Advanced Numerical Analysis
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Lecture - 40
Solving Ordinary Differential Equations - Initial Value Problems (ODE-IVPs): Basic Concepts

How to solve these problems? My lectures are going to be, of course, centered on algorithms, but the derivation of algorithms. I am more worried about how these algorithms are derived rather than what are these algorithms. I want to derive Runge-Kutta methods, 1 class of algorithms which are based on Taylor series. The other class of algorithms based on polynomial or Vieta's theorem, multistep methods or predictor-corrector methods on the class of algorithms.

I will briefly touch up on orthogonal collocations, then we will move on to talk a little bit about convergence or numerical stability of these algorithms. Why 1 algorithm has better properties than the other. So comparing the algorithms. What is the basis for comparing the algorithms? After that, we will spend time on some special applications like there are methods of converting a boundary value problem into initial value problem. They are called as shooting methods.

We will look at shooting methods and then if time permits, we will have a peek at what are called as differential algebraic systems. Differential algebraic systems are 1 in which you have solve simultaneously differential equations and algebraic equations. In fact, a problem which is very, very often encoded in chemical engineering. Though it is very, very important, we can probably get time only to touch up on some algorithms, some ideas of di systems.

So let us begin our journey into ODE-IVP. Last class I talked about a general set of ODI-IVP.
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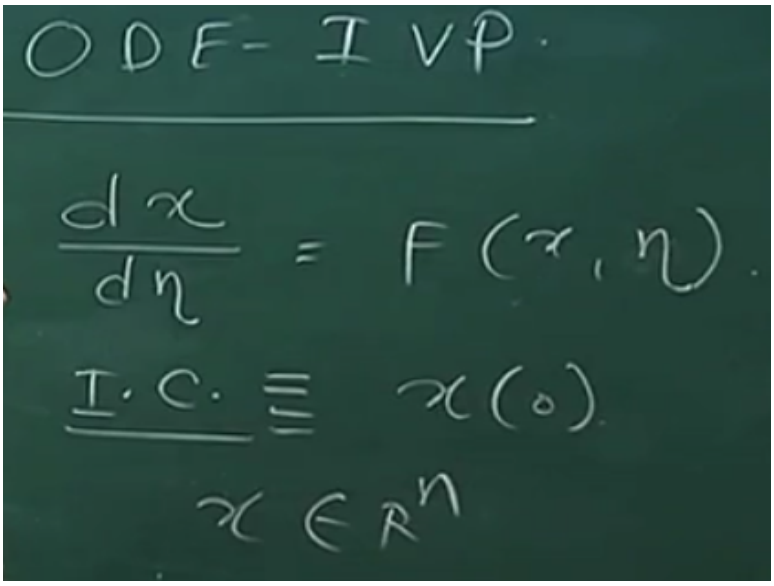

Which is dx/dt=F(x, t), initial condition corresponds to x not, x belongs to Rn, n dimensional vector and I want to find out the time trajectories or I want to find out spatial trajectories. So actually to generalize I had made a small modification. I had just said here some independent variable eta at time 0 or at special coordinate 0, whatever it is at a initial condition is known to you, you want to integrate this differential equation over some finite interval.

I want to integrate this differential equation over a finite interval in independent variable eta. That is my problem. Before we begin talking about the methods of solving like we discussed a little bit about existence of solution, uniqueness of solution and so on when we talked about solving linear algebraic equations or towards the end, I gave a lecture on existence of solutions for nonlinear algebraic equations. I am going to very, very briefly mention about this aspect.

Not really get into deep into this. Now it is very, very important. There are 3 issues that are primary concern in the beginning.

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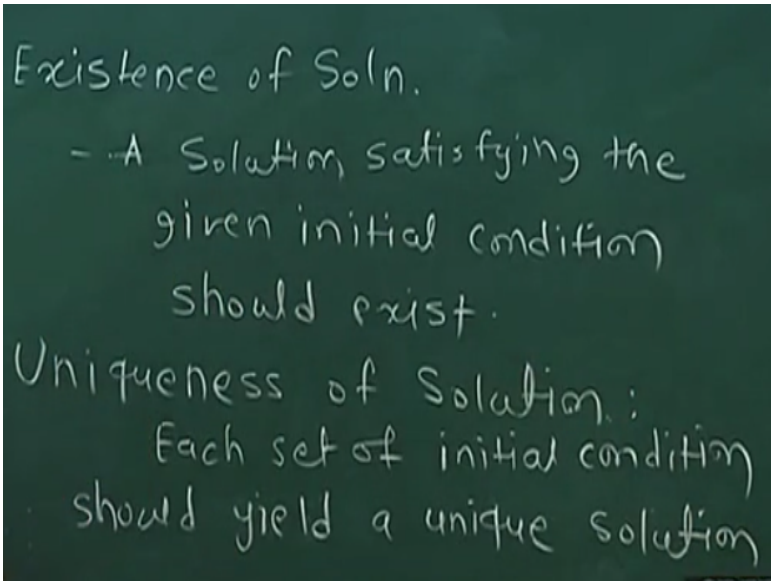

Existence of solution, that is solution or a solution, first essential thing that a solution for a given differential should exist. Typically, except for some differential equations which have been conceived by mathematicians, typically most of the differential equations that you want to solve are some models of a physical system. No physical system exists and just like a physical system has different behavioral patterns for different starting conditions.

