energy balance or in this particular case an energy balance; but another other cases we might have a mass balance or a momentum balance as well; so, if **how** we get this equation, is if we were to take a small control volume; in this particular block what we will see is that, energy gets transferred to this control volume through conduction and energy gets transferred out of this control volume through conduction again.

So, this particular control volume is going to interact with all of its neighboring control volume; it is going to interact with the two neighboring control volumes in the x direction and two neighboring control volumes in the y direction; that is what is going to happen **in order to** in order for this particular equation to be obtain in this system.

And so, the value of temperature and this control volume is going to depend on the value of temperature on this control volume, that intern will depend on this control volume so on and so forth up to this particular boundary; likewise, this will also go back up to this particular boundary; this will go on up to this boundary; and this goes on up to this particular boundary.

So, the temperature that we get in **at** any location within this block is going to be determined by the boundary conditions at all of these boundaries; all the boundary condition at these boundaries are going to affect the evaluation of temperature in this particular location; so, what happens is that there is, no direction in which this particular

system is evolving; this system the values that we are going to get r dependent on all the 4 boundaries, indeed when we look at the boundary conditions for the system, we had written the boundary conditions that at this particular guy is, at some α this guy is at some value β over here we have t dash as certain quantity and over here, we had given t dash or $\frac{dt}{dz}$ by $\frac{dt}{dy}$ as certain other quantity.

So, the value at this temperature is determined by all of the four boundaries; so, what we need to do is, we need to solve the entire problem for the domain along with the boundary condition simultaneously; so, there is no evaluation in either x or y direction in one of the characteristic direction; all the four boundaries are going to determine the value of temperature in any small control volume, that we can take **in this** in this particular domain.

So, that is what happens when we have an elliptic equation; what we have in in case of a hyperbolic equation is that, the values are going to change in time. So, in time, how we are going to be governed is, we are going to be governed by an initial condition in time; and based on the initial condition that we give in time, we are going to propagate in into the future.

So, **what we are going**, what is going to happen in this particular; this particular type of a problem is that, we are going to evolve **along** along the time axis, but not just are we going to be evolving around a time axis, the solution is also going to evolve around the x axis as well, because it is an initial value problem in x , we are given an initial condition at x equal to 0; starting from that particular initial condition, the values along the x direction are going to get determine.

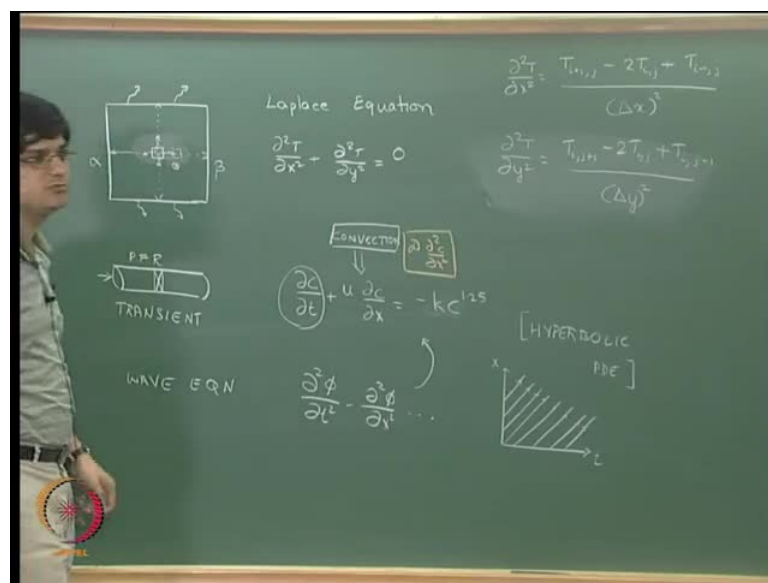
So, what happens is that, the solution **so** at any location in the plug flow reactor at any time is going to be determined by the initial condition at the inlet of the reactor; and the initial conditions that we specified at time t equal to 0; so, based on the condition at time t equal to 0 and based on the conditions at x equal to 0, this particular solution is going to evolve in both time and x ; in fact, if you recollect the way this hyperbolic PDE's were solved **in** in the math course, there is one of the methods for solving this type of a problem was **to define** to define what is known as characteristic curves.

And for this particular problem...; and again we will take this thing in **in** the next lecture is the characteristic curves essentially look like straight lines with a slope u and the solution evolved along these characteristic curves.

