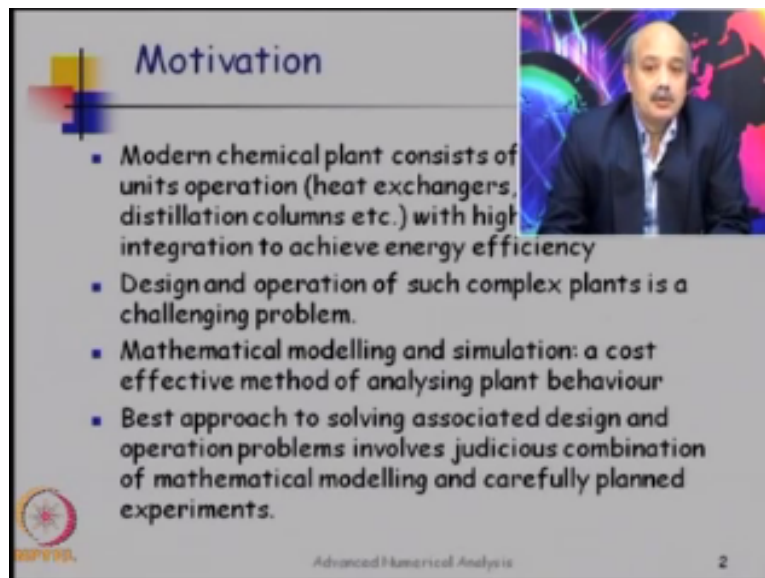


**Advanced Numerical Analysis**  
**Prof. Sachin Patwardhan**  
**Department of Chemical Engineering**  
**Indian Institute of Technology – Bombay**

**Lecture – 01**  
**Introduction and Overview**

Welcome to the world of numerical analysis, I am Professor. Sachin Patwardhan from Department of Chemical Engineering at IIT Bombay and these are series of lectures delivered on advanced numerical analysis in NPTEL phase 2. So, this is my first lecture, this is an overview of the course and next 1 hour also, I am going to present a bird's eye view of what we are going to study in this course.

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The slide is titled "Motivation" and features a video inset of Prof. Sachin Patwardhan in the top right corner. The main content consists of four bullet points:

- Modern chemical plant consists of units operation (heat exchangers, distillation columns etc.) with high integration to achieve energy efficiency
- Design and operation of such complex plants is a challenging problem.
- Mathematical modelling and simulation: a cost effective method of analysing plant behaviour
- Best approach to solving associated design and operation problems involves judicious combination of mathematical modelling and carefully planned experiments.

At the bottom left is the NPTEL logo, and at the bottom center is the text "Advanced Numerical Analysis". A small number "2" is visible in the bottom right corner of the slide.

World of numerical analysis is pretty involved and complex and probably some of you have already have some introduction to this. This is meant to be a course, which is Advanced Course, we will introduce you many of the things in a different light and I hope, it will help you throughout your academic career. So, let us begin our journey with the motivation. In chemical plants it can; now, you have large number of interconnected units like heat exchangers, reactors, distillation columns.

And these days, the chemical plants are very tightly integrated to achieve high energy efficiency or high material efficiency, which makes it very complex to handle, to operate, to design and it is not possible to do it without doing mathematical modelling. So, design and operation of such

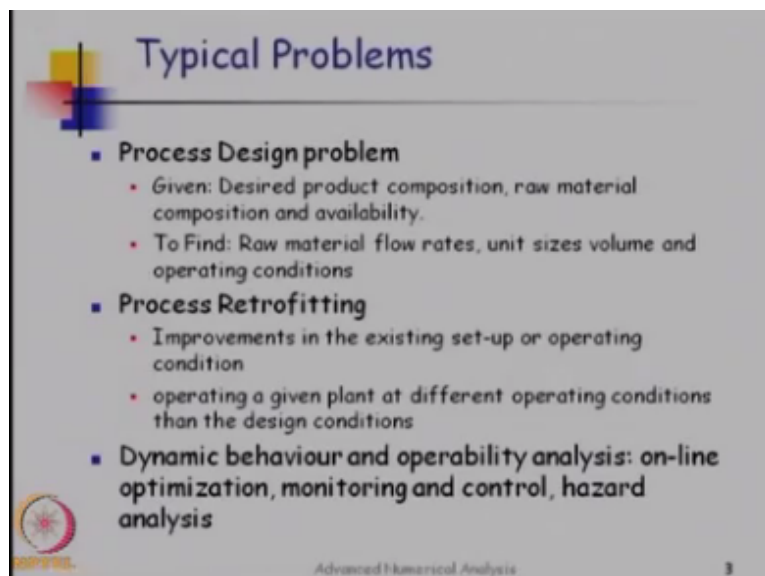
complex plant is always a challenging problem and mathematical modelling and simulation has become a very, very handy tool.

A very cost effective method of analysing behaviour of such plants, so in a real design problem or a real operation problem, we have to judiciously blend mathematical analysis with experiments. It is not possible to rely only on experiments; it will be not correct to rely only on mathematical modelling. What we are going to do is to plan experiments very carefully using mathematical models.

So, mathematical modelling has become a backbone of modern chemical engineering, design and operation. Now, these models have to be solved either offline or online and when you have to solve this models under a variety of conditions, variety of problems, you need to use numerical tools. Most often, you cannot solve these problems analytically, so numerical problems is at a; or numerical solutions is at the heart of mathematical modelling and simulation, which is in effect used for designing and operating chemical plants.

Now, what are the typical problems that we encounter? Let us look at some of the problems that a chemical engineer would typically have to face, when he goes to a chemical plant. Well, one problem is of course, a design problem, you may have to design a new section of a plant or if you are part of a consulting firm, which design chemical plants, you have to design a new plant under; you know you are given some desired product composition you are given some raw material availability.

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**Typical Problems**

- **Process Design problem**
  - Given: Desired product composition, raw material composition and availability.
  - To Find: Raw material flow rates, unit sizes volume and operating conditions
- **Process Retrofitting**
  - Improvements in the existing set-up or operating condition
  - operating a given plant at different operating conditions than the design conditions
- **Dynamic behaviour and operability analysis: on-line optimization, monitoring and control, hazard analysis**

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And then, you have to find out unit sizes, you have to find out flow rates, you have to find out operating conditions, so coming up with a base design from which a mechanical engineer or other engineering departments can take over is what is the job of Chemical Engineer coming up with the basic flow sheet design. So, this normally involves models for different linear operations.

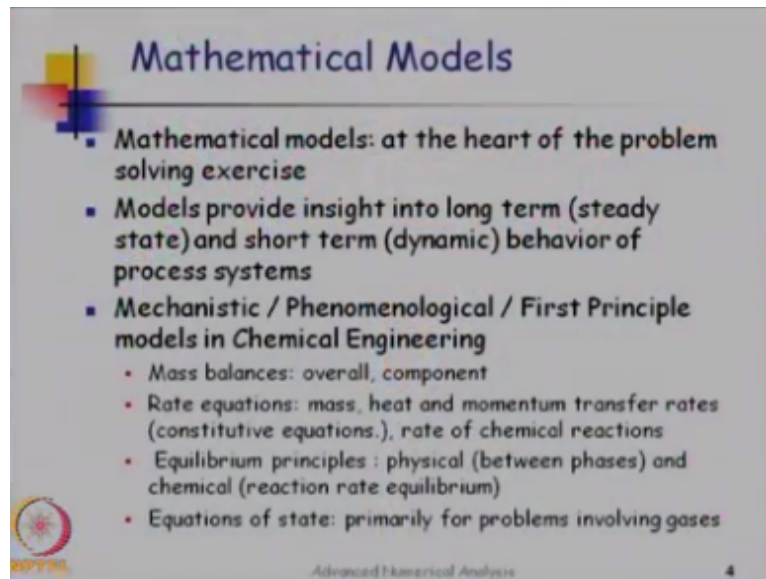
You have to connect all these models into a giant mathematical model into a big model, which could be 100's and 1000's of equations, they need to be solved under a variety of conditions, so this is one of the problems that you normally encounter. The other problem could be that you are already employed in a plant and then you know, you have to do process retrofitting.

So, retrofitting involves improvement in the existing operating conditions, so you have a plant, which is operating and then some modifications are necessary because maybe the input conditions have changed, maybe you know, the feed quality has changed or you need to ramp up, you need to operate the same plant at different conditions than what it was designed for because of the market conditions.

So, retrofitting is another problem for an existing plant and a problem that always comes when your operating plant is control or online optimization. So, dynamic behaviour and operability analysis is integral part of operating any complex chemical plant, you have to; first of all you have to monitor and control the plant, you have to make sure that it is operating safely, you may have to carry out hazard analysis, conduct what-if studies.

You may want to do online optimization, run the plant in an optimal way and all these exercises cannot be done without mathematical modelling and subsequently, solving these mathematical models using numerical analysis. So, numerical analysis is at the heart of all these exercises that we have to undertake as a chemical engineer. Now, what are mathematical models?

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## Mathematical Models

- **Mathematical models: at the heart of the problem solving exercise**
- **Models provide insight into long term (steady state) and short term (dynamic) behavior of process systems**
- **Mechanistic / Phenomenological / First Principle models in Chemical Engineering**
  - Mass balances: overall, component
  - Rate equations: mass, heat and momentum transfer rates (constitutive equations.), rate of chemical reactions
  - Equilibrium principles : physical (between phases) and chemical (reaction rate equilibrium)
  - Equations of state: primarily for problems involving gases

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Mathematical models could be in different forms, we have models that give insight into long term behaviour, so these are typically energy and material balances and we look at the steady state conditions and the design problems or in retrofitting problems, you might want to only restrict yourself to steady state models that means, we ignore the transient behaviour or short term behaviour.

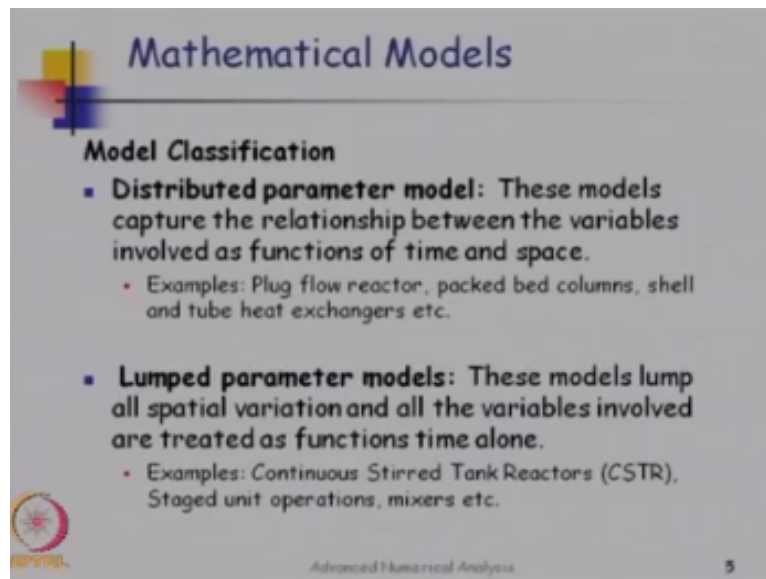
Whereas, when you are studying operation of a plant, when you are trying to control the plant, you cannot ignore the dynamics, so in that situation, the short term behaviour or the transients become very, very important and then, we have to; we have to solve the mathematical models in time and possibly, time and space, okay. So, what kind of mathematical models that we are going to study, what we need in this particular course?

Mostly these models are going to be coming from first principles or they are from; or they are often called as mechanistic models or phenomenological models, so these models come from you know, mass balances, component balances, this is something that you have been doing for; as you know in your courses and various courses at Chemical engineering. So, this could be you know, models are composed out of you know, rate equations, mass, heat momentum transfer.

There are constitutive equations, then chemical reaction rate equations, there could be equilibrium principles used while doing a modelling between different phases, also you may have to use equations of state, if for systems involve gases or multiple phases, so the models that you actually use for doing this design operation dynamic simulation are quite complex.

They are constructed out of these fundamental concepts of energy mass material balances, rate equations and equilibrium models.

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**Mathematical Models**

**Model Classification**

- **Distributed parameter model:** These models capture the relationship between the variables involved as functions of time and space.
  - Examples: Plug flow reactor, packed bed columns, shell and tube heat exchangers etc.
- **Lumped parameter models:** These models lump all spatial variation and all the variables involved are treated as functions time alone.
  - Examples: Continuous Stirred Tank Reactors (CSTR), Staged unit operations, mixers etc.

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Well, from a mathematical viewpoint, how do I classify these models? Well, we can have variety of classifications but one classification that is relevant to this course, which will of course, show up in a different way in terms of classes of model equations that we are investigate; is distributed parameter models and lump parameter models, so by this classification, you know we are looking at 2 classes.