A model also has different behavioral patterns for different starting conditions. For a specified initial condition, a solution should exist for the given differential equation that is very, very important. If may happen that you have done a wrong modeling, solution does not exist, physical system, of course exist, you have developed a model for the physical system and there are some wrong assumptions or there is something wrong which you are understanding of the system and no solution exist for the initial condition that you are specified.

Now if the solution exists, we are worried about one more thing. We are worried about the uniqueness of the solution. Once I have existence of the solution, I am worried about uniqueness. Here concern is each set of initial condition. Uniqueness of solution is another important aspect of the solutions of differential equation, now you might wonder why am I worried about existence and uniqueness which appear to be very, very mathematical concepts.

Actually they are just abstractions of something that we know from the reality. First of all, the behavioral pattern exists for a real system, so if the model represents a real system, a solution should exist for a given initial condition. Second thing that we know is that this I would call something like a principle of determinism. That if you for most engineering systems, if you start with same initial condition, you will get the same identical behavior.

Very, very important, you will not get different behaviour under identical conditions. That is mathematical way of saying it that a solution should be unique. I should not get different solution for same initial condition, does not make. I should get identical behavior for identical initial conditions. The third important aspect is continuity of solution with respect to initial condition.

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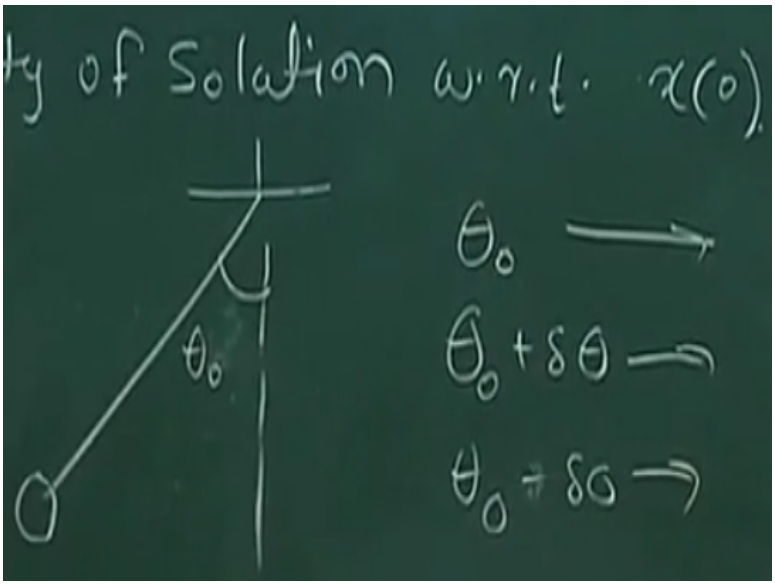

The third aspect is continuity of the solution with respect to initial condition. We want that the solution of the differential equation should depend continuously on the initial condition. Now when I talk of continuity, you think of that epsilon delta definition and then you might think this is complex, it is not. If you try to understand what is it trying to quantify or abstract, then it is not so difficult. What do you know about continuity?

About continuity what we know is that will a small perturbation in the input will change result in a small perturbation in the output. A bounded change in the input will lead to bounded change in the output, is what we are worried about in the continuity. A function when it is continuous in a

very crude way of saying a small change, any amount of small change should lead to a small change in the function value.

Now we know from working with real systems that even though we demand uniqueness of the solutions, when you actually perform experiments, you can never repeat identical conditions. Even if you decide that that is how you do the simple experiment that you have a pendulum and then you want to understand motion of the pendulum, you start from some theta. You want to start from some theta 0 and then you have developed equation for governing the pendulum.

You have to understand those equations. Even if you want to repeat the experiment from same theta 0 every time, it is impossible to conduct an experiment which will be every time starting from same theta 0. If you do 10 experiments, it will be some theta + delta theta every time. Now what is important what we know from physics, what we know from observations, is that minor change in the initial conditions leads to minor change in the solutions.

It does not lead to significant drastic change in the solution. If a minor change in the initial condition leads to a drastic change, that does not happen, in real systems. If you change the initial condition of the system slightly, the solution that you obtain, if I start from theta 0, next time I start from theta 0+some delta theta, then next time I start with theta 0-delta theta. The solutions that I get for each one of these cases of the motion of the pendulum will be close.

