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

Lecture - 12
Solving ODE - BVPs Using Finite Difference Method

In our last lecture, we were looking at Taylor's series approximation and using Taylor's series approximation for problem discretization. So we looked at solving non-linear algebraic equations of this form. So what is discretization process involved here. I want to point out what is the original operator, what is the discretized operator and how we are solving a problem, which is not the original problem, but a different problem, that I want to point out here.

One thing which I stressed in the last lecture was polynomial approximation actually is the cornerstone of approximating different problems or discretizing different problems in numerical analysis and Vieta's theorem gives us the foundation, why we can approximate a continuous function using a polynomial function. Now how do you do it? Vieta's theorem is only an existence theorem, it does not tell you how to construct polynomial approximation.

So we said we are going to look at 3 different ways of constructing polynomial approximation. One of them is Taylor's series approximation and then we looked at example of multivariable Taylor series that was developing Newton's method for solving non-linear algebraic equations.
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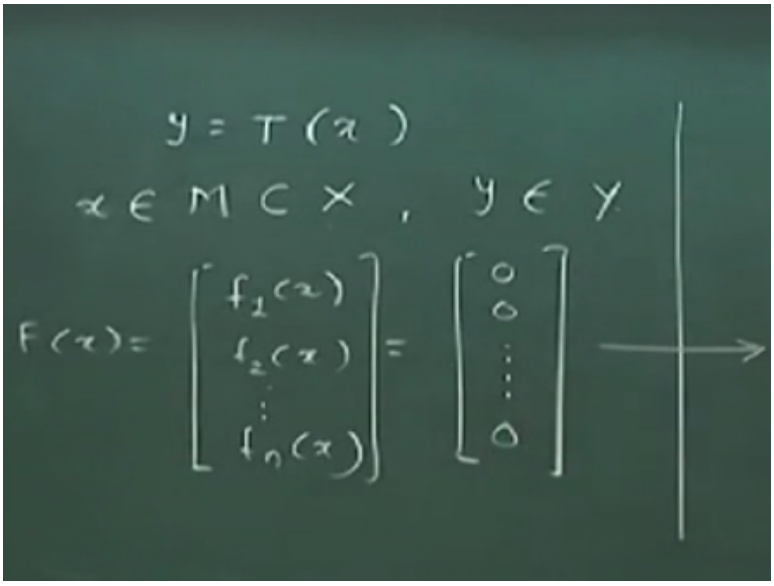

What I had been talking about earlier is that you have this y=T of x where x belongs to a subset M of X, X is our vector space, and x is the range and y is the range. This is the original problem and then I said that we actually end up solving y tilda=T cap, x tilda. We end up solving a different problem than what we started with. So I just want to just oppose the 2 things what we wanted to do here actually to solve f of x = f1x, f2x.

I wanted to solve this problem using Taylor's series approximation where this original n non-linear equations and n unknowns is not analytically solvable in general, maybe there are some cases where you can solve, but in general this is not analytically solvable. We come up with a simplified problem.

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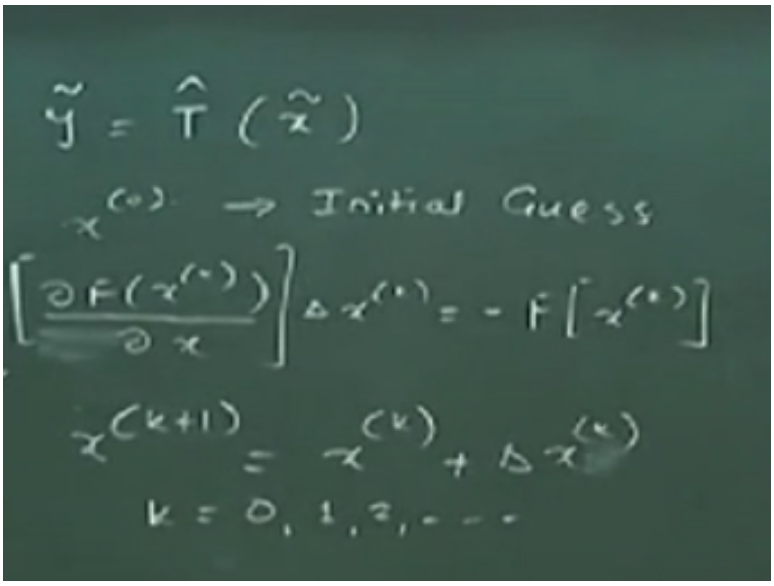

We started with a guess solution, x not, and then we solved this problem dou f/dou x. So this is my initial guess. So I wanted to solve this problem. This is the original simultaneous non-linear equations. Actually, the way I end up solving this is by approximating. So this is my T cap. What is T cap here? T cap here is a sequence of linear algebraic equations, which are constructed from the original problem.