One that deals with variation in time and space, so distributed parameter models capture relationship between different variables not just in space but also in time. When I say space, it could be in multiple dimensions not just single dimension, so for example, Plug flow reactor or a packed bed column or even a shell and tube heat exchanger can be modelled as a distributed parameter system.

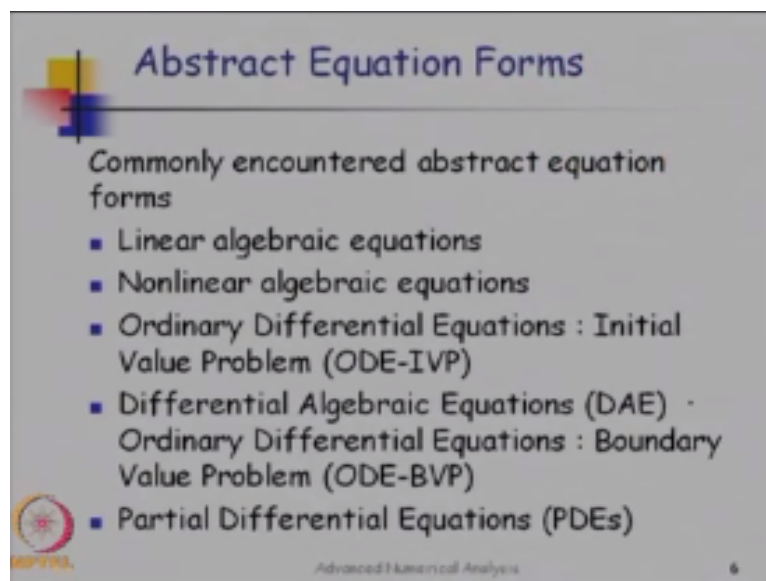
So, this will depend upon situation, in some cases, you might use very, very simple lumped parameter model for a shell and tube heat exchanger but there are situations where you may want to use more complex distributed parameter model. So, one class of models that we are going to encounter in this course are distributed parameter models. The other class of models, which we very often study in chemical engineering, a lumped parameter models.

For example, stirred tank reactors or many stage unit operations, mixers, so these are models with ignoring you know, spatial variation and if necessary, we only consider variation in time

alone. So, see we are looking at transient behaviour only time comes into picture, if you are looking at steady state behaviour, you may get only algebraic equations in this case. So, there are 2 broad classes of models that are encountered in chemical engineering.

And we are going to study these models; we are going to study how to solve different subclasses belonging to these 2 broad classes of models. Well, if we examine from a mathematical viewpoint, what are the equation forms that we encounter, when we are going to do this course. Well, when you do a course in mathematics or let us say courses in mathematics in your first or second year of engineering, we start looking at only abstract equation forms.

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And it is important that you relate those at abstract equations forms to what you see in the mathematical models. So, what a kind of equation forms that you commonly encountered in chemical engineering models; well, one is linear algebraic equations, where we study linear algebraic equations maybe even before we enter an engineering program, what; you study as you enter an engineering program.

And chemical engineering is solving nonlinear algebraic equations, so very often we have to deal with a single variable or multi variable nonlinear algebraic equations, thermodynamic relationships for example, many times nonlinear equations. The other class of problem that you encounter in modelling chemical engineering unit operations is ordinary differential equations.

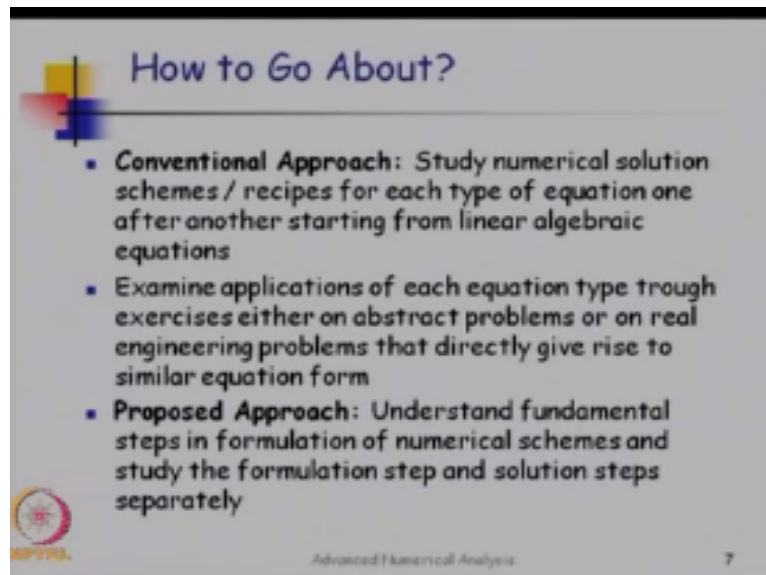
Typically, an initial value is given and then we are supposed to find a solution of first, second, third or higher order ordinary differential equation. The other class of problems that are

encountered particularly in distributed parameter systems or differential equations with boundary value problems; you also may have equations, which are differential and algebraic equations.

So, differential algebraic systems DAE's, so this is differential algebraic systems are mixtures of algebraic and differential equations, while ordinary differential equations boundary value problems are one in which boundary conditions are specified partially at one boundary and remaining at other boundary and we are expected to solve these kind of differential equations. So, these kind of problems typically arise, we are solving say, plug flow reactor models or distributed parameter systems.

And other models that we often encounter while modelling chemical engineering unit operations or partial differential equations, so these models they may not come in isolation. In real problem, when you are actually trying to solve a problem associated with a section of a chemical plant, you may get mixture of all of them not just one of them in isolation. Nevertheless, when we study these equation forms, we often study them in isolation.

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**How to Go About?**

- **Conventional Approach:** Study numerical solution schemes / recipes for each type of equation one after another starting from linear algebraic equations
- Examine applications of each equation type through exercises either on abstract problems or on real engineering problems that directly give rise to similar equation form
- **Proposed Approach:** Understand fundamental steps in formulation of numerical schemes and study the formulation step and solution steps separately

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And then we understand how to attack more complex problems, where combination of these might be encountered. Now, how do you go about doing this, how do you go about studying these equation forms? Well, if you look at many of the approaches presented in textbooks are written for engineers, a conventional approach is study numerical recipes for each type of equations.

That means, you start by saying; Well I am going to first look at linear algebraic equations and the tools for solving linear algebraic equations then, we move on to say nonlinear algebraic equations having studied linear and nonlinear algebraic equations, we look at ordinary differential equations, then initial value problems typically, you begin with. Then, you might want to move on to study ordinary differential equations with boundary values.

And then, typically a course would end with set of partial differential equations, so methods for partial differential equations, methods for ordinary differential equations and so on. So, if we look at it from this viewpoint, one can get a view that there are separate methods for solving linear equations and for partial differential equations or boundary value problems but this is not exactly; so when you start looking at these methods from a different viewpoint.

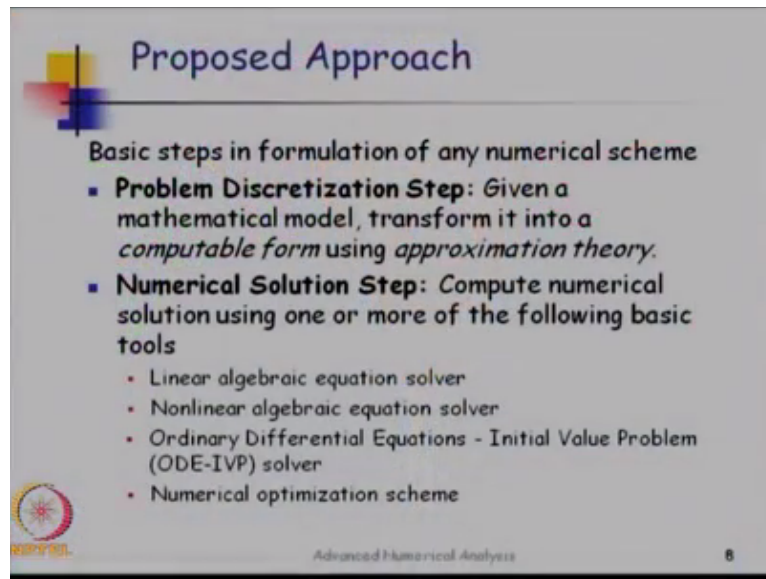
So, in the conventional approach, how do you; where do you encounter all these applications? So, after we have studied each one of these equation types that is numerical methods for solving each one of these equation types, then in exercises or in the in the sample examples, you will encounter real engineering problems or it could be, you might come across some abstract problems in terms of some  $x, y, z$  variables, which do not make physical sense.

So, these problems are then used to form of the concept that you have studied for each equation type. In this course on advanced numerical analysis, we are going to be different, we are going to look at it in a completely different manner. So, what I am going to do is; I am interested in understanding what are the fundamental steps involved in formulation of a numerical scheme and then how do you come up with a recipe or a solution approach to solve a particular problem.

So, if you take a critical view point of all the methods then, you come across certain threads which are common and from that you can actually built a different way of studying numerical analysis. So, what I am going to do here is you know, look at 2 different steps separately. If you look at all the numerical methods that are used for solving, you know different type of problems that are encountered.

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**Proposed Approach**

Basic steps in formulation of any numerical scheme

- **Problem Discretization Step:** Given a mathematical model, transform it into a *computable form* using *approximation theory*.
- **Numerical Solution Step:** Compute numerical solution using one or more of the following basic tools
  - Linear algebraic equation solver
  - Nonlinear algebraic equation solver
  - Ordinary Differential Equations - Initial Value Problem (ODE-IVP) solver
  - Numerical optimization scheme

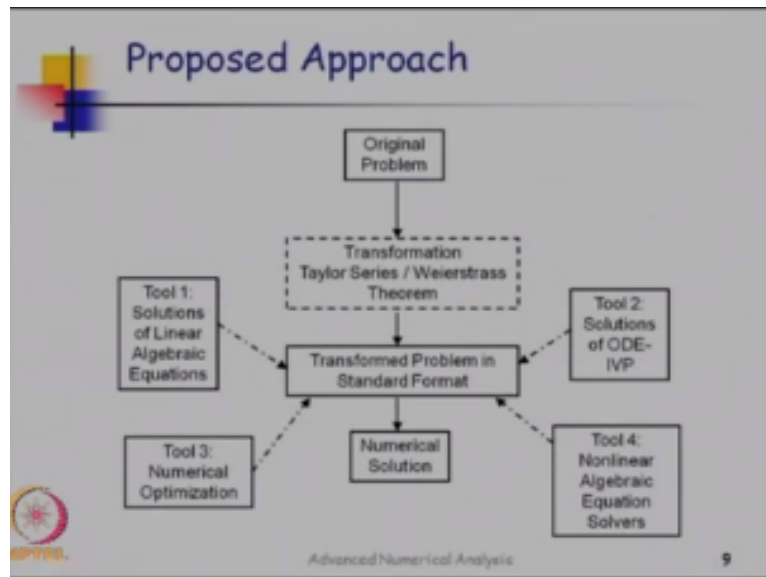
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And you know, make analysis, what kind of; what is the first step and what is the second step, so what do you realize is that invariably a first step is you know, model transformation, so many times you have models that cannot be directly or many times your mathematical problems that cannot be directly solved using existing methods, when I mean to say that could not be directly solved, I mean to say that they cannot be analytically solved.

If they cannot be analytically solved, you have to construct approximation; approximate solutions but to construct approximate solutions, you have to first convert a given problem into a computable form; a computable form is one to which known computation tools can be applied. Now, this problem transformation is carried out using tools or using approaches developed in approximation theory, a well-developed branch of Applied Mathematics.

Approximation theory is used to transform a problem into computable form and then you actually use different tools to attack the transform problem and construct numerical solution, so these tools are; you know linear algebraic equation solver or nonlinear algebraic equation solver, it could be ordinary differential equation, initial value problem solver or it could be a numerical optimization scheme.

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So, when you actually construct, receive or when you construct a numerical scheme to solve a problem, you first transform it into a form that can be dealt with; that can be tackled with one of the standard tools and then you use one or more of these tools in combination to come up with a solution of their transform problem. So, this is; if I just put this into pictorial form, then you have an original problem.

This original problem might be a partial differential equation, then you take this original problem use principles developed in the approximation theory and transform it to what I have called here in a standard form; a standard form is what I mean by my standard form here is a computable form okay. So, this original form might be a partial differential equation when I transform it, it might turn out to be set of linear algebraic equations or set of nonlinear algebraic equations.