This you know, the way of quantifying this mathematically is saying that the solution is continuous with respect to the initial condition. If I perturb the initial condition a little, the solution will get perturbed a little, very, very important. Perturbation in the initial condition can occur when you are solving a differential equation. Somebody might, I have given initial condition which has some variable is one-third.

Somebody might decide to do it 0.33, somebody might do it 0.333, somebody else might do it 0.3333, and the solutions that you get should not drastically change because he takes 0.33 and she takes 0.333, they should be close by, similar solutions. So third aspect which is important is

the solution continuous with respect to initial condition. I am not going to go too deep into this. I am just going to state 1 theorem.

Which talks about the continuity aspect, existence, uniqueness and continuity. So we will define something called a region.

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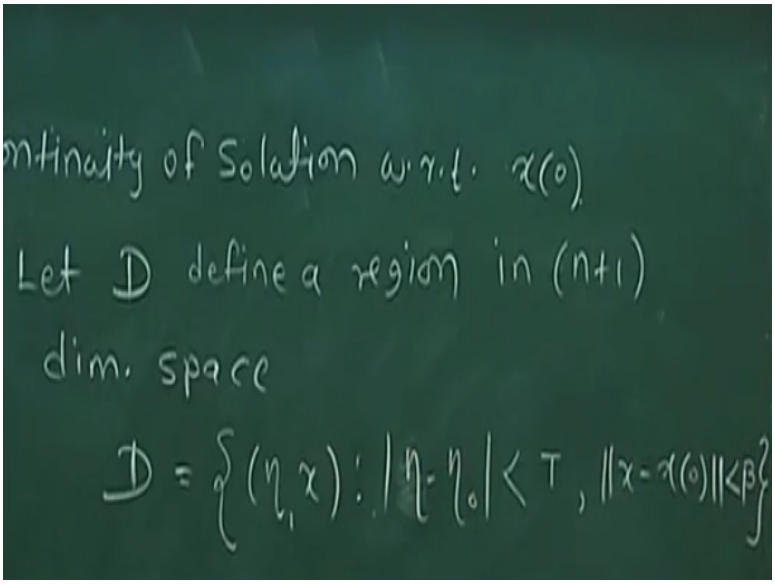

I am defining a region in n+1 dimensional space, n+1 dimensions because x is an n dimensional vector, eta is a scalar parameter, time, space, whatever dou/dou x, dou/dou t whatever you are looking at. It could be time, it could be space depending upon what you are looking at and looking at a region, the region is defined using norms. This is using only 1 norm. This is using absolute values because eta 0 is the initial point where you are starting.

The value of x at eta 0, so this should be actually x eta 0, x-x eta 0. Then let us see what these theorem says of existence of solutions.

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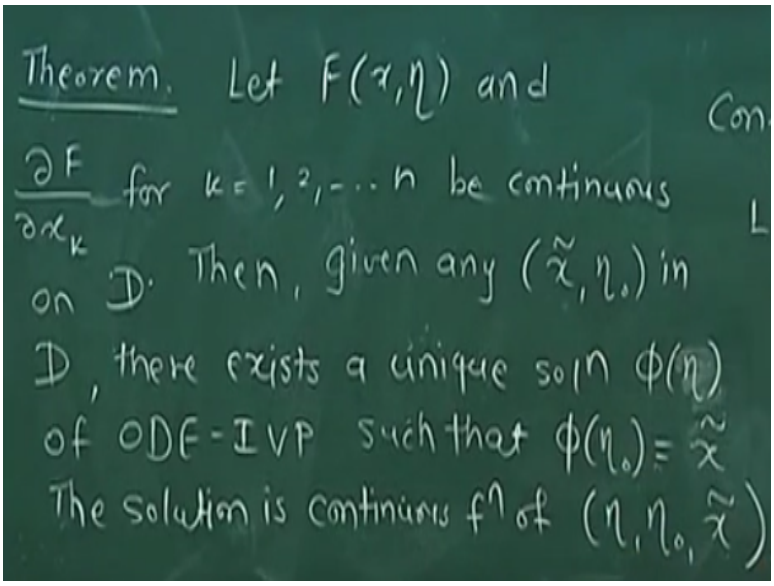

Now this theorem gives a condition under which a unique solution exist. It says that if F and its first partial derivative that is dou f/dou xk, F is a function vector, its partial derivative with i-th component of x that is also a vector. This is also a vector. This partial derivative of the function vector with i-th component of x is also a vector. We are saying that if this function vector and its partial derivative is continuous function on domain on the set d that we have defined.

If it is continuous, then actually x tilde here is the initial condition. I am starting with the initial condition and initial value of the independent variable and it also says that the solution is continuous function of the triplet. Detailed statement you can see here. What I want to point here is that how do I judge. The problem what is the importance of this theorem. Importance of this theorem is that I am able to judge about existence and uniqueness of the solution and continuity of the solution without actually having to solve it, solve the problem.