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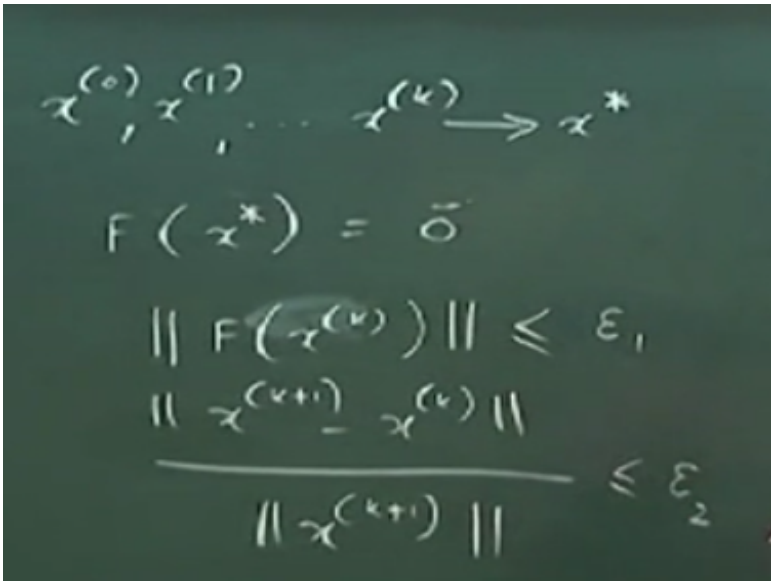

What we hope is that this sequence will finally go to x0 x1… xk will tend to x*. What is x*? x* is my solution of the original problem. So I hope that f of x*=0 vector. I hope to converse to this solution x*. So this one is my Newton's method here. I hope that the sequence of vectors, which

is generated by this method will eventually converge to x*. What is x*? X* is the solution, so how do we check whether convergence has occurred.

Typically, we keep checking for convergence whether f of x has become really small where epsilon 1 and epsilon 2 are typically very, very small numbers. So we keep checking whether the convergence has occurred and we want to know whether the vector where the sequence is converging, whether that solves this problem, =0. We actually cannot check in the computer exactly =0, so we check for a norm. This could be any norm. This could be infinite norm.

This could be 1 norm, 2 norm whatever you like to use, any one of the norms can be used. Original problem has been approximated using Taylor's series and then the approximate problem is solved and then we hope that the sequence generated in the approximate solution will tend to the solution of the true problem. Now I have just introduced this Newton's method here. We will be revisiting Newton's method again much more in detail.

There are many modifications to make it converge and how can you accelerate. We will talk about it later. Right now I am introducing Newton's method just as an application of Taylor's series approximation. About 1 or 1-1/2 month later, we will revisit this Newton's method much more in detail, solving non-linear equations much more in detail, but the point to convey here is this was achieved through Taylor's series approximation.

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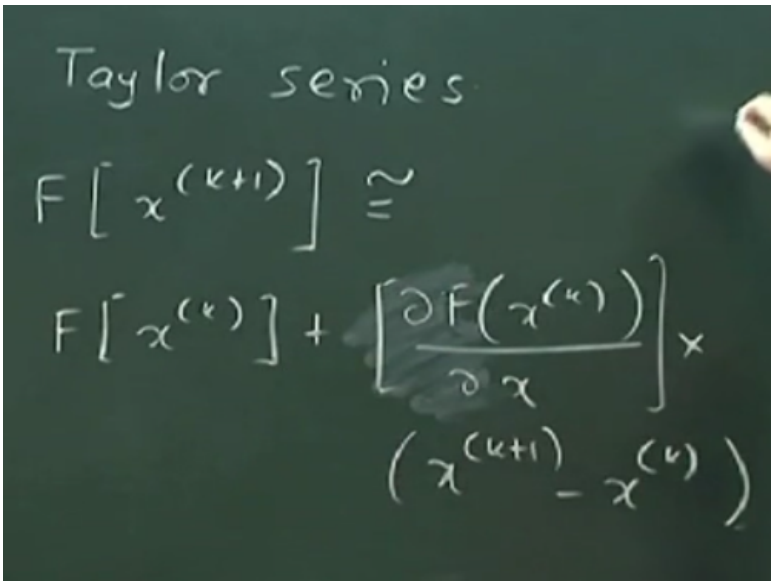