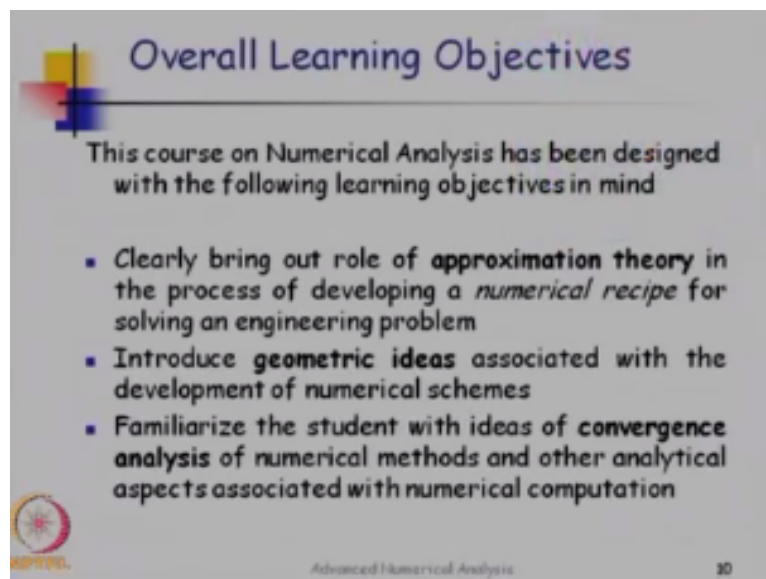
So, the original problem that you want to solve and the transform problem do not have same equation type, you have a partial differential equation here, you have a set of nonlinear algebraic equations here, so to solve this nonlinear algebraic equations, you may have to use; you may have to use special tools that are developed for solving nonlinear algebraic equations, these tools for solving nonlinear algebraic equations in turn might use linear algebraic equation solver.

So, you know it is not that I am going to use just one tool, so I am going to use multiple of these tools to attack this transform problem and then come up with a solution, which is a numerical

solution of my original problem. So, what we are going to study in this course is 2 steps, well how do I take the original problem and transform it into a solvable form or a computable form.

Now, this process actually in the conventional approach get mixed up with various; you know receipts that are developed for a specific equation types, we are going to separate it and view it as a separate step. So, this means unlike the conventional approach, I am not going to look at partial differential equations at the end of my course or boundary value problems at the end of my course.

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**Overall Learning Objectives**

This course on Numerical Analysis has been designed with the following learning objectives in mind

- Clearly bring out role of **approximation theory** in the process of developing a *numerical recipe* for solving an engineering problem
- Introduce **geometric ideas** associated with the development of numerical schemes
- Familiarize the student with ideas of **convergence analysis** of numerical methods and other analytical aspects associated with numerical computation

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I will begin right in; you know attacking these problems right in the beginning and we will just transform them into forms that can be solved using one or more of these standard tools, so that is the approach that we want to take. So, what are the overall learning objectives for this numerical analysis course? Okay, well I am assuming here that you have had some exposure to this numerical method prior to doing this course.

Well, if you have not had does not matter, this course will give you; you know from scratch, a different viewpoint of numerical analysis but if you had some prior experience with numeric analysis well it will enrich your understanding. So, the first thing that I want to do here is to clearly bring out the role of approximation theory in the process of developing a numerical receipt for solving an engineering problem.

This word is you know I am deliberately using this word numerical receipt, it is like you know at the end of the course, you should realize that forming a numerical scheme is like cooking up

some dish and you know; if you know the basic ingredients, you can actually combine and then come up with a particular dish, so you often have to be a good cook to come up with a numerical receipt to solve the problem and to be a good cook you have to understand the foundations.

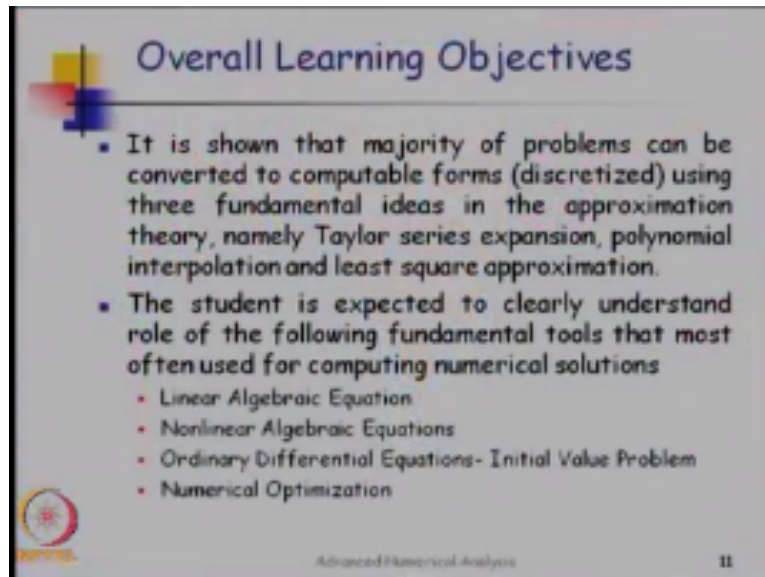
So, the first step is; you know problem transformation, which is based on the approximation theory. The next step is of course solving it but in solving it, there are 2 aspects; one is of course the algebraic aspect of the problem, how do you actually write the algorithms and so on but often there are very, very interesting geometric ideas associated with these numerical schemes.

And if you get understanding of these geometric ideas; if you understand you know, if you can visualize some of these, if you can use your; you know power of visualization then actually that can help you to construct solutions much better. So, unlike a traditional course, I would like to stress a lot on explaining many geometric ideas that are associated with development of numerical schemes.

So, this will actually help in developing a deeper understanding of numerical recipes and finally an aspect that we do not try to stress in a first course is analysis of convergence or convergence analysis of numerical methods or error analysis, there are also other analytical aspects that are associated with the numerical computations and I would like to stress these numerical; these aspects along with the numerical aspects; convergence aspects or along with numerical aspects.

Though we may not get too much deep into these but we will nevertheless study this to some extent, so that you have a taste of what goes in; you know understanding the convergence behaviour of these schemes. So, all these 3 aspects are very, very important when it comes to; coming up or one when it comes to concocting a new numerical scheme. So, if you take a critical look at many many numerical schemes that are available in the most of the textbooks.

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**Overall Learning Objectives**

- It is shown that majority of problems can be converted to computable forms (discretized) using three fundamental ideas in the approximation theory, namely Taylor series expansion, polynomial interpolation and least square approximation.
- The student is expected to clearly understand role of the following fundamental tools that most often used for computing numerical solutions
  - Linear Algebraic Equation
  - Nonlinear Algebraic Equations
  - Ordinary Differential Equations- Initial Value Problem
  - Numerical Optimization

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You will see that you know there are some fundamental 2 or 3 ideas that are used in developing the compatible forms okay. One of them; one dominant idea that is you find in numerical methods is using Taylor series expansion. So, approximations carried or carried using Taylor series expansion is one dominant way of doing approximation. The other method or other approach that is used is polynomial interpolation.

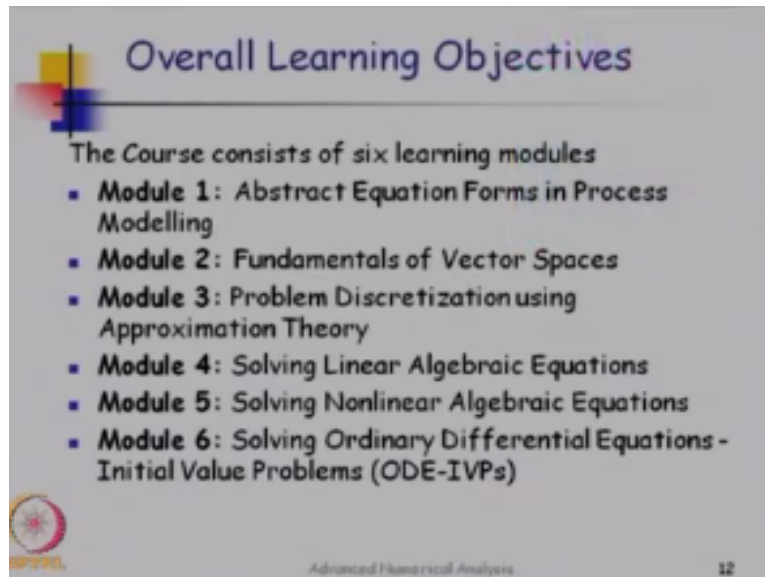
And the third you know; pillar of approximation or problem simplification, problem discretization is least squares approximations, so the problem transformation is carried out mainly using these 3 fundamental tools or fundamental ideas; one is Taylors series expansion, other is polynomial interpolation and least square approximation and we are going to study them pretty much in detail, so as to understand their role in problem transformations.

Then, after that we are going to get in depth understanding of 4 different numerical tools. Well, once you transform the problems, there are a variety of ways of attacking the problem to get a numerical solution. So, if you look at what are the tools available today, well we can come up with 5 different classifications, I have just mentioned 4 of them here; one is linear algebraic equations, other is nonlinear algebraic equation, ordinary differential equations, initial value problem and numerical optimizations?

So, I need these 4 toolkits with me to come up with a numerical scheme and then the fifth one, which is not mentioned here or which is not going to be part of this course is stochastic methods that goes much beyond scope of this particular course and would probably need a separate course to see how stochastic methods can be used to solve the transform problem. We

are going to concentrate mainly on linear algebraic equations, nonlinear algebraic equations and ordinary differential equations, initial value problems or ODE IVP as they are known.

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The slide is titled "Overall Learning Objectives" and features a decorative graphic of overlapping colored squares (yellow, red, blue) on the left. The text on the slide reads:

The Course consists of six learning modules

- **Module 1:** Abstract Equation Forms in Process Modelling
- **Module 2:** Fundamentals of Vector Spaces
- **Module 3:** Problem Discretization using Approximation Theory
- **Module 4:** Solving Linear Algebraic Equations
- **Module 5:** Solving Nonlinear Algebraic Equations
- **Module 6:** Solving Ordinary Differential Equations - Initial Value Problems (ODE-IVPs)

At the bottom left of the slide is a circular logo with a star-like pattern. At the bottom center, it says "Advanced Numerical Analysis" and at the bottom right, the number "12".

Along our way, we will also pick up fundamentals of numerical optimization, I do not intend to have a separate module on numerical optimization but we will; on our way, we will pick up tools for numerical optimization. So, this course consists of 6 learning modules, the first one actually here I am talking of the course ideally what it should consist of. Well, I will then, at the end of this slide, I will tell you what I am going to lecture on.

But this course, initially should begin with relating abstract equation forms to process models okay. So, if I am delivering this course to finally year undergraduate students, I would spend first 2 or 3 lectures talking about different mathematical models that they have already studied and what abstract equation forms that arise from these mathematical models. The second module is going to be completely different from what you do in a conventional numerical methods or numerical analysis course.

A few lectures; these few lectures are going to be devoted to fundamentals of vector spaces. Now vector spaces, we start studying vector spaces probably even before we enter our engineering programs, so by the time we come into engineering programs, we are familiar with 3 dimensional vector spaces and mostly we continue using 3 dimensional vector spaces, maybe you study you know, different coordinate systems which probably you do not study when you are in your school.

But more or less, the idea of vector space remains confined to 3 dimensional vector spaces but in mathematics, in the field of functional analysis the idea of vector spaces has been very, very profoundly developed into; you know a rich concept where a large subset of objects can be looked upon as vector spaces and we are going to get some peek; some you know understanding of these generalized vector spaces which are not just 3 dimensional vector spaces but 4, 5 or n dimensional or even infinite dimensional vector spaces.

In fact, these vector spaces, a fundamental role in formulation of; or in understanding of numerical schemes and this is what I mean, when I am saying that I want to stress upon geometric ideas. The geometric idea is that you understand in 3 dimensions can be extended to spaces of higher dimension and that is what we are going to have a peak at in the second module. The third module is going to be problem discretization using approximation theory.

So, significant numbers of lectures are going to be devoted to problem transformations. So, here you know I will start with the models which could be a nonlinear set of algebraic equations, which could be a partial differential equation, which could be an ordinary differential equation, boundary value problem; I am going to transform it into a computable form. So, unlike a conventional course, where these PD's or boundary value problems are discussed at the end will encounter them right in the beginning of this course.