I do not want to solve the problem. I do not want to solve the differential equation problem. I just want to look at a differential equation and make a judgment whether solution exist, is it unique, and if it is unique, then the third thing is, is it continuous with respect to initial condition, time and spatial coordinate, expertise my initial condition, is the solution continuous with respect to x tilde, is it continuous with respect to t not, is it continuous with respect to t.

Now, of course there is one more aspect, which I am not talking about right now. This solution corresponds to the real system behavior. I am not talking about that right now. I am just saying that in real system what I know that a solution exists, it is continuous with respect to perturbations in the initial condition. If I slightly start a little later with the same initial condition, I will get a similar solution.

If you think of 2 people doing experiments on 2 different pendulums, which are identical, they start at different points in from the initial condition, the solution will not be different, if the systems are identical. I can judge about the existence of the solution just looking at continuity of F and continuity of the first derivative with respect to each of the elements of x. I will just give an example, then we will move on to solving the problems.

Bifurcations, we are talking about the behavior in the neighborhood of some steady state conditions. Even then, uniqueness if these conditions are met, solution will be unique. Bifurcations, you are talking about the steady state behavior under some parametric variation. Do not confuse bifurcation with existence and uniqueness. In bifurcation, we are looking at the local behavior of all the solutions in the neighborhood of some steady state point.

Each 1 of them could be a unique solution starting from a unique initial condition. If you start from an initial condition and it will get a unique, from the same initial condition, you will get the same solution. If you start from the same initial perturbation from the bifurcation point, you will get the same solution, that is important. See if it is unstable reactor, if you perturb from the unstable point in the same way, you will get the same solution.

You cannot get a different solution. For example, this is an unstable system. I am trying to balance it on my hand. This is an unstable operating point. This is an inverted pendulum and if I put it like this, it is a stable system. So this is an inverted pendulum. If I perturb it slightly, the way it will behave, if I do the same perturbation every time, it will behave in the same manner every time. That is what I am worried about.

Let us see a brief application of this theorem on a specific example. What are these I am writing here in a very mathematical way that there is a region in which the solution, region of interest. Region of interest is there in every physical system. For example, if I am working with concentrations, concentrations cannot be negative. So you have to work with in the positive quadrant when you work with concentrations.

There is no meaning for the solution or meaning for the differential equation when it goes to the negative point, same way about temperature, pressure, all these physical variables. Unless you start talking about perturbation variables, perturbation variables can be positive or negative, but absolute variables had been positive. So we have to worry about existence of solution in certain regions of state space. Let us look at this 1 specific example.

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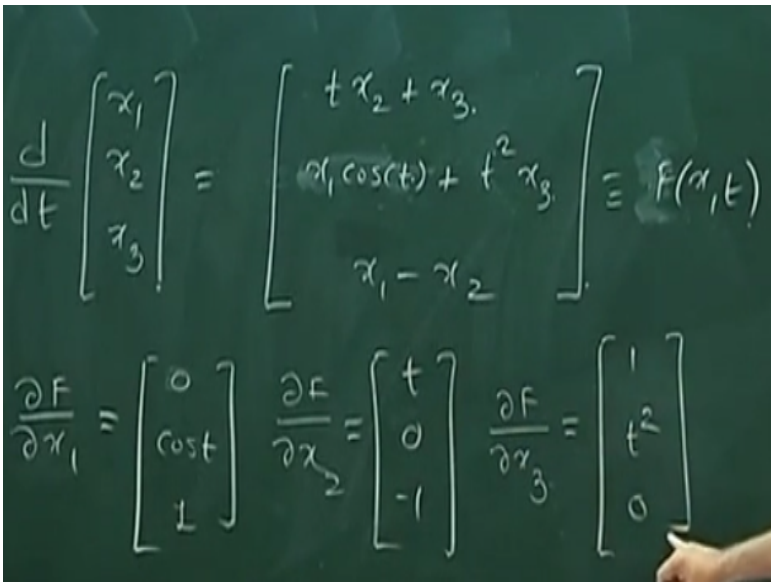

So this corresponds to F(x, t). I am giving you some differential equations right now. I am not worried about whether this corresponds to a physical real system. It is a mathematical example. Now I want to apply our theorem without having to solve, I want to judge whether the solution will exist for every x and t, for every initial condition x not, t not, if I start from that will the solution exist, will it be unique, will it be continuous with respect to x not, t not and t.

Now this theorem asserts, I just wanted to understand the application of the theorem. If you are interested in knowing the proof of the theorem, we can refer to books on differential equations

where the proofs are given, but for us as engineers, we are just worried about knowing whether a solution exist for the given problem. First of all, we have to see whether each 1 of them, is it a continuous function. Is this a continuous function of x1, x2, x3, and t.