So the basis for this was using Taylor series. So what we have done is f of xk+1 has been actually approximated as f of xk+dou f/dou x evaluated at xk, so this into. If you take a close look at Newton's method what we have done is we have approximated xk+1 in the neighborhood of xk, so when I start with x0 and then instead of solving for f of x=0, I solve a linearized approximation of this set of equations and that gives me xk+1.

So x0 will give me x1, then I substitute into the sequence, I linearize that x1, I get x2. I linearized that x2 I get x3. So this is a sequence of vectors, which I generate by local linearization. So original problem, which are solving non-linear algebraic equations, was solved by constructing the sequence of linear algebraic equations and approximations from the foundation of applied mathematics or the applied engineering mathematics.

Because we cannot most of the time solve the original problem. We have to approximate by some means and convert into a computable form, that computable form is then used to construct an approximate solution. Now let us look at next application of Taylor series. Now I am going to look at solving boundary value problems, ordinary differential equations boundary value problems or partial differential equations using Taylor series approximation.

So I will be converting my boundary value problem either into a set of algebraic equations or a partial differential equation. I will be converting it into either algebraic equations or I might be

converting them into a set of ordinary differential equations and so on. So I will convert it into a standard form, which then can be attacked using a standard tool. What the standard tool that is used here, when you are Ax=B?

So here each 1 of this problem is just solving linear algebraic equations. Each 1 of them is like solving A. If I want to put a notation here Ak delta xk=Bk. In abstract form, I am solving these kind of problems. This is a matrix n x n matrix delta xk is a vector, Bk is a vector. These vectors are changing, this matrix is changing, but I am solving them repeatedly to come up with the solution of the non-linear algebraic equations.

Now let us look at problem discretization using or boundary value problems discretization using Taylor series approximation. What I want to convey here is that now, I am going to develop this method of approximating local derivatives using Taylor series, which is something I am sure you have done within your undergraduate. All of you are aware of forward different approximation, backward difference approximation, central difference approximation.

All these approximations local approximations we are aware and then you may have used it to actually simplify some boundary value problem or if you have done some work on numerically solving this. now what is that I have to convey? What I have to convey here that the tool that you are using to discretize boundary value problem or to discretize partial differential equation, the same as the tool that is being used to construct Newton Raphson method or Newton's method.

Underlying ideas are the same. Problem is different, application is different, but basically we are using Taylor series approximation. So now let us look at. Now this problem is like that I have.

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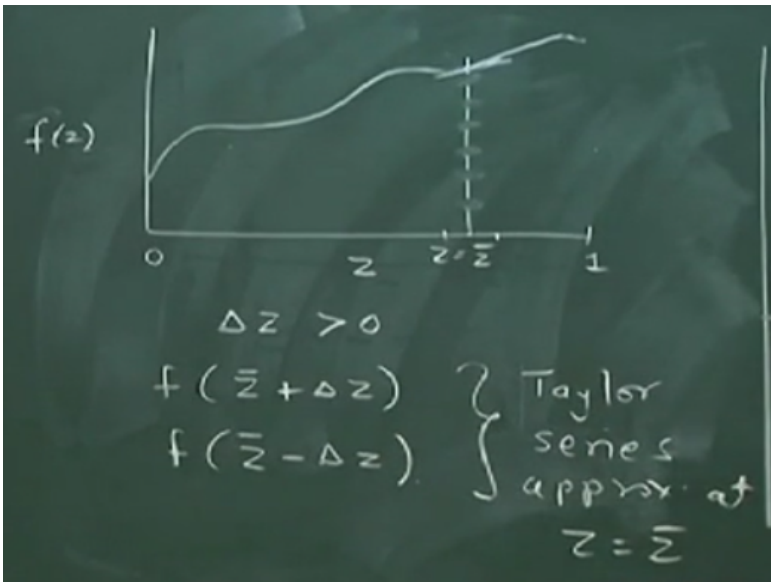

Let us for the time being take set of differentiable functions on interval 0-1. So this is 0-1 and I have some continuously differentiable function and this is some point, let us this is z=z bar. This is a point. At this point, I want to construct a local approximation of derivative of this function sometime, which you know very well, how this is, then I am sure power difference backward difference has been taught to you at some point.