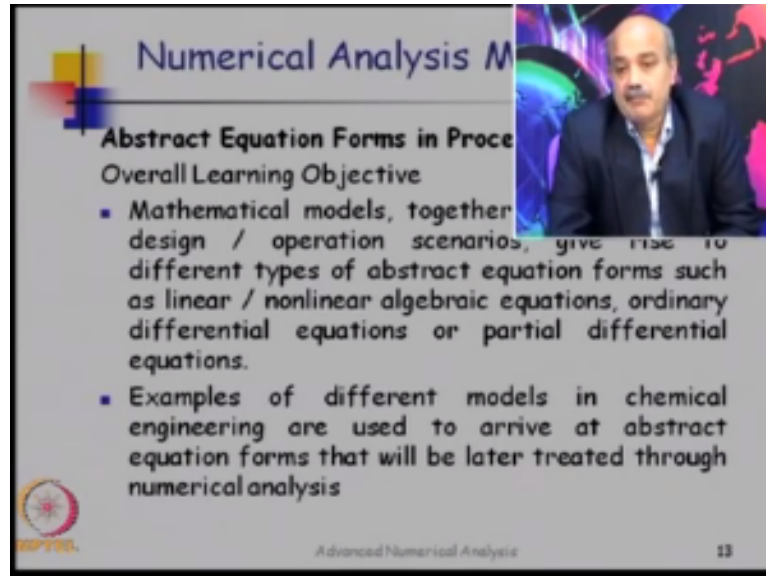
And we will transform to the computable forms, once we have this standard compatible forms which could be set of linear algebraic equations, which could be set of nonlinear algebraic equations or ordinary differential equations initial value problems, then we need to know how to solve them. So, module 4 is going to look at variety of numerical tools for solving linear algebraic equations, then we move on to tools for solving nonlinear algebraic equations.

And finally we end with tools for solving ordinary differential equations initial value problems. So, ideally this course should consist of these 6 modules well, but when I am going to deliver these set of lectures, I am assuming that you are already well familiar different model forms that you encounter in chemical engineering. So, the modules 1 though I have mentioned here, I am not going to really start with module 1.

My lectures will start in module 2 that is fundamentals of vector spaces. In the next few slides, I will very briefly touch upon what should go into model 1 but the second lecture onwards, will

start looking at vector spaces; generalized vector spaces and what role they play in numeric analysis okay. So, moving on; well, how long will this journey be; it is going to be a long journey, we would deal about 48 lectures, 1 hour lectures to understand this variety of aspects of numeric analysis.

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**Numerical Analysis M**

**Abstract Equation Forms in Process Modelling**

**Overall Learning Objective**

- Mathematical models, together with design / operation scenarios, give rise to different types of abstract equation forms such as linear / nonlinear algebraic equations, ordinary differential equations or partial differential equations.
- Examples of different models in chemical engineering are used to arrive at abstract equation forms that will be later treated through numerical analysis

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So, let me get into a little more details of module 1, so the module 1 will consist of abstract equation forms in process modelling, so what all objective would be you know, mathematical models in chemical engineering together with variety of designer operating conditions, they give rise to different types of abstract equations or equation forms like ODEs like partial differential equations.

And so, we must in the beginning associate abstract forms with a real problem because as we go along, we just start looking at abstract forms, we lose track of the engineering problems except when we look at some you know, examples or when we look at or when we solve some exercises apart from that we lose connection with the engineering problems. So, in the beginning, it is good to have connection with these models.

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**Module 1: Learning Objectives**

Examine examples of models commonly encountered in chemical engineering problems and relate them to abstract Equation Forms

- **Linear Algebraic Equations**
  - Steady state material balance equations lumped parameter models of sections of a chemical plant
- **Nonlinear Algebraic Equations**
  - Steady state energy and material balance equations for lumped parameter models of sections of a chemical plant
- **Optimization Based Formulations**
  - Estimation of reaction kinetics parameters
  - Estimation of mass transfer / heat transfer correlations

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And then we need to know which type of equation forms will be treated through in this course. So, if you just want to have commonly encountered examples, so linear algebraic equations, where do we get linear algebraic equations in chemical engineering systems? So, many many times, we have to solve steady state material balance for a lump parameter model, for a section of a plant and this will give rise to a set of linear algebraic equations  $Ax = B$ .

Nonlinear algebraic equations of course, you must have studied in your courses, in the third year, when you study, you know mass transfer heat transfer courses or linear operation courses mainly, where we encounter models which come through energy and material balance for one unit or a section of a plant which consists of multiple units and these give rise to nonlinear algebraic equations.

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**Module 1: Learning Objectives**

Examine examples of models commonly encountered in chemical engineering problems and relate them to abstract Equation Forms

- **Ordinary Differential Equations - Initial Value Problem (ODE-IVP)**
  - Dynamic simulation of lumped parameter models of individual unit operations like reactors
  - Dynamic simulation of section of a plant
- **Differential Algebraic Equations**
  - Dynamic simulation of lumped parameter models of individual unit operations like distillation columns
  - Dynamic simulation of section of a plant
- **Partial Differential Equations**
  - Design / Simulation of packed bed columns and plug flow reactors

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Very often we have to solve problems using optimization tools for example, estimating some rate parameters, say reaction kinetics parameters or estimation of mass transfer or heat transfer correlations. So, these problems have to be solved using tools that are used for optimization; numerical optimization, so these are optimization based formulations and ordinary differential equations, initial value problems arise when you start looking at control at dynamic simulation of a chemical plant.

Or when you want to do HAZOP analysis using dynamics; dynamic simulators, so, these problems in abstract terms are nothing but solving coupled ordinary differential equations subject to given initial conditions or given input scenarios, then you may end up with not just differential equations, you may end up with algebraic differential equations. Well, common example is distillation columns, where you have a phase equilibrium giving rise to algebraic equations, which could be highly nonlinear.

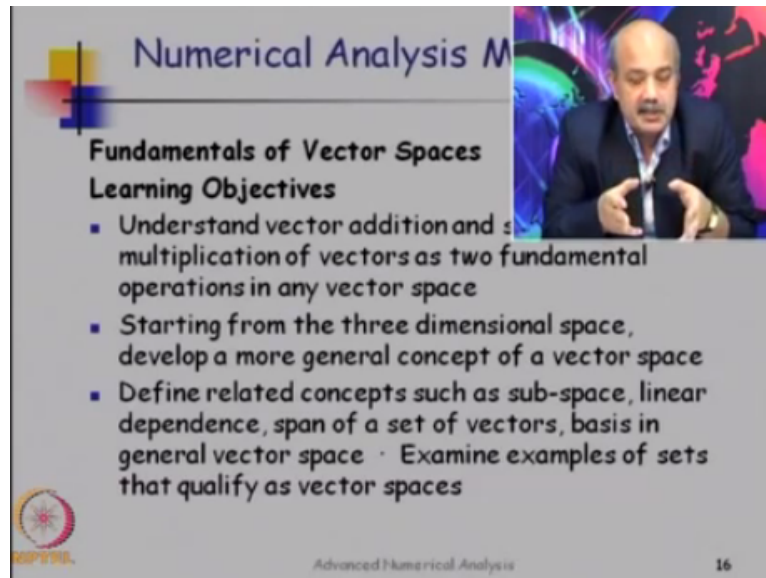
You have differential equations coming from dynamics on the trace, temperature dynamics, composition dynamics, material balance on the trace. If you want to simulate the dynamic behaviour not just do the design, then you get differential algebraic equations coupled equations and these equations are notoriously difficult to solve than the differential equations alone or algebraic equations alone.

So, these are the situations where you know these differential algebraic equations arise, when you have phenomena which are operating at different time scales, so some phenomena are fast, some phenomena are slow and in such situations, the slow phenomena you retain them as differential equations, the fast phenomena you can neglect the derivatives and you know approximate those equations associated with those equations as algebraic equations and that gives rise to differential algebraic equations.

If you want to do detail analysis of; let us say some reactor; plug flow reactor or a packed bed column, then you do not have option but to use partial differential equations, whereas when you are doing a very gross analysis, you know taking it just as a unit in a plant and doing energy material balance, you can probably neglect those variations but if you want to study one unit operation in detail, you often have to use you know, distributed parameter models that is partial differential equations.

So, these partial differential equations arise when you are looking at packed bed columns, plug flow reactors and so on. So, in the beginning, it is good to make these associations to understand where these abstract equation forms arise but as I said my lectures are going to start from module 2 because these are meant for somewhat advanced users, in the final year of a chemical engineering undergraduate program or maybe first year of a graduate program of chemical engineering.

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**Numerical Analysis M**

**Fundamentals of Vector Spaces**

**Learning Objectives**

- Understand vector addition and scalar multiplication of vectors as two fundamental operations in any vector space
- Starting from the three dimensional space, develop a more general concept of a vector space
- Define related concepts such as sub-space, linear dependence, span of a set of vectors, basis in general vector space · Examine examples of sets that qualify as vector spaces

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Well, here we begin with fundamentals of vector spaces, so what are the learning objective? So, first thing is I would like to understand 2 fundamental operations; vector addition and vector and scalar multiplication and see how these operations hold in any vector space. What I mean by any vector space? I am going to define sets, which are called as vector spaces where these 2 operations hold and these sets are going to be other than the familiar 3 dimensional vector spaces.

For example, I would introduce set of continuous functions over some domain say 0 to 1 or I might introduce, I meant start talking about a set of continuous functions over 0 to infinity, these kind of functions; these kind of sets arise when we are solving differential equations, partial differential equations and if you have understanding; basic understanding or of the geometric understanding of these underlying spaces, then it is much easier to develop the solutions for these kind of equations.

So, we are going to look at these abstract notions of vector space and generalize vector spaces like function spaces. So, a vector in this vector space is a function for example, you know set of

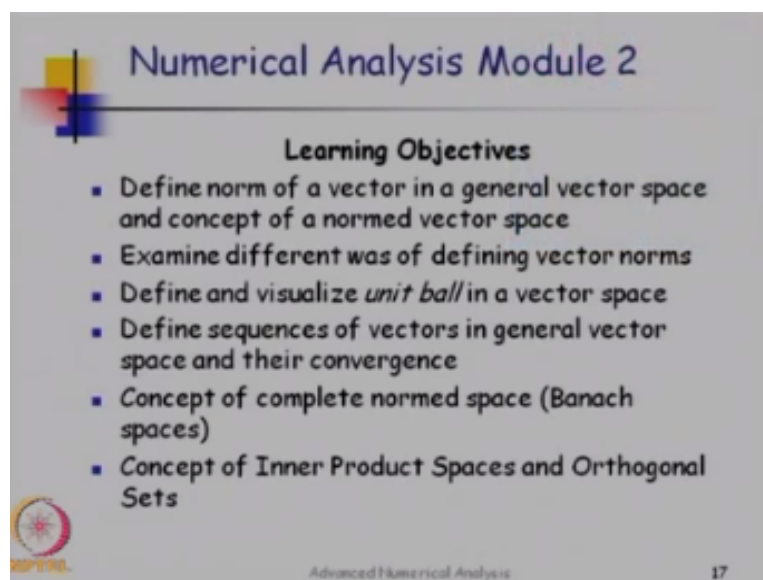
all continuous functions over 0 to  $2\pi$  okay and say  $\sin x$  is a vector in this set or  $\cos x$  or  $\cos 2x$  is a vector in this set of continuous functions. Well, another vector could be just a line,  $A + Bt$  defined over 0 to  $2\pi$  and so on, or some polynomial defined over 0 to  $2\pi$ .

So, these sets are generalized sets not just 3 dimensional vector spaces that you are familiar with and what you will study in this particular module as how these sets to qualify to be called as vector spaces and how the geometric ideas that hold in 3 dimensions can be extended to these higher dimensional spaces. So, we will go on to generalize the concepts such as subspace, such as linear dependence, such as span of vectors, what is the basis in a vector space and so on.

And we will examine examples of different sets that qualify to be vector spaces or that qualified to be subspace of a vector space and so on. So, this is; this is beginning of the geometric generalization; this grand geometric generalization was carried out probably 60, 70, 80,100 years back in the domain of mathematics and if you have some idea about the generalizations, then it becomes very, very easy to understand underlying foundations of numeric analysis.

So, that is why first few lectures are going to be devoted to understanding these generalized sets. Well, when we work in a 3 dimensional vector space, what are the things that you actually need? Well, we need; when you work with vectors, we need to know about length of the vector okay. So, when you move on to generalize vector spaces, we define something called norm of a vector, which could be viewed as a generalization of concept of length of a vector.

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**Numerical Analysis Module 2**

**Learning Objectives**

- Define norm of a vector in a general vector space and concept of a normed vector space
- Examine different ways of defining vector norms
- Define and visualize *unit ball* in a vector space
- Define sequences of vectors in general vector space and their convergence
- Concept of complete normed space (Banach spaces)
- Concept of Inner Product Spaces and Orthogonal Sets

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So, we are going to distil out essential properties that define length in 3 dimensions and generalize them to this concept of norms. Is there a unique way of defining a norm? What we will find out is that a norm can be defined in multiple ways okay. The way we define the so called length in 3 dimensions is one way of defining norm, it is a special case. Now, it is good to do visualizations in 3 dimensions or 2 dimensions, one can do visualizations.