If you examine all of them, these are continuous functions of x1, x2, x3 and t. So first condition is that F(x) eta should be continuous function of the dependent variable. The second condition is I have to worry about 3 vectors. What are the 3 vectors, 1 is dou F/dou x1, this is the first vector, dou F/dou x1 turns out to be 0 cos t and 1, dou F/dou x2. There are 3 different vectors, which I should look at. This is my F(x, t), dou F/dou x1, dou F/dou x2, dou F/dou x3.

If these partial derivatives are continuous functions or continuous function vectors, you can see for examining these function vectors, you can see that these are continuous functions. Since these are continuous functions, we are guaranteed that a unique solution exists for this particular set of differential equations, starting from any initial condition, any time, t not. Moreover, if you perturb initial conditions by small amount, the solution will be perturbed b a small amount.

This we know from analysis of this particular F(x, t) and important aspect, I am going to leave it at this point, just the idea of doing this or sensitizing you about these fundamental issue, you might be solving a problem, which does not have a solution or in some region, solution may not exist because in some region, continuity of this might be lost. So you should at least be aware of that one can examine without actually having to solve whether solution exist, is it unique and will small changes in the initial conditions, will it lead to small changes in the solutions.

That you can just decide looking at the continuity of these vectors. Let us move on to solving this. Let us say that we have, for given problem, solution exist, it is continuous and all that. So now we move on to the algorithms. So before I start with the algorithms, I want to talk about some basic concepts, which we will be using throughout.

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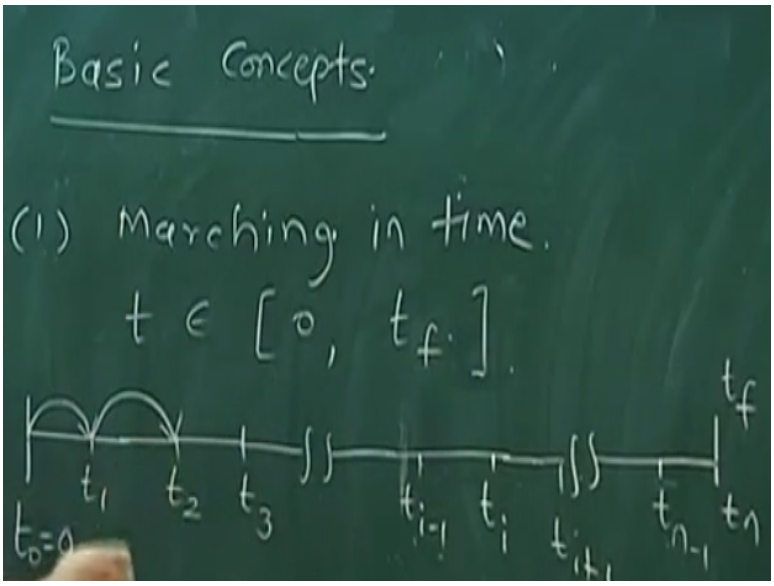

First thing is marching. Now what I am going to do is for the sake of notational simplicity, I am going to just go back here and not worry about the integration with the respect to the spatial coordinates, I am going to call this as t, and I am going to say at time=0, but the same things can be worked out when you are starting integration with special coordinate with space part=0. The other special coordinate is at 0.

Everything that I am going to say about time in the context of integration over a special coordinate, same things can be applied. Marching in time, if you want to read it every time as marching in the independent variable is fine. Now I want to solve this problem typically from over an interval t belonging to sometime 0 to some tf. I want to see how a reactor concentration profile is when I give a step change in the feed flow rate or feed concentration.

Whatever variable of interest that is me, over a period of time, from time 0 to next 30 minutes. I have this model, differential equation model. I am playing with it, it is like a toy with me, I give a change in the input, I record, I want to integrate and find out concentration profile, temperature profile, as a function of time. That is what is the assignment which I have given to you as computing assignment.

We are supposed to find it as a function of time, so actually it is the entire function that I want to find out. When you do this numerically, it is not possible often to solve this problem over the

entire interval that you intend to solve. I might be wanting to find out the trajectory for next one hour, but when I integrate, I do not solve 1 initial value problem which is starting from initial condition at 0 and then entire trajectory over the entire interval.

What I do is I divide, subdivide, I want to reach here, so this is my tf, I subdivide this into say t1, t2, t3, …. What I do is I subdivide this interval from 0 to tf into smaller intervals and I go marching in time, which means I integrate from time 0 to time t1. I solve 1 initial value problem with this as my initial condition at time 0 and I reach only up to time t1, this t1 could be for example I want to integrate the differential equation over 1 hour.

But I make a small step from 0 to 1 minute. Then the condition at the end of 1 minute is the initial condition for the next problem, so I march from here to here 1 minute to 2 minute, 2 minute to 3 minute and likewise I go on hopping in time. Now it is not necessary that these steps should be uniform. They can be non-uniform, depends upon the problem at hand. So I go marching in time and instead of solving 1 initial value problem, I solve multiple initial value problems, 1 after another, sequence in time.