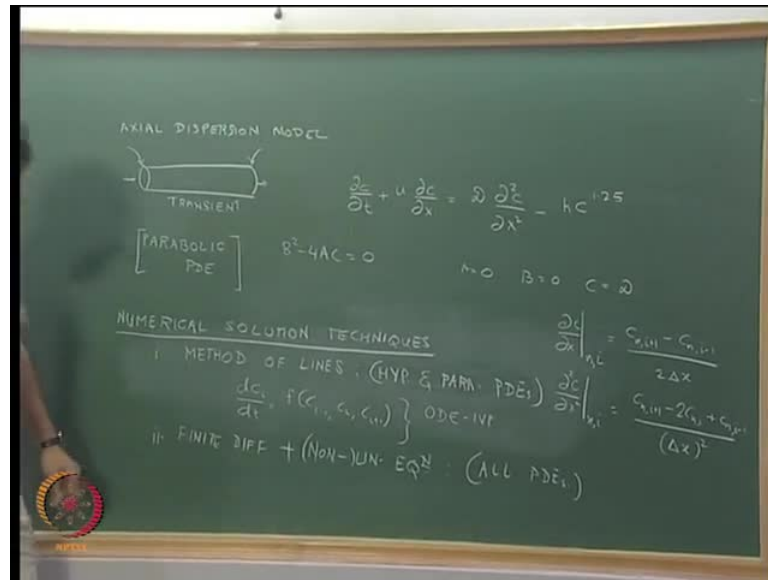
And the commonality between the wave equation and the first order hyperbolic equations are the act both of these equations are going to evolve along the characteristics; and we start off with a solution along each of these characteristic and we evolve in to the future; **the solutions along these characteristic**, if this is the t axis and this is the x axis, the solution along these characteristics are governed by the initial conditions at x equal to 0; the solution along these characteristics are governed by the initial condition at t equal to 0; and there is net evaluation of the overall system along this characteristics.

Physically another thing that is different is that, these are convection dominated system, this is the convective term and there is no diffusion term over here, so this system of equations are driven by convection that takes place **into** into the system; now, let us compare this type of a plug flow reactor with an axial dispersion reactor; again we are going for a transient model; now, let us look at what was different when we solved the boundary value problem and the initial value problem **in** in the previous two modules - **module 7 and module** module 8 and module 7 respectively.

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So, what was different in case of the boundary value problem or the axial dispersion reactor from the plug flow reactor was, one the presence of the diffusion term, the second or the axial dispersion term; the second thing that was different in those two problems is that, the values of the boundaries had to be specified at the two different boundaries.

So, what we had to do in solving the boundary value problem is that, **the temperature or sorry** the concentration was specified at the inlet boundary and dc by dx equal to 0 was specified at the outlet boundary; and both these boundary conditions determined how this particular solution is going to evolved; so, the solution in the x direction was determined by both the boundaries, **it was**, it did not have the freedom to move about the way it had the freedom to move about in an initial value problem; so, it was kind of hinge at both these ends the solution was however the solution in the time direction is going to be determine only by the initial conditions in time, there is no boundary condition that is actually specified in time.

So, what happens in this type of a problem in parabolic PDE's is that, the solution evolves around along time, whereas it is fixed along in the space by the boundaries; so, if we were indeed to look at the characteristic equations and if this was t and this was x , the x it is going to be fixed between 0 and 1, and our solution is going to evolve only around along the time dimensions; so, this is essentially what is going to be different, when we

talked about parabolic PDE's and when we talk about the hyperbolic PDE's; in parabolic PDE's the things are only moving along the time direction.

So, what it means when it comes to solving these problems using a numerical technique is, we can use the property that the solution is evolving along one direction in order to convert the PDE's into ODE's.

So, what happens is that, **the** the parabolic PDE's and the hyperbolic PDE's can be converted into ODE's using what is known as the method of lines; when it comes to solving the elliptic PDE's, we cannot use the method of lines, we have to indeed use **the** the finite difference method in order to solve this type of problems. And of course, when I say the term finite difference method, it can be replaced by finite volume or finite element methods also; those are something we are not going to cover in this particular course.