And maybe if you understand visualizations in 2 and 3 dimensions, then you might be at least able to do some imagination and or extend your imagination to see what is happening in a higher dimensional space or a function space, so that is what we are going to look at in this part. Well, when you are dealing with numerical analysis, a thing that you have to you invariably encountered is convergence of a numerical scheme.

So, we have to understand whether a particular; we start with a guess solution and we construct a new solution from an initial solution, so whether this sequence of vectors that you get in the process of generating approximate solutions, is it converging to some point, is it going to somewhere; is it going somewhere in the same space, we need to examine this thoroughly when it comes to understanding numerical behaviour of solutions.

So, in abstract terms, we are going to look at sequences of vectors okay and we also have to talk about conversions in fact, when you talk of conversions of vectors, we have to talk of nearness of 2 vectors and if you want to talk of nearness of 2 vectors, you have to find out distance between the 2 vectors and this is where the concept of norm becomes very, very vital. So, the ideas that we use in 3 dimensions need to be generalized to higher dimensions.

Well, we will look at very briefly at the concept of a normed space that means a space on which a norm is defined so and we will also have; you know we will also understand very briefly what are called as Banach spaces or the complete normed spaces. Well, these spaces you may not encounter later the concept of Banach space may not be required throughout the course but it is good to have understanding of this idea, when we start looking at; when you start generalizing the concept of a vector space.

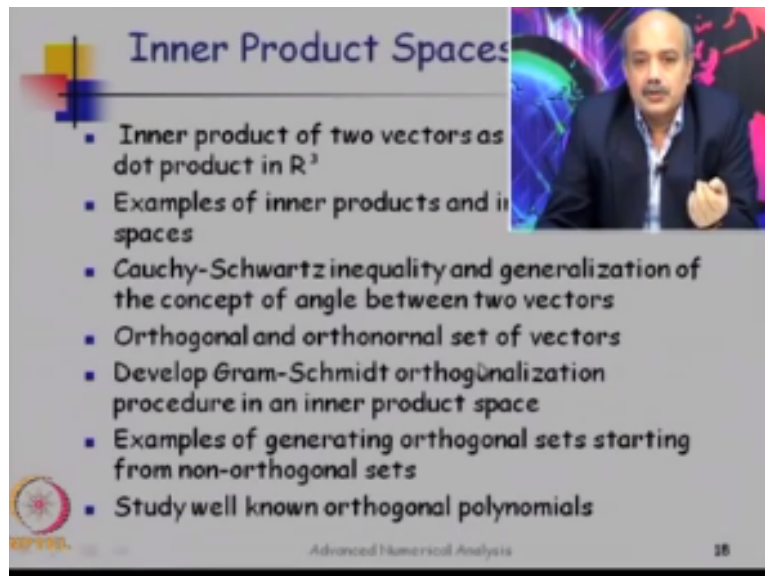
The most important concept that we use in 3 dimensions; when we do geometry in 3 dimensions is orthogonally, okay, we like to work with orthogonal sets, we like to work with you know coordinate definitions, which are orthogonal to each other;  $x$ ,  $y$ ,  $z$  or you know

coordinates that we normally take or you know is a orthogonal coordinate system, so orthogonality that is so useful in 3 dimensions is also useful when it goes to other spaces like function spaces, okay.

So, we need to generalize the concept of orthogonality to higher dimensional spaces to other spaces and this is done through what is called as inner products, so we are going to define a special class of spaces vector spaces called as inner product spaces okay that is a vector space, a set of objects on which an inner product is defined. Well, when it comes to a 3 dimensional space, all of you would be familiar with a dot product okay.

So, when I am generalizing the; when I am generalizing the idea of vector space from 3 dimensions to some other; you know some other sets, which are more general sets, I also would like to have ideas, which are similar to a dot product okay. So, this inner product is going to give me something similar to a dot product in fact, what we will see is that dot product is one way of defining an inner product.

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The slide is titled "Inner Product Spaces" and features a list of bullet points. In the top right corner, there is a small video inset showing a man in a dark suit speaking. The slide also includes a logo in the bottom left and the text "Advanced Numerical Analysis" and "18" in the bottom right.

- Inner product of two vectors as dot product in  $\mathbb{R}^2$
- Examples of inner products and inner product spaces
- Cauchy-Schwartz inequality and generalization of the concept of angle between two vectors
- Orthogonal and orthonormal set of vectors
- Develop Gram-Schmidt orthogonalization procedure in an inner product space
- Examples of generating orthogonal sets starting from non-orthogonal sets
- Study well known orthogonal polynomials

So, inner product is a generalization is a grand generalization, which will help us to generalize the concepts of orthogonality; orthogonal vectors in general spaces, function spaces and so on. So, we are going to look at inner product spaces; inner product spaces are generalization of 3 dimensional vector spaces with dot product defined in them. So, we are very, very familiar with dot product, we use dot product to define angle between 2 vectors in 3 dimensions.

And when we move on to more general spaces, set of functions, set of the polynomials, we need this concept we need something like dot product, which is going to be this inner product in these spaces. So, we are going to look at variety of inner product spaces, so there are different ways of defining inner product that not only one way. In 3 dimensional space, you only know one way of defining an inner product.

But there are other ways of defining inner products and we will look at those different methods of defining inner products. Well, one of the fundamental equation that we use in 3 dimensions is that  $\cos \theta$  angle between any 2 vectors is dot product of two unit vectors in two directions. So, if I have a vector A and B, I find out we need vectors along A, I find a unit vector along B and then I take a dot product, which gives me  $\cos \theta$  between A and B.

A generalization of this particular concept in inner product spaces is nothing but the so called Cauchy Schwarz inequality; the name Cauchy Schwarz inequality might sound very intimidating but this is a very fundamental result in inner product spaces and it will help us to define angle between 2 vectors. So, here a vector as I said is going to be a function and then we need to talk about orthogonal functions okay.

So, so see you might have come across some statements in your undergraduate education saying that  $\sin \theta$ ,  $\sin 2 \theta$ ,  $\sin 3 \theta$ , these are orthogonal to each other, why they are orthogonal? Okay, so if you understand the concept of inner products and inner product spaces, this will no longer be a mystery okay. So, generalization of concept of angle between any 2 vectors is achieved through inner product.

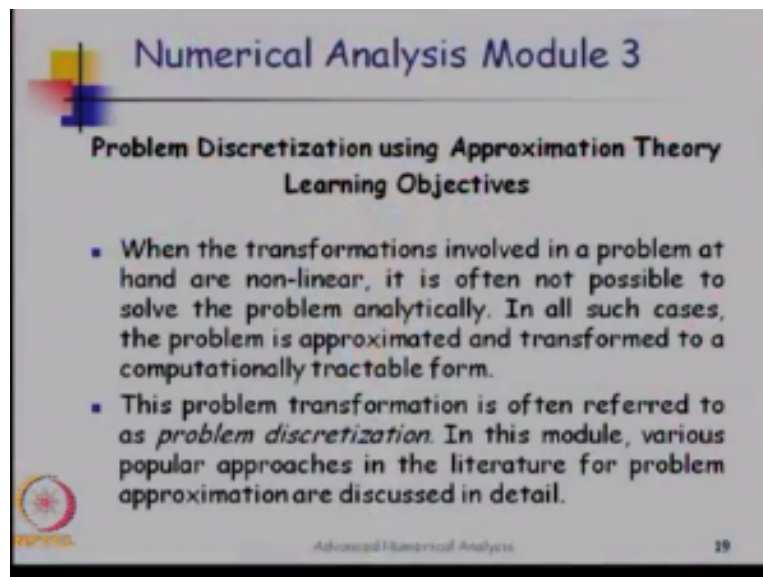
And then the Cauchy Schwarz inequality is a fundamental inequality, which is nothing but generalization of the fact that  $\cos \theta$  is dot product of 2 vectors through unit vectors in 3 dimensions okay. So, we are going to study this Cauchy Schwarz inequality then we will look at variety of orthogonal or orthonormal sets that are very often used in numeric analysis. For example, Legendre polynomial or Lagrange polynomial, now these names we encountered in maths courses.

And often we do not know why they are they are called orthogonal sets or why they are called as orthogonal polynomials. If you start from fundamentals of vector spaces, you will get in depth understanding as why these sets are called as orthogonal sets. Well, it is not always that

you have a set of vectors, which are orthogonal okay but if you have a non-orthogonal set of vectors, then one can systematically construct a set of vectors that is orthogonal.

For example, in 3 dimensions, you may have come across this method called Gram Schmidt orthogonalization okay, which is you start with 3 vectors, which are not orthogonal and starting from these vectors, one can systematically construct 3 new vectors which are orthogonal to each other, okay.

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The slide is titled "Numerical Analysis Module 3" and "Problem Discretization using Approximation Theory". It lists two learning objectives: 1) When transformations are non-linear, analytical solutions are often not possible, so the problem is approximated into a computationally tractable form. 2) This transformation is often called "problem discretization", and the module discusses various approaches in detail. The slide also includes a logo in the bottom left and the text "Advanced Numerical Analysis" and "19" in the bottom right.

So, constructing an orthogonal set from non-orthogonal set, this process is called Gram Schmidt orthogonalization and this we are going to study in a general inner product space, it is very useful to get again insight into how different orthogonal sets are developed and then we will look at examples of generating orthogonal sets starting from non-orthogonal sets. So, from inner product spaces, we then move on to the third module.

Now, this is going to be a very, very important module in this course, I would say heart of this course. How do you discretize the problem using approximation theory? So, as I told you in the beginning, it is often not possible to solve a given problem in its original form. Most of the times, the problem that you have is not a linear, which means it could consist of nonlinear algebraic equations, nonlinear differential equations, nonlinear partial differential equations.

Well, when where you have linear differential equations, linear partial differential equations you can many times construct solutions analytically, at least for some idealized situations. This becomes very, very difficult even if there are slight nonlinearities and it may not be possible to



have analytical solutions, this means you have to construct numerical solutions. To construct numerical solutions, we have to first transform into standard forms.


See, this is because we do not have tools to solve all kinds of problems; we can only tackle certain types of equation forms. So, first step is to convert a different problem into a problem, which can be tackled using standard tools okay and then we attack the problem to construct the solution okay. So, by hook or crook by some means, by using multiple ideas together from approximation theory, we actually transform the problem to a computable form.

Is there a unique way of doing this? Obviously not, a given problem can be transformed into a computable form by variety of means and if you have to choose between different means of transformations, you have to have in depth understanding of how these transformations are done. Why do you choose one over the other, whether I should use a Taylor series approximation or whether I should use interpolation?

Unless you know the foundations, it is difficult to make these choices, so it is good to have a basis of foundation of you know; approximation theory. This step of model transformation is often referred to as problem discretization and in this module; in this set of lectures, we are going to look at popular approaches that are available in the literature for approximations or approximate a given problem to computable forms.

So, first thing that I want to do here before I begin this transformation is to show that actually different problems that you encounter in numeric analysis, they are only seemingly different. Once you start viewing these problems from the viewpoint of vector spaces; generalized vector spaces they do not really appear different problems, one can come up with a grand generalization that there is a one single problem, well in a particular vector space this problem will be called as set of algebraic equations.


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## Numerical Analysis Module 3

### Learning Objectives

- Study how unification of problem representation can be achieved using vector space concepts
- Understand concept of problem discretization to computable forms
- Understand fundamentals of polynomial approximation of a continuous function
- Study Weierstrass approximation theorem: approximation of continuous functions using polynomials



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In the particular vector space; in another kind of vector space a similar problem will be called as solving differential equations initial value problems, in some other vector space this problem will be called as; a problem which is partial differential equation okay. So, if you understand this grand generalization very briefly, then it helps us to develop discretization in a better way into the computable forms.

So, basic problem you can show is that is nothing but operator operating on a vector giving another vector and there are 3 problems associated with this fundamental equation is either given the operator and a vector find the solution, so given operator, say  $T$  operating on a vector  $X$  find  $Y$ , the second problem that you encounter is given operator at  $T$  and  $Y$  find  $X$  that means, I know the solution, I know the effect, I want to find out the cause, so operator at  $T$  when it operates on  $X$  gives me  $Y$ .