So now I just want to put it in the context of Taylor series, so that the connections become clear. So this is my interval and locally I want. What we do is around this point, we take some small perturbation. So let delta z greater than 0 be a perturbation and I want to look at Taylor series expansion of f z bar+delta z. I want to look at Taylor series expansion of z bar+delta z. I also want to look at Taylor series expansion of z bar-delta z.

So I want to expand this function. now this function, which I am looking at should be continuously differentiable once, twice, thrice, depending upon the order of approximation that you develop. So I want to develop Taylor series approximation in the neighborhood of z=z bar. And then use that further to discretize boundary value problems. I am going to change that notation a little bit instead of using f here.

This is because further when I develop boundary value problems, I want to use a particular notation. So I am going to use here u, u is a continuous function, continuously differentiable function.

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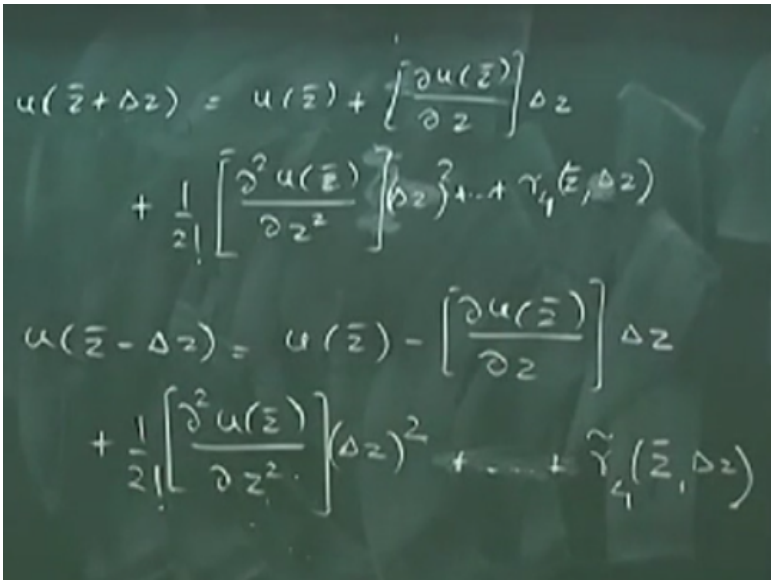

If I take uz bar+delta z, I can write this as uz bar+, so the notation here means that we are actually computing all these derivatives at z=z bar and so on. So I am going to write terms up to third order and then say R4z bar delta z. So similarly I can write u z bar-delta z that is uz bar-, so here delta z square. So I am expanding each one of these scalar valued differentiable functions, either Taylor series expansion in the neighborhood of z=z bar.

What we know about Taylor series, is that the derivatives of original function and derivatives of the approximation are identical at z=z bar. This is something which we know about a Taylor series function. I am going to use this property to construct approximations. There are multiple ways I can arrive at approximation starting from these 2 equations. So equation #1 and equation #2, 1 way is I rewrite this equation as dou, actually we can write exact differentiable.

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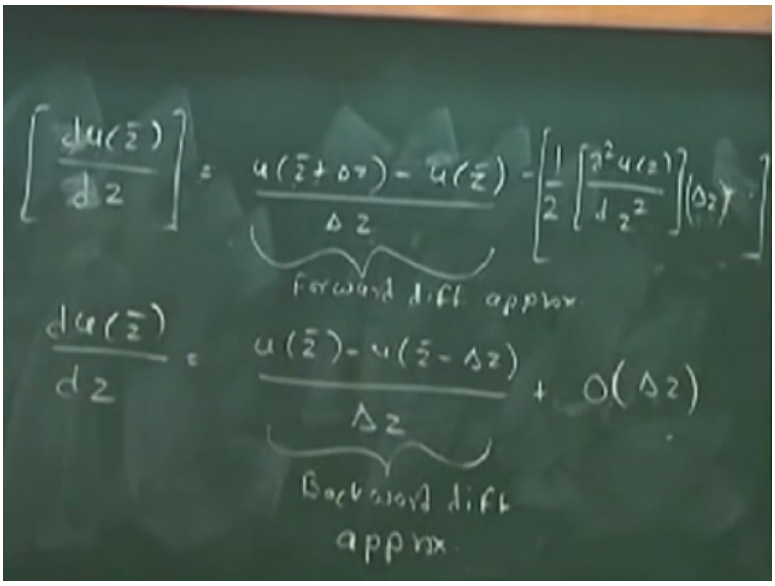