The end condition, the final condition of the first initial value problem will be the initial condition for the next initial value problem and so on. This is how even the problem, which you are supposed to solve in the part of the computing assignment is to be solve, so you go marching in time.

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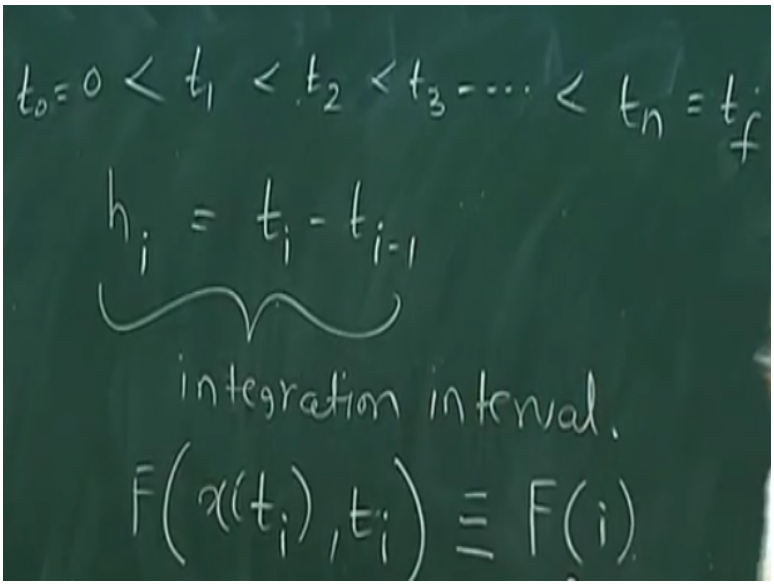

As I said, the way you do this is t0=0<t1<t2<…. The difference between this that ti-t(i-1), let us call this hi, this we call as integration interval. This we call as integration interval. So one of the major problems in solving ordinary differential equation initial value problem, is how do I choose integration interval appropriately. We will talk about this in some detail at a later point. What is the basis for choosing integration intervals?

But remember that you are never going to solve the problem in 1 shot. We are going to solve the problem by marching in time, by subdividing into sequence of multiple initial value problems, and the final value of the last problem is the initial value for the next problem. That is how we are going to solve it. It is like saying that if you want to go from here to the gate, you are never going to jump in 1 shot from here to the gate.

We are going to go in steps, steps could be variable depending upon whether it is a up the slope, or down the slope, the pace could be variable, you might be running, you might be sometimes walking, but you are never going to go in 1 shot. We will go in steps and the difference between any 2 steps, we will call it as integration step size. This is the first important concept. Just a notation that I am going to use throughout before I move on.

So this let us say function F evaluated at x(ti), this function vector F evaluated at x at ti, and time ti, I am going to denote this as F(i). This is neither superscript nor subscript. This is a vector, it

can have a superscript, it can have a subscript. I am talking about a time index. Here when I write F(i), which means function vector F evaluated at time ti using x(ti) and time ti. I am going to use this short hand notation Fi for this.

Similarly, I am going to use short hand notation x(ti) as x(i), that means value of the vector x at time ti, instead of writing every time ti, ti, makes my notations very, very complex. I am going to use this. Similarly, whenever I get a Jacobian matrix, I am going to say dou F/dou x evaluated at x(ti), ti when this matrix appears, if it is evaluated at time ti, I am going to just call this as dou F/dou x subscript i, subscript i will indicate that it has been evaluated at time ti.

This is to simplify the notation as we go along, because the notation can become very, very complex when you are trying to solve ODE initial value problem. This is the notation, please keep this mind. This is what we are always going to look at. The second important concept that I want to mention here is explicit algorithm and implicit algorithm. There are 2 classes of algorithms, which we are going to look at, some of them are called as explicit, some of them are classified as implicit.

Right now, I am not going to derive, after some time we will derive algorithms, some of them will turn out to be explicit, some of them turn out to be implicit. Right now I am not going to derive the algorithms, while giving the idea, I am going to take 1 simple algorithm, which all of you probably know from your undergraduate mathematics is Euler's method. I am going to illustrate what is an implicit Euler method and explicit Euler method.

This is just introducing the terminology, 1 is the marching in time, second is explicit and implicit. This I need when I go along.