So, the solution techniques that we are going to talk about, first one is called method of lines; what we do in method of lines is, all the spatial derivatives we represent them as numerical derivatives; so, we represent partial c by partial x at location i and at time n, let us call it time n, and location i as $c_{n,i+1} - c_{n,i-1}$ divided by $2 \Delta x$; we will represent **double c** double square c by double x square at n, i as $c_{n,i+1} - 2c_{n,i} + c_{n,i-1}$ divided by Δx^2 ; and once we represent that what we are going to have, we will have the equation as $\frac{dc_i}{dt} = \text{sum function } f \text{ of } c_{i-1}, c_i, c_{i+1}$; by doing this what we have really done is, we have converted a partial differential equation into an **ordinary differential equation** sorry into **an** ordinary differential equation.

Now, this is an ordinary differential equation in time; so, this results in an ODE initial value problem; so, the idea is that, we had developed **in** in the numerical derivatives part of this course, we are going to implement them on the spatial derivatives and **convert them in into** finally the convert the overall PDE into an ODE initial value problem; once it is converted into an initial value problem, we can use any of the numerical techniques that we covered in the module 7 of this course; specifically, we can take either the Runge-Kutta method or the Adam-Moulton's method or backward difference formulae in order to **then** march forward in time; now, this method of lines is applicable as you can imagine it is applicable only to the hyperbolic type of an equation, where we can actually

represent $\frac{dc}{dx}$ as a numerical derivative, $\frac{dc}{dx}$ by $\frac{c_i - c_{i-1}}{\Delta x}$ as a numerical derivative, and with that representation we convert this PDE into an ODE.

Same thing we can do that for a parabolic PDE; so, the method of lines are going to be applicable to only to hyperbolic and parabolic PDE's; and the second method that we are going to talk about is going to be use finite difference plus a non-linear equation solving technique; and in that particular case, what we are going to do is, we are going to write the overall PDE as a finite difference, for example, this t let us consider t at any location i, j the x location is i , the y location is j , in that case, $\frac{\partial^2 t}{\partial x^2}$ can be represented as $\frac{t_{i+1,j} - 2t_{i,j} + t_{i-1,j}}{\Delta x^2}$; likewise, $\frac{\partial^2 t}{\partial y^2}$ can be represented in a similar manner.

We can represent $\frac{\partial^2 t}{\partial y^2}$ as $\frac{t_{i,j+1} - 2t_{i,j} + t_{i,j-1}}{\Delta y^2}$; and once we do that and substitute in this particular equation along with the boundary conditions, **we will have**, so if we split this in n zones and this in m zones, we will have n multiplied by m equations in n multiplied by m unknowns; that we can solve using our linear equation technique or a non-linear equation techniques and finally we will end up getting the actual solution for this problem.

So, this finite difference method is the only method for that we are going to deal with in this course that is applicable for elliptical equations, but the same finite difference method can be applied to parabolic as well as to the hyperbolic PDE's; so, the finite difference **will** be applicable to all PDE 's; and **it is** in the context of the finite difference and the method of lines is where we are going to talk about the differences between the parabolic PDE's and the hyperbolic PDE's; as we said what happens in case of parabolic PDE's is that, there is this particular diffusion term; in case of hyperbolic PDE's, this diffusion term is absent, we do not have this diffusion term in the hyperbolic PDE's; what that basically means is that, when it comes to stability of this PDE's, it has certain very important criteria that we need to satisfy with respect to the stability; what happens is that, lack of this diffusion term is going to make this hyperbolic PDE's unstable under certain conditions; whereas, the presence of the diffusion term is going to make the actual dispersion model going to more stable under those same conditions

We will talk about these things in in the third lecture of this module. In the second lecture of this module, we are basically going to concentrate on solving the elliptic

equation using the finite difference method and then we are going to concentrate on solving both parabolic as well as hyperbolic PDE using method of lines; and the third module of the third lecture **sorry** of this module, we are going to consider the difference between hyperbolic PDE's and parabolic PDE's when we are going to use a finite difference plus non-linear equation solving technique

That is going to what we are going to cover with respect to the theory of PDE's; and then the final one or two lectures we are going to take numerical examples, specifically when we are going to talk about the finite difference methods; we will talk how we can convert the PDE's into linear or non-linear equations; **how we solve**, how we use say a Newton-Raphson's method to solve this non-linear equation and because it is a multivariable Newton-Raphson's method; how we can actually imply the linear equations solving techniques, specifically the gauss elimination technique and the tridiagonal matrix algorithm in order to solve in the non-linear equation to a **certain** certain technique; so, that is really you how we are going to proceed **in the next** the last three lectures of this particular course .

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