We do not have to, these need not be partial derivatives. These can be exact. These are not partial variables. This is only one variable so I can write d here, no need to take partial derivatives. Du/dz at z=z bar, I can rewrite this as uz bar+delta z-uz bar, so 1 way is I can write du/dz bar as uz+delta z-uz bar/delta z+some terms, this involves second order derivatives and all the higher order terms. I could choose to neglect the terms.

If delta z is very, very small, I can choose to neglect terms of order delta z and higher and then I get an approximation, which is forward difference approximation. So this is my forward difference approximation. So I choose to neglect terms of delta z and higher order. If delta z is very small, so I am in a very small neighborhood of z bar, I could actually approximate this, I could use this sort of approximation for the local derivative

The same way, I could rearrange the second equation. So the first equation I get like this, the second equation would give me duz bar/dz, right now just remember that I am writing to= that is because this + something, if you do not neglect it, this is exact equality. The moment we choose to neglect this delta z and higher order terms, then local approximation of this, this is the forward difference. So likewise I can develop a backward difference approximation using this.

So this will become uz bar-z bar-delta z/delta z. So + the terms which you take on this side. So these terms are of order delta z, delta z square, delta z cube and so on. So when the first term, the

order of this is the smallest term that we are neglecting. So in this case delta z, we are neglecting. In this case also, delta z higher, we are neglecting. So this becomes my backward difference approximation, but these 2 approximations are somewhat inferior because we are neglecting terms of the order delta z and higher.

If there was approximation where we could neglect terms of delta z square and higher, then that will be a better approximation of the local derivative than these approximations. So that turns out to be the central difference approximation, so the way you derived central difference approximation is we subtract equation 2 from equation 1, and then we arrive at the central difference approximation.

In central difference approximation, what will happen is that this second derivative here will vanish. If I subtract from this term, this is positive, this is positive, this will vanish, but a third order derivative will remain and what we get here is after doing the subtraction and rearranging.

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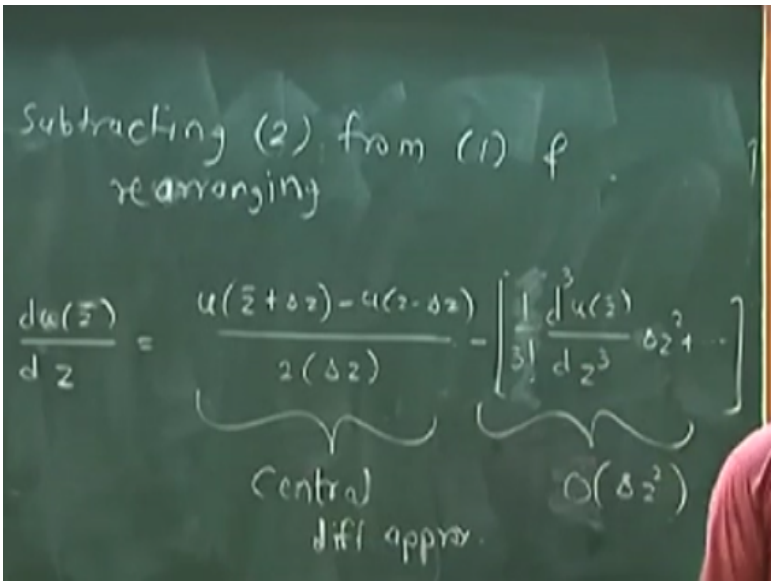

So here what you get is. When you subtract equation 2 from equation 1 and do a rearrangement, you will see that the terms of delta z disappear, in the residual you get the first term, which is delta z square, so the way we write is that this is order of delta z square, so the terms delta z square and higher are neglected and what you get here is the central difference approximation. So this is my central difference approximation.