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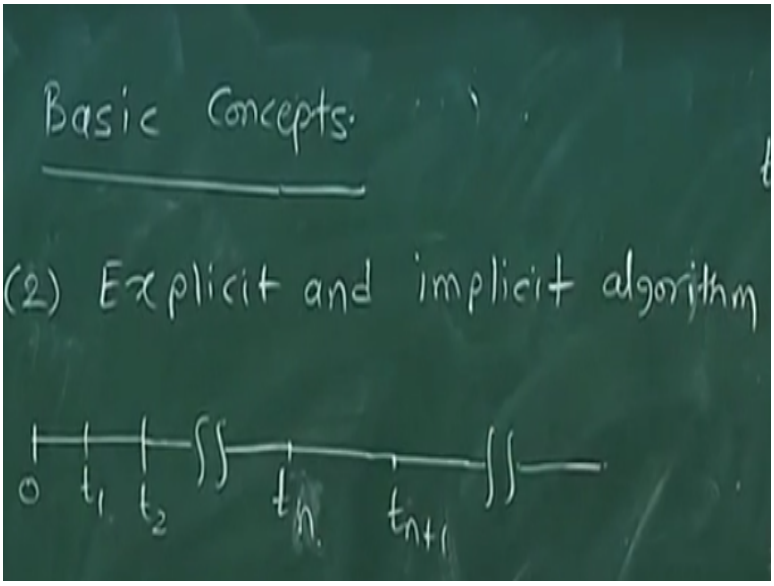

Second basic concept that I wanted to know is. Now I have this differential equation, just look the differential equation. I have this differential equation, let us say I have done some integration and I have reached a point at tn. Now tn need not be the last point, tn is some intermediate point, I want to go to some other final condition, tn is some point where I have reached. I want to solve initial value problem, which is over the interval t belongs to tn+1.

I have started from time 0, t1, t2, I have come to point tn and then my problem is to go to tn+1. I have reached here; I want to go to tn+1. What I want to do is I have reached up to point tn and then I want to go to point tn+1, so I have broken down my initial value problem into sequence of initial value problems. I have somehow solved up to point tn. I want to go from tn to tn+1. The simplest algorithm you know from your undergraduate is Euler's method. Let us go to Euler's method.

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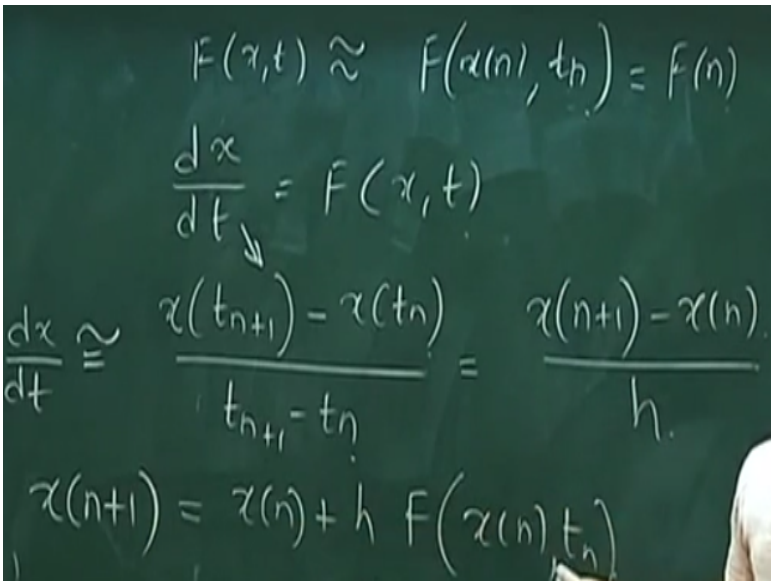

Now I can approximate the left hand side using x(tn+1)-x(tn). This is an approximation of the left hand side. Now let us take the simplified case where h is constant difference between. We are taking equal size steps. Left hand side can be written as x(n+1)-xn/h. With our new notation, the left hand side can be approximated, so I would say that dx/dt is approximated like this. Now comes the question, first of all remember we are only solving this problem approximately.

In most of the cases when F(x) is nonlinear, it is not possible to solve the problem exactly analytically. The true solution is more than often times is not know. Now question is how do I approximate the right hand side. This is a function of x and t. Now the question arises is whether I should use value of x. This is my initial point. I know what is xn here. At this point, I can evaluate the function vector F, because xn is given to me, it is known to me.

Time tn is known to me, but if you look at a differential equation carefully, actually it requires the function derivative, the derivative vector that is F(x, t) at each point in this, is not it. When you integrate actually you should know at each point, but we do not know what is the future value. You are currently at time tl, you are advancing in time. We do not know the future value; you make a simple approximation that the derivative over this interval can be approximated.

One simple approximation is F(x, t) over the entire interval is approximately=F(xn, tn). You take the initial value, find the derivative at the initial point, local derivative and if you make this

approximation, this we call as F(n), then with this approximation, I can write explicit Euler Algorithm, this is x(n+1), I am just rearranging the equations x(n+1)=xn+x*. Do you agree with me? I have just combined these 2 approximations and arrived at this algorithm.