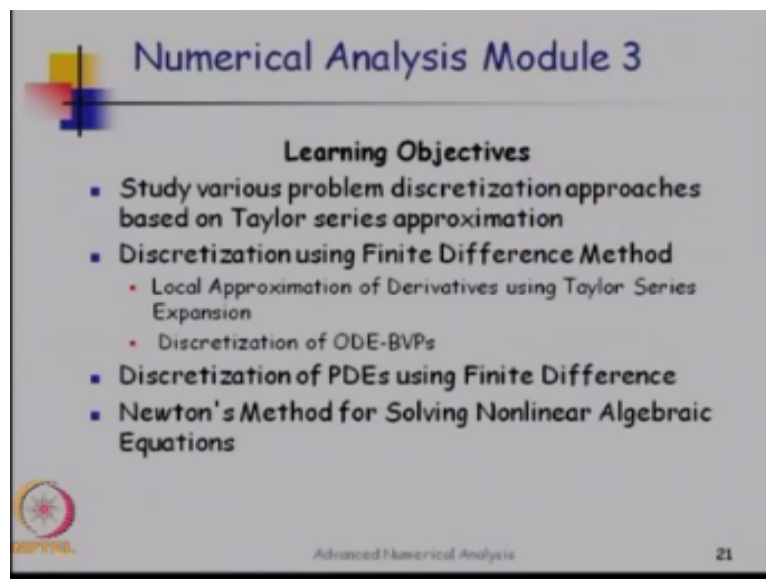
I know  $Y$ , I know  $T$ , I want to find out  $X$  these are called as inverse problems. The first problem where you look at or you are given operator and you are given  $X$ , you find out  $Y$  is called as direct problems. Our course is mostly going to be dealing with inverse problems that is given an operator operating on a vector and you are given  $Y$  the effect then you want to find out because that is  $X$ , then you know we will look at specific tools that are used in problem approximation.

What it turns out is that the backbone of approximation is approximating a given function using set of polynomials okay. It is the fundamental theorem in approximation theory called as Weierstrass approximation theorem and this lays the foundation of all the problem discretization methods that are used in numerical analysis okay. So, this particular theorem

states that any continuous function over a finite domain can be approximated with arbitrary degree of accuracy using a set of polynomials okay.

So, it does not tell you which polynomial to use, it just tells you the existence of such a polynomial approximation, well it is up to us to construct the polynomial approximations but the study of Weierstrass theorem very briefly, we will give you the foundation of how this whole business is done of approximating or how transforming a problem; original problem into a computable form.

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The slide is titled "Numerical Analysis Module 3" and lists the following learning objectives:

- Study various problem discretization approaches based on Taylor series approximation
- Discretization using Finite Difference Method
  - Local Approximation of Derivatives using Taylor Series Expansion
  - Discretization of ODE-BVPs
- Discretization of PDEs using Finite Difference
- Newton's Method for Solving Nonlinear Algebraic Equations

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So, we will just very briefly look at the Weierstrass approximation theorem and then we will one by one start looking at commonly used polynomial approximations okay. So, which is the most commonly used polynomial approximation? As I said, the most commonly used polynomial approximation is Taylor series approximation, so this is used in variety of numerical tools for example, for solving or developing this method called method of finite difference.

Method of finite difference is used for discretization of ordinary differential equations, boundary value problems ODE BVP, they get transformed into set of algebraic equations, this method is also used for transforming partial differential equations into set of algebraic equations okay. So, we will also study this method in a different context for example, you probably are familiar with Newton's method or sometimes called as Newton Raphson method for solving nonlinear algebraic equations.

And again this method originates from Taylor series approximation that is approximating a nonlinear differential equation or nonlinear set of equations locally using Taylor series and then converting into a set of a sequence of linear algebraic equation problems. So, we will look at Taylor series approximation as a fundamental tool and how it is applied to do problem transformations.

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**Numerical Analysis M**

**Learning Objectives**

- Study various problem discretization based on Polynomial Interpolation
  - Lagrange Interpolation
  - Piecewise Polynomial Interpolation
  - Interpolation using Linearly Independent Functions
- Study discretization using orthogonal collocations
  - Discretization of ODE-BVP
  - Discretization of PDE's
- Study Orthogonal Collocations on Finite Elements

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A variety of problem transformations transforming a partial differential equation, transforming boundary value problem, transforming set of nonlinear algebraic equations, then we continue our journey into other type of approximation. The second most important or not second most important equally important approximation is polynomial interpolations. So, in the beginning we will have a brief understanding of Lagrange interpolation.

Well, it is a large vast area and then we cannot do justice to every aspect of interpolation; I am just going to give you a brief introduction to some important concepts. So, we will begin with Lagrange interpolation, we will move on to piecewise polynomial approximations or interpolations or not approximations, piecewise polynomial interpolation and then we will also look at not just polynomial interpolation, we will also look at function interpolations, okay.

So, linearly independent functions are used to construct interpolating functions and then we will look at problem discretization using this approach. So, I am going to again look at a boundary value problem, ordinary differential equation boundary value problem and discretize it using interpolation polynomials or I am going to discretize a boundary value partial differential equation using interpolation polynomial.

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**Numerical Analysis M**

**Learning Objectives**

- Study various applications of least squares approximations including problem
- Develop analytical solution of linear least square problem
- Study geometric interpretation of Linear Least Squares Approximation
- Projection Theorem in a general Hilbert space
- Function approximation based models and formulation of parameter estimation problem

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So, this is my next task that is study how interpolation plays a role in problem discretization in particular, we are going to look at this method of orthogonal collocations, which is a very powerful method used in solving variety of chemical engineering problems and then have a brief probably look at orthogonal collocations on finite elements. So, the third important tool or third important approach that is used for problem discretization is least squares.

So, we are going to study various ways of approximating problems using method of least squares. First, we will develop analytical solution of linear least square problem okay look at its geometric interpolations, this will give us insight that is very, very valuable that can be you know extended when we understand approximations in higher dimensional spaces and then we will actually extend this idea to general spaces or general Hilbert spaces.

So, the fundamental to this least square approximation is the idea of projections. Now, projections we normally study in engineering, engineering drawing or we study projections even starting at a school where you were to project find a nearest point in a plane from a given point outside the plane, so projections are very, very important and how do these idea projections is used in the problem approximation is what we want to study next.

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**Numerical Analysis M**

**Learning Objectives**

- Least square formulation for linear models
- Nonlinear in Parameter Models and Method
- ODE-BVP / PDE Discretization using Minimum Residual Method
  - Method of Least Square
  - Galarkin's Method
- Discretization of ODE-BVP / PDEs using Finite Element Method
- Understand various types errors that arise in problem approximation and computation of approximate solution

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So, we will also have a brief peek at function approximation based models and the formulation of the parameter estimation problem and in this before we move on to the main; the remaining part that is understanding the tools, we will also look at least square problems for linear in parameters models, least square formulations for nonlinear in parameters models, so in particular we are going to look at a method called Gauss newton method.

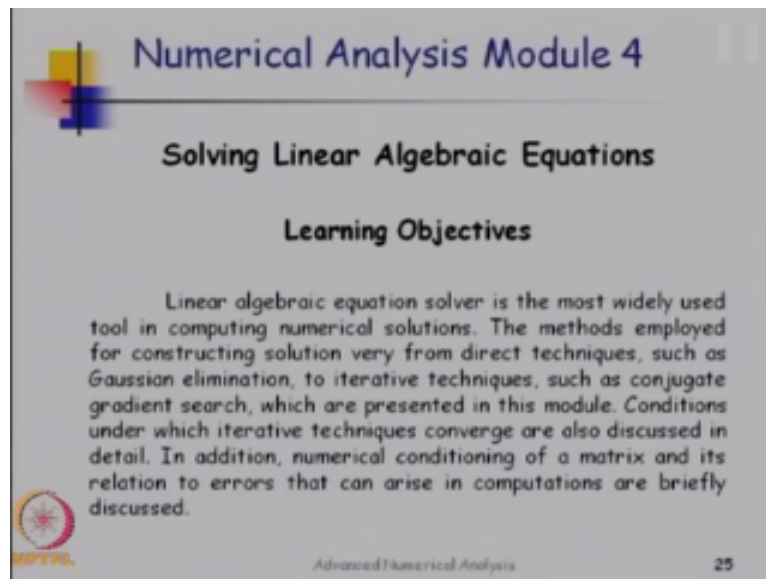
So, this Gauss Newton method is a combination of least squares and Taylor series, so we look at this Taylor series approximation and least square approximation, so we are going to look at this method and then finally move to problem transformations, which we have been already looking at that is how do you transform a boundary value problem or how do you discretize a partial differential equation using method of least squares.

So, these methods are known as method of minimum residual methods, so a popular method in this class is Galarkin method and we will have; we will study this method; actually the discretization of ordinary differential equations boundary value problems or partial differential equations using least square approach leads to the so called finite element methods, we will not go in depth into this but we will have a very brief introduction to what element; finite element method using and how it is related to least square approximation.

So, with this, we will come to an end to of our module, which talks about problem transformations, so this will almost we come to half of the course, now what remains to be done is attack the problems which are transformed. Before that, we will very briefly look at what are

the errors that come up in problem transformations and what are the approximation errors and what it is bearing on the solutions; numerical solutions.

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The slide is titled "Numerical Analysis Module 4" and "Solving Linear Algebraic Equations". It lists "Learning Objectives" and provides a detailed paragraph about linear algebraic equation solvers. The slide also includes a logo in the bottom left and the text "Advanced Numerical Analysis" and "25" in the bottom right.

**Numerical Analysis Module 4**

**Solving Linear Algebraic Equations**

**Learning Objectives**

Linear algebraic equation solver is the most widely used tool in computing numerical solutions. The methods employed for constructing solution vary from direct techniques, such as Gaussian elimination, to iterative techniques, such as conjugate gradient search, which are presented in this module. Conditions under which iterative techniques converge are also discussed in detail. In addition, numerical conditioning of a matrix and its relation to errors that can arise in computations are briefly discussed.

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So, after having done this; after having transformed the problem now we begin our journey into tools okay. The first tool that we are going to look at is solving linear algebraic equations and here well, you might wonder, we have been solving linear algebraic equations since school days what is so new about it, what am I going to learn about it, maybe you are already familiar with Gaussian elimination.

And then in Gaussian elimination you may have studied even some advanced things like when you know, how to do pivoting and so on but there is much more to linear equation solving than just Gaussian elimination. There are many other methods; there are iterative methods for solving linear algebraic equations and we are going to have look at them, even optimization methods based methods or numerical optimization based methods are used to solve linear algebraic equations and we will be studying those equations.

But apart from studying these numerical schemes, I am going to discuss one very important thing here that is matrix conditioning; matrix conditioning talks about how well posed or how ill posed a given problem is; a given set of linear equations are and then that gives your insight into behaviour of the numerical solution, it may happen that you have ill posed problem and then the solution that you compute numerically is not quite reliable.

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**Numerical Analysis Module 4**

**Learning Objectives**

Study conditions for Existence of Solutions of System of Linear Algebraic Equations

- Geometric interpretation of system of linear equations: row picture and column picture
- Geometric interpretation of solution from different viewpoints
- Geometric interpretation of singular matrix case
- Row space, column space, null space and their relation with solutions of linear algebraic systems

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You should be able to differentiate between ill posed problem and not reliable solution and well posed problem but mistake that you have made in computing the solution okay, so this is possible using the concept of condition number or matrix conditioning and we are going to have a look at these; the concept of conditional numbers as a part of this module, so we will begin with the study of conditions for existence of solutions for linear algebraic equations.

We move on to the geometric interpretation of the solutions very, very important, so I look at the problem through 2 pictures; a row picture and a column picture. We will look at the solution from a 2 different viewpoints; geometric viewpoints, we will interpret the what is the meaning of a singular matrix geometrically and here essentially in the beginning we will just have a some understanding of 4 fundamental subspaces associated with the matrix; row space, column space, null space and left null space.

So, up to now, we were not talking about any numerical scheme where our solution scheme, we were talking about problem transformation and just now I started about solving linear algebraic equations but even in the beginning, I am talking about geometric ideas and now we will move into numerical schemes okay, the first time in this course will be encountering actual numerical schemes.

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**Numerical Analysis M**

**Learning Objective**

Study direct solution techniques for linear algebraic equations

- Gaussian Elimination and LU Decomposition
- Number Computations in Direct Methods: number of multiplications and divisions and their relationship with computation time

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So, first of course, I am going to look at Gaussian elimination very briefly and LU decomposition and will spend some time on the number of computations that are required in carrying out a Gaussian elimination process and see whether you know, there are methods that can even improve that can even reduce the number of computations.