What it says is that vector x at time point tn+1 is function of xn and derivative computed with respect to xn. This algorithm is called as explicit Euler algorithm. On the right hand side, everything is known to me, xn is initial value known to. I have arrived at that xn by some means and now I am getting new value xn+1. When you go from xn+1 to xn+2, what will happen? Xn+2 will be function of xn+1, xn+1 would be known to you, so you start from n0.

What will happen if you start from x0, x1 will be known to you after you implement this step. Then when you go to x2, x1 is known so go to x2 and so on. So you go on marching in time, very, very simple way of implementing the algorithm. Somebody might say, well, I do not really agree that, you should take this approximation. How can you say that the derivative in the time is going to remain constant?

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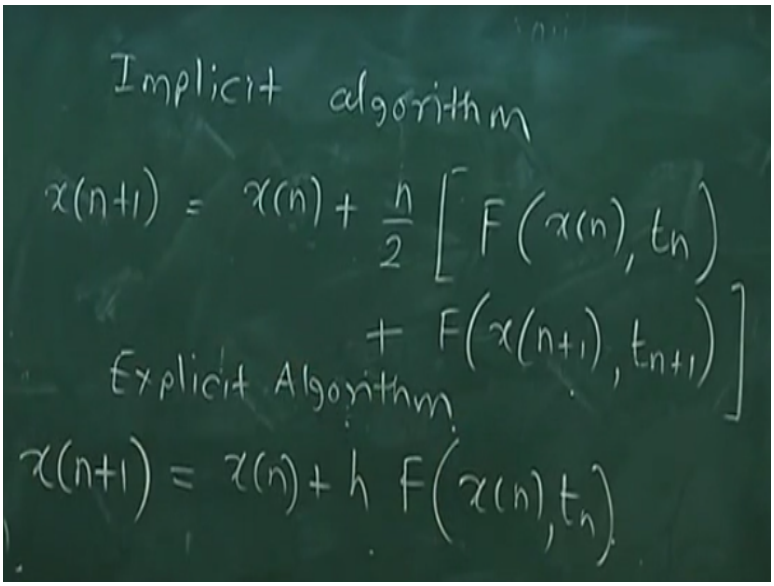

He would come up with an approximation x. He would say no, no I should take the derivative at n point, not at the beginning point. Third person may say, well that is not right. You should take average of initial point and the end point. Now let us take that view. I want to take average of this

+1/2, let us say this is a better approximation. Now if this is the better approximation, then I am just taking the derivative at initial point. What is my algorithm?

My algorithm becomes x(n+1) = xn+h/2 F(x(n), tn)+Fx(n+1), tn+1. What is the trouble with this algorithm? Trouble with this algorithm is that xn+1 appears on the left hand side and on the right hand side. How will you solve this problem? In general, F is a nonlinear operator. You take a reactor or you take a distillation column, F will be a nonlinear operator. How will you solve this problem? I want hear louder.

Newton-Raphson, or successive distributions or optimization, it is a nonlinear. Now once you have developed this algorithm, this equation is a nonlinear algebraic equation with what is unknown, x(n+1) is unknown, xn is known to you, so this is computable. This part is computable what is not computable is this because x(n+1) is not known to me. I am marching in time. I do not know what is the future value.

So I have to guess my future value and do iterations to solve this problem. I have to solve this problem iteratively and this particular algorithm is an implicit algorithm. It is not an explicit algorithm. Here you have an explicit solution of x(n+1) in terms of xn. Here you do not have an explicit solution. So this is categorized as implicit, while this particular algorithm is categorized as explicit algorithm. This is implicit algorithm; this is explicit algorithm.

This is easier to solve; we will see after some time does it give great solutions. It is less accurate. You have to use very, very small h, this 1 is difficult to solve, every time you have to solve a nonlinear algebraic equation gives great results, numerical stability is excellent. So what is difficult to solve actually gives you dividends, more accurate better results, easy to solve, you have to be very, very careful in choosing h. I am not saying you cannot use this.

Unless you use h to be very, very small, this explicit algorithm will not work. Here the calculations are more because you have to choose small h, your calculations are more because you have to do iterative calculations. You get nonlinear algebraic equations. So just look at this. I

am solving an ordinary differential equation, subject to initial conditions. I am marching in time. So one giant ODE-IVP is converted into sequence of ODE-IVPs.

Each one of them inside requires iterations, nonlinear algebraic equation to be solved. Look at the complexity of calculations. But this is better than this. So we tend to use this rather than this or you can use this, no doubt, but you have to choose h to be very, very small. So you have to understand the differences and then use which 1 to use when and so on. We will, of course, get into those details when you use which 1, why and so on.

So this basic terminology will get on to the algorithm development from the next class. There is 1 more concept called stiffness of algorithm or stiffness of differential equations, but we will come to stiffness of differential equations a little later. These 2 are initially good enough to get started. We will develop these algorithms numerical methods of integrating differential equations and then, we will move on to analysis part, when is one better than the other and so on.