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**Numerical Analysis M**

**Learning Objective**

Introduction to Direct Methods for Linear Systems

- Block Diagonal Matrices
- Thomas Algorithm for Tridiagonal and Block Tridiagonal Matrices
- Triangular and Block Triangular Matrices
- Solution of a Large System of Equations by Method of Partitioning

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So, the main focus in this part is going to be introduction to the iterative methods but before that we will look at some special methods for solving linear algebraic equations and these are going to be called methods for sparse linear systems. So, many problems have very nice structure, sparse systems are one in which lot of elements are zeros and there are only few nonzero elements in a big matrix.

In solving problems, which are large scale let us say you are doing simulation of a section of a plant, you may have thousands of equations and when you actually start solving them, let us say by Newton's method you linearize them, when you linearize them, you get linear set of equations which are say  $1000 + 1000$  or  $10,000 + 10,000$  but this matrix, which is  $10,000 + 10,000$  may not be fully populated, it will have many many 0s and it is possible to take advantage of this structure and then come up with special schemes.

So, these are called as schemes for sparse linear systems and we are going to look at just few of them, it is an iceberg and we can only touch the tip of the iceberg, so I am going to look at block diagonal matrices, I am going to present the Thomas algorithm for tridiagonal matrices and block tridiagonal matrices, we will look at triangular matrices and block triangular matrices but as I said, this is only a brief introduction and we are going to move on to the iterative schemes.

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Numerical Analysis M

Learning Objective  
Study Iterative Solution Techni  
Linear Algebraic Equ

- Derivation of Iterative Algorithms: Jacobi, Gauss-Seidel and Relaxation methods
- Convergence Analysis of Iterative Methods
- Eigen values and speed of convergence
- Convergence results for special forms of matrices

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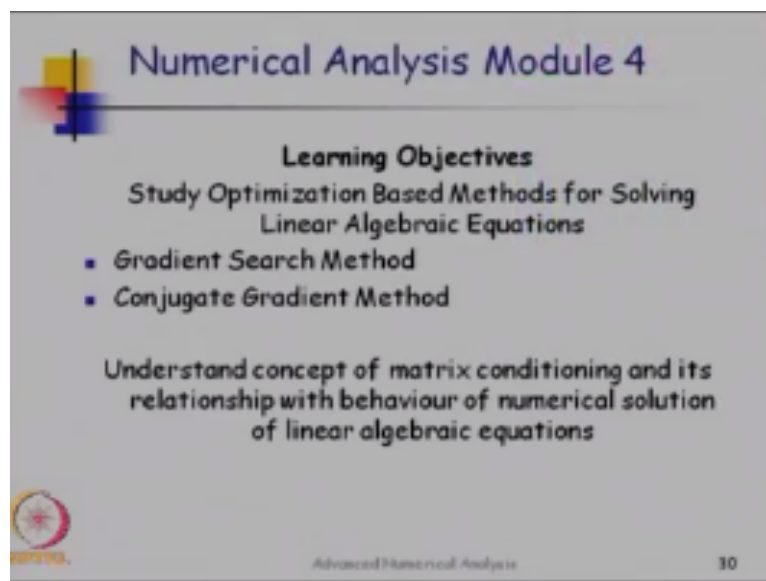
The main thing here is to familiarize you with the notion of sparse matrices and then maybe when you encounter them, you will remember to use them in your application. The study of iterative solutions of or study of; solving linear algebraic equations using iterative solution scheme is the next component that we will look at. So, there are variability of iterative schemes, you start with the guess solution and then you iteratively refine the solution and finally you approach the true solution, this is the iterative approach.

And this we are going to study different methods; very popular methods in this category are Jacobi method or Gauss-Siedel method or the relaxation method, so we will study these

methods their algorithms but more importantly, we will study the convergence analysis of these iterative schemes. I am going to spend quite a bit of time in understanding the convergence of these schemes.

The question is; if I start with a particular guess what is the guarantee that the solution iterative scheme will converge to the solution of solving linear algebraic equations? So, that will be you know; that will be analysed systematically using concept of Eigen values and we will see the rules of Eigen values in speed of conversions or the conversions itself and then we will look at some special form of matrices that enhance convergence.

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We then move on to optimization based schemes for solving linear algebraic equations okay, so here I am going to use a numerical optimization tools such as gradient search method or conjugate gradient method to solve set of linear algebraic equations that is solving  $Ax = B$  is going to be done using optimization, it turns out that in many situations, this can be a very fast tools particularly, when you are solving large set of equations.

And in the end of this module, I am going to understand; I am going to present the concept of matrix conditioning or condition number of a matrix and its relationship with behaviour of numerical solutions of linear algebraic equations. So, we will end with a deeper understanding into how good or how bad a numerical solution is and we associate that with the conditioning of the matrix.

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**Numerical Analysis Module 5**

**Solving Nonlinear Algebraic Equations**

**Learning Objectives**

Majority of models for engineering and real world systems are nonlinear and this leads to systems of nonlinear algebraic equations, which have to be solved numerically. Such systems of equations have to be solved by iterative numerical techniques. In this module, variety of iterative methods used for solving nonlinear algebraic equations are presented in detail. Towards the end, a brief introduction is given to convergence analysis of these methods, which is based on the contraction mapping principle.

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We then move on to the next tool the next tool that I am going to study is going to be solving nonlinear algebraic equation. So, in this toolbox, well nonlinear equations are more often encountered than the real equations, most of the real engineering problems or real engineering models consist of nonlinear coupled equations you do not have them in single variables, you have multiple variables, which are coupled which give rise to couple nonlinear algebraic equations.

If you are modelling section of a plant and understanding the steady state behaviour of energy and material balance, it might be thousands of coupled nonlinear algebraic equations that need to be solved simultaneously that is very, very important. In this method, in this particular module we will look at variety of iterative methods that are used for solving nonlinear algebraic equations okay.

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**Numerical Analysis Module 5**

**Learning Objectives**  
Study Method of Successive Substitutions

- Formulation of derivative free iterative search schemes
- Formulation of Jacobi, Gauss-Seidel and Relaxation Iterations

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In the end, we will also have a brief introduction to the convergence analysis of these methods based on a famous principle in function analysis called as contraction mapping principle. so again this is just a brief introduction to let you; to tell you that what goes in in understanding the convergence analysis of this scheme. So, we will begin with the method of successive substitutions, this is one of the very preliminary methods, which is used.

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**Numerical Analysis Module 5**

**Learning Objectives**  
Study Newton-type (local derivative based) Methods

- Univariate Newton Type Methods
- Multivariate Secant or Wegstein Iterations
- Multivariate Newton's Method and Damped Newton Method
- Quasi-Newton Method with Broyden (rank one) Update of Jacobian Matrix

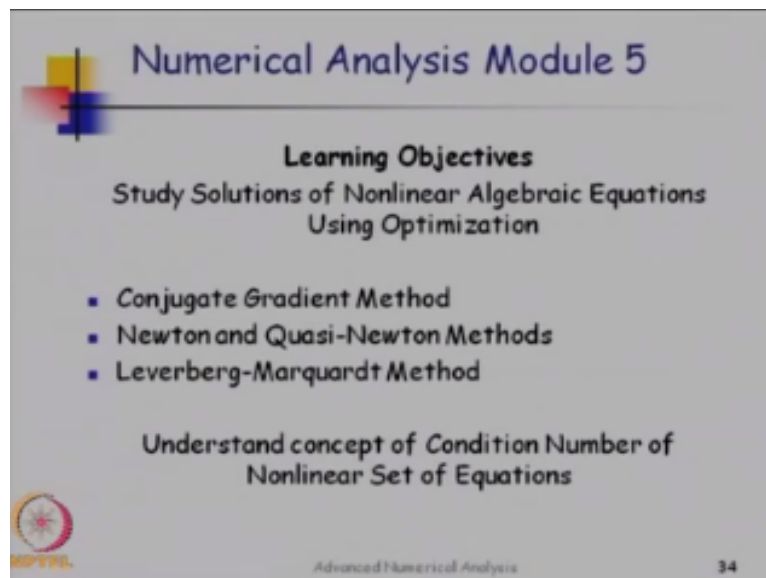
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These are derivative free methods, so there are a variety of derivative free methods like Jacobi iterations or Gaussian iterations or relaxation iterations, we will study these methods and then from this, we will move on to derivative based iterative methods. The well-known derivative based internet methods are Newton's method, so we will first look at Univariate Newton type methods, where you find out the local derivatives either exactly or approximately.

Then, we will formulate a multivariate secant method which is an approximate derivative based method or popularly known as Wegstein iterations, then we will move on to the well-known Newton's method and look at its variations like damped Newton method, you can try to improve the convergence behaviour or we will develop numerically more friendly versions of Newton's method, which are you know called as Quasi-Newton methods or with rank 1 updates of the Jacobian matrix.

The problem with newton method is that you have to compute derivative matrix; Jacobian matrix; if there are any questions and  $n$  variables every iteration, you have to compute an  $n$  cross  $n$  matrix and this can be numerically quite complex, if you have thousands of equations. This Quasi-Newton method allow you to do approximate update of the Jacobian, so they construct a new Jacobian using the old Jacobian and this way they save computations, so we are going to have a brief introduction to this Quasi-Newton methods.

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The slide is titled "Numerical Analysis Module 5" and lists the following learning objectives:

- Study Solutions of Nonlinear Algebraic Equations Using Optimization
- Conjugate Gradient Method
- Newton and Quasi-Newton Methods
- Leverberg-Marquardt Method

Understand concept of Condition Number of Nonlinear Set of Equations

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Then, we move on to solving nonlinear algebraic equations using optimization; optimization; numerical optimization is a powerful tool which is used for solving nonlinear problems, nonlinear algebraic equations. One of the popular method in this class is conjugate gradient method, so we will have a brief look at conjugate gradient method, this is a gradient based method, there is a hessian or second order derivative based method which are called in this category, they are called as Newton's method.

We also have Quasi-Newton method which are again simplifications of Newton's method or Hessian based methods, so we will have a brief peek or brief introduction to Quasi-Newton

methods and finally we will look at a method called Levenberg-Marquardt method, which is combination of the gradient method and Newton's method, so you use gradient when it is helpful to use gradient, you use Hessian when you it is helpful to use Hessian. So, it is a merger of the 2 methods.

And we will just understand this, towards the end we will just briefly understand the concept of condition number of set of nonlinear equations, you cannot have one condition number you can define a local concept of condition number here, which is conceptually similar; qualitatively similar to what we have done for linear algebraic equations. So, before we wind up this particular module, we look at 2 important aspects.

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Numerical Analysis M

Learning Objective  
Study conditions for existence nonlinear algebraic equations and the convergence of Iterative Methods

- Contraction mapping theorem
- Convergence of Successive Substitution Schemes
- Convergence of Newton's Method

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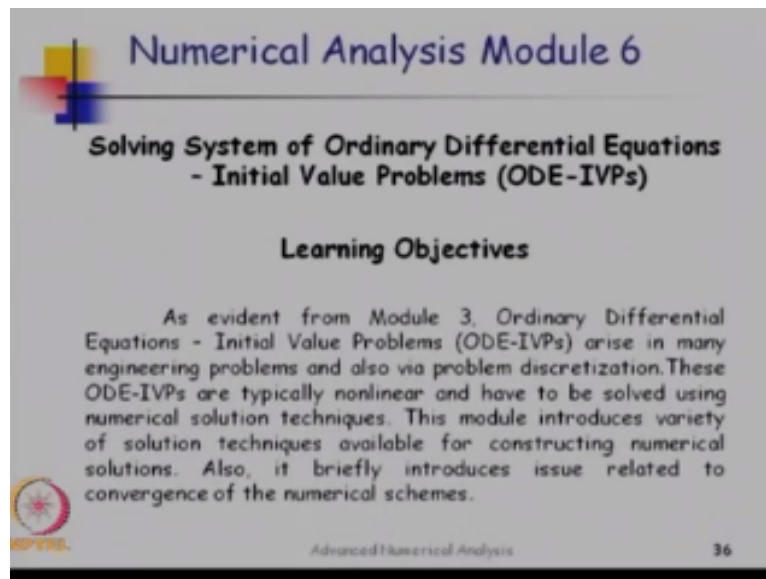
One was existence of solution of nonlinear algebraic equations and its relation to convergence of iterative methods okay, in the; when we started studying linear algebraic equations, we began with the conditions for existence of solutions we never talked about this, when we started solving nonlinear algebraic equations. Here, I want to give a brief introduction to the conditions of existence of solutions.

And what is its relation to convergence of iterative methods, we look at contraction mapping principle or contraction mapping theorem, we will apply to understand convergence of method of successive substitutions, we will also see how contraction mapping principle can be used to analyse Newton's method or Newton-Raphson method and with this, we have come to or we will come to an end of module 5, which is on solving nonlinear algebraic equations, so we



move on to the last tool that will be discussed in this course that is solving ordinary differential equations initial value problems.

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**Numerical Analysis Module 6**

**Solving System of Ordinary Differential Equations - Initial Value Problems (ODE-IVPs)**

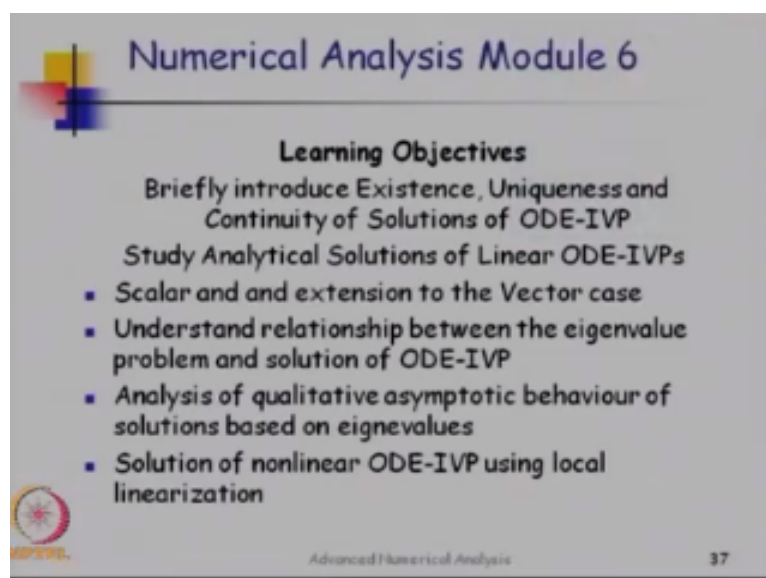
**Learning Objectives**

As evident from Module 3, Ordinary Differential Equations - Initial Value Problems (ODE-IVPs) arise in many engineering problems and also via problem discretization. These ODE-IVPs are typically nonlinear and have to be solved using numerical solution techniques. This module introduces variety of solution techniques available for constructing numerical solutions. Also, it briefly introduces issue related to convergence of the numerical schemes.

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So, this is another fundamental tool, which can be used to attack or to solve the transform problem, so what are the learning objectives? Here, as it is evident from problem transformation module that many situations when you transform a problem, you get ordinary differential equations initial value problems, so this is one of the fundamental model type or equation type, which needs to be dealt with.

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**Numerical Analysis Module 6**

**Learning Objectives**

Briefly introduce Existence, Uniqueness and Continuity of Solutions of ODE-IVP

Study Analytical Solutions of Linear ODE-IVPs

- Scalar and extension to the Vector case
- Understand relationship between the eigenvalue problem and solution of ODE-IVP
- Analysis of qualitative asymptotic behaviour of solutions based on eigenvalues
- Solution of nonlinear ODE-IVP using local linearization

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And we have to arrive at or we have to develop special methods to solve this class of problems. So, in the beginning, we will very briefly introduce the conditions for existence and uniqueness of solutions of ordinary differential equation initial value problem, this is a very, very brief



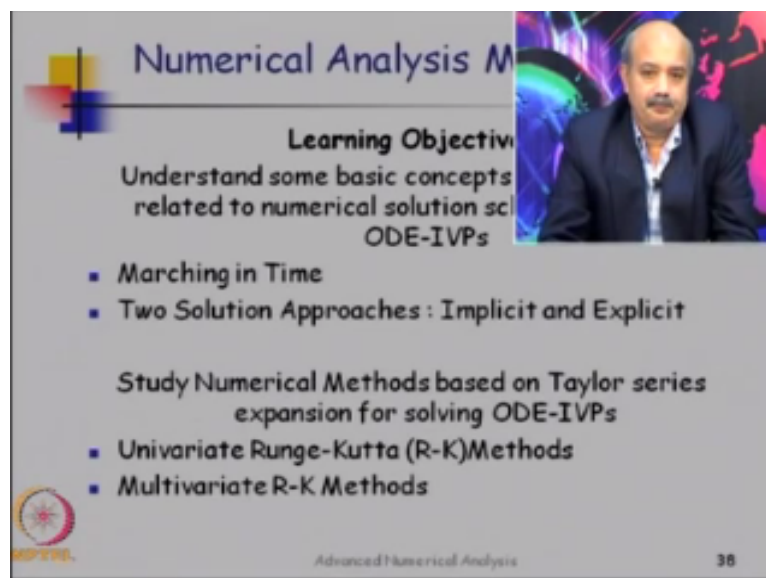
introduction and then we immediately move to study of analytical solutions of linear ordinary differential equations in multiple variables.

Well, you might wonder, why am I doing this analytical solution in a course, which is meant to be for constructing numerical solutions. Well, this analytical solution part gives in depth understanding how local solutions behave also, this is going to help us when we understand or when we analyse convergence behaviour of numerical schemes for solving ODE IVP, so as a background to develop numerical schemes, I am going to solve analytically linear ordinary differential equations given initial conditions.

So, I will start with a scalar equation, move on to vector equations and then what is critical here is that I want to relate; so what are these kind of equations? I am going to look at  $dx/dt = Ax$ , where  $A$  is a matrix and then I want to understand relationship between the Eigen values of matrix  $A$  and analytical solution of this differential equation  $dx/dt = Ax$ , then actually you can get the Eigen values of this matrix, I can qualitatively tell how the solution is going to behave asymptotically as time goes to infinity.

So, just looking at the Eigen values we can analyse the behaviour of the solutions and this elegant part we are going to study briefly and then, what is the relationship of linear equations and local linearization through Taylor series approximation is what we are going to look at here at end of this sub module. We now move to the proper numerical methods for solving ODE IVP.

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**Numerical Analysis M**

**Learning Objective**  
Understand some basic concepts related to numerical solution schemes for ODE-IVPs

- Marching in Time
- Two Solution Approaches : Implicit and Explicit

Study Numerical Methods based on Taylor series expansion for solving ODE-IVPs

- Univariate Runge-Kutta (R-K) Methods
- Multivariate R-K Methods

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So, before that we need to understand some basic concepts like marching in time, how do you develop a solution, you want to solve a problem, you want to integrate differential equations from some time; 0 to time infinity, you actually do it in small steps, this is marching in time, so we will talk about this. If you look at the methods; for solving numerical methods for solving ODE initial value problems, there are 2 classes.

One is explicit methods, other are implicit methods, so we will just have understanding of what is an implicit method, what is an explicit method and then we move on to study and important class of methods, which is based on Taylor series approximation, popularly these methods are known as Runge-Kutta methods, they actually arise from Taylor series approximation and this is where I relate it to the approximation theory part that we have done earlier.

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Numerical Analysis M

Learning Objectives  
Study Numerical Methods Based on  
Interpolation for solving

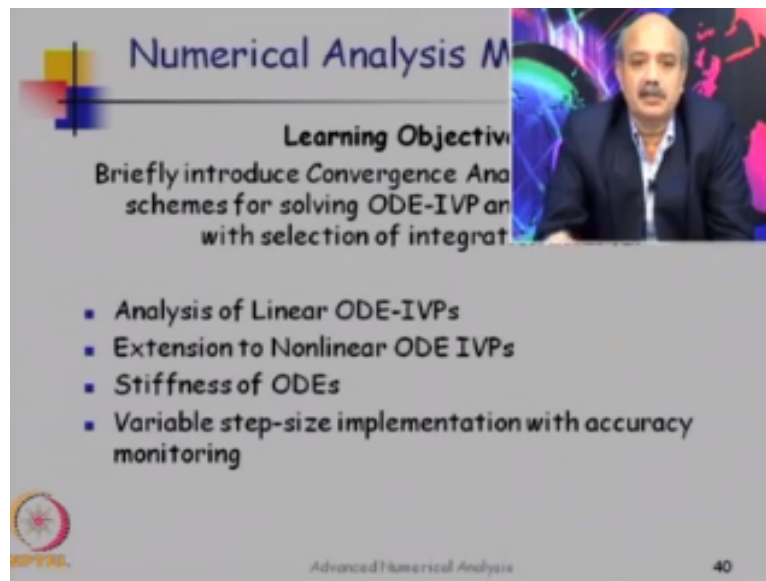
- Multi-step Methods
  - Examples of Multi-step methods
  - Predictor-Corrector Algorithms
  - Multivariate Case
- Numerical Solution using Orthogonal Collocations

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So, we will actually derive here Runge-Kutta methods starting from basics, initially for a scalar case and then move on to the multivariate case. We then move on to the next important method, which is based on polynomial interpolation. So, again you will see that the ideas of; ideas of approximation theory are playing a role, when you are actually solving ordinary differential equation initial value problem.

So, those ideas are so fundamental, they just are everywhere in numerical analysis, so we are going to study methods called as multi step methods okay or popularly known as predictor corrector methods okay. We will develop; we will derive these algorithms starting from scratch, starting from interpolation polynomials and first for the scalar case and see how they can be generalized to multivariate case.

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**Numerical Analysis M**

**Learning Objective**  
Briefly introduce Convergence Analysis schemes for solving ODE-IVP and with selection of integration step size

- Analysis of Linear ODE-IVPs
- Extension to Nonlinear ODE IVPs
- Stiffness of ODEs
- Variable step-size implementation with accuracy monitoring

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And then move on to solving initial value problems, ordinary differential equation initial value problems using orthogonal collocations. Well, after that we actually have a brief look at convergence analysis of numerical schemes for solving initial value problems, ODE initial value problems and what is its relationship with selection of integration step size, when you are integrating nonlinear differential equations, one of the key things is how do you select integration step size, okay.

To greater understanding into this, we have to have some understanding of you know convergence analysis, so we will analyse of course, linear ordinary differential equation initial value problems use and we will apply approximate solutions to these linear problems, we already know their exact solutions and then we can compare exact solution with approximate solution and get insights that is the reason I introduced analytical solution of linear ODE IVP in the beginning.

Then, we will see how this can be extended to nonlinear ODE IVPs; we will look at few concepts which are important in solving these equations like stiff ordinary differential equations. So, stiffness of ODEs is what we look at and then finally we look at what are called as variable step size implementation of these ODE IVP schemes with accuracy monitoring, so these are all involved concepts of course, most of the tools that we use today, most of the programs are available will have these built in tools you should know when to use, which one to use, why to use particular choice.

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**Numerical Analysis Module 6**

**Learning Objectives**

- Introduction to numerical solution approaches for solving Differential Algebraic System of Equations (DAEs)
- Introduction to a scheme for solving ODE-BVP using ODE-IVP solvers (Shooting Methods)
- Error Convergence Analysis of Numerical Solvers for ODE-IVPs


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If you have a stiff differential equation, you should use a particular tool, if you have you know variables, which are; which have too much difference in their timescales, you should use variable steps as implementation and so on. So, these things become very, very important when it comes to; in the end I am going to talk about solving differential algebraic equations, we have studied differential equations, we have studied algebraic equations, nonlinear algebraic equations just a brief look at how do you solve differential algebraic equations, if they are encountered together.

Then, we will look at a special method for solving ordinary differential equations boundary value problems called method of or a shooting method. So, actually you use an initial value problem solver to solve the boundary value problem okay, so how this is done to look at this method and then again, we look at convergence analysis of solvers for ODE IVP. So, this brings us to an end of this 6 modules; introduction to these 6 modules.


So, if I want to sum up what is; what is you know overall learning objective in this course in this; well, first is you should know how to transform a mathematical problem at hand into a computable form using of course, principles of approximations here that is the almost half the course is devoted to that, then understand basic properties of different tools particularly 3 different tools solving linear algebraic equations, solving nonlinear algebraic equations and solving ordinary differential equations subject to or given initial values or initial conditions ODI IVPs.

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## Overall Learning Objectives

- Understand how a mathematical problem is transformed to a computable form
- Understand properties of basic tools used in solving the transformed problem along with their limitations
- Concoct a recipe for constructing a numerical solution of a transformed computable form



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Understand different methods of different numerical schemes for solving these standard class of problems and understand their limitations, so that if you understand their limitations, if you understand their strengths, if you understand how they are developed you have been much better position to employ them, use them to concoct a recipe. Finally, what I wanted to learn or to understand is that a numerical scheme is actually like a recipe and we are going to be a cook who will actually be able to cook a recipe; cook a recipe for a given problem.

So, you have these fundamental tools you have some fundamental tools coming from approximation theory, use a combination of them, first combination of tools from the approximation theory to transform the problem, then you solve the transform problem using standard tool kits that you have okay. So, this journey is going to be fairly long, it is about 48 lectures and we begin our journey from the next lecture. Thank you.