So this central difference approximation is preferred over forward difference or backward difference that is because in forward difference or backward difference, you neglect terms of the order delta z and higher. In this case, we neglect terms of delta z square and higher. So this is a better approximation than forward difference or backward difference approximation. What about second derivatives.

I could use this idea, Taylor series approximation to approximate the second derivative here. if I rearrange these equations, I just have to be careful what I eliminate, if I rearrange these equations, you can subtract and rearrange and you can develop the second order difference equation.

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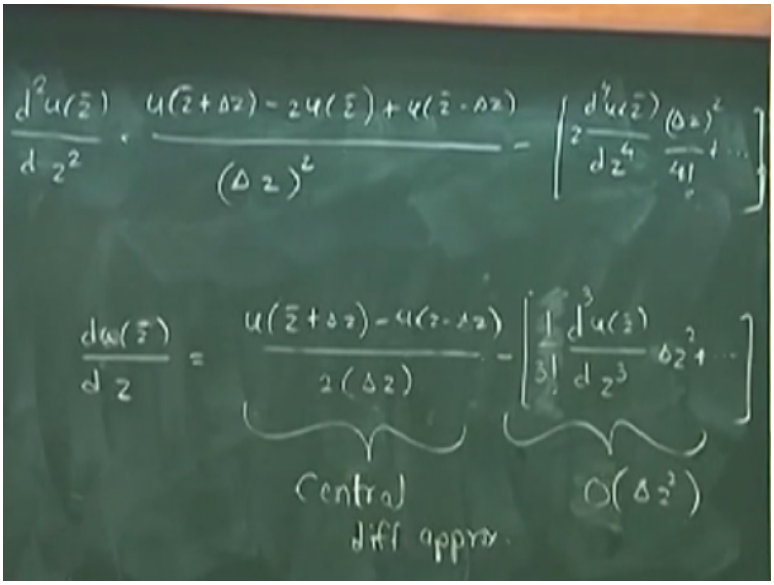

So you can develop this d2u/dz square=uz + delta z (z bar + delta z)-2u. so this is my approximation of second order derivative or d2u/dz square at z=z bar and this 1 is the residual term. You can see here; this is again of the order of delta z square. So the order of approximation in central difference and order of approximation in the second order derivatives is identical. So we prefer to use this and this together.

We normally do not use the first order approximation except at some points, we will come to that, when we use the forward difference or backward difference, but typically we use these 2

together because the order error in both of them is identical. So far so good, how do I use this to solve a problem, which is a boundary value problem, let us go to that. Now what is the general boundary value problem.

I am going to write it in the generic form and then we will come to specific examples.

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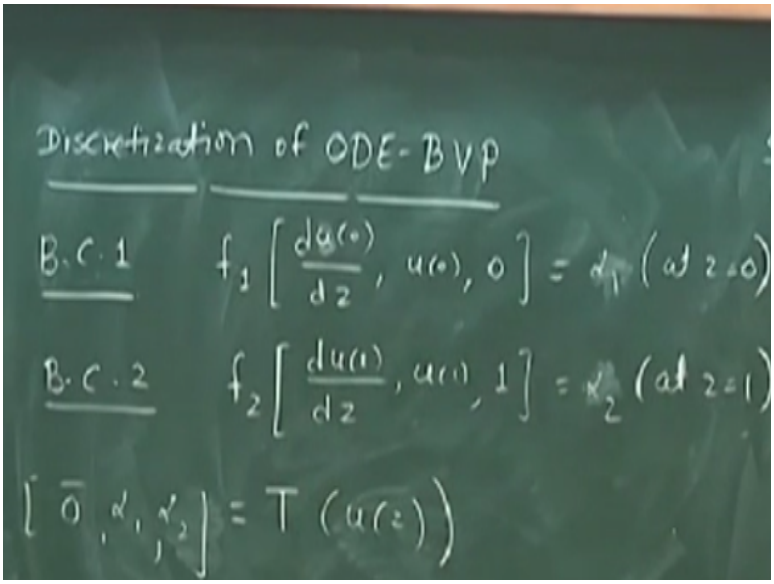

So now I am concerned about discretizing a boundary value problem using Taylor series approximation and the concept that I developed just now, I am going to use them to solve this problem. Now let us write this generic problem here. So I am writing the generic boundary value problem, which we encounter normally in engineering, chemical engineering or most of the engineering problems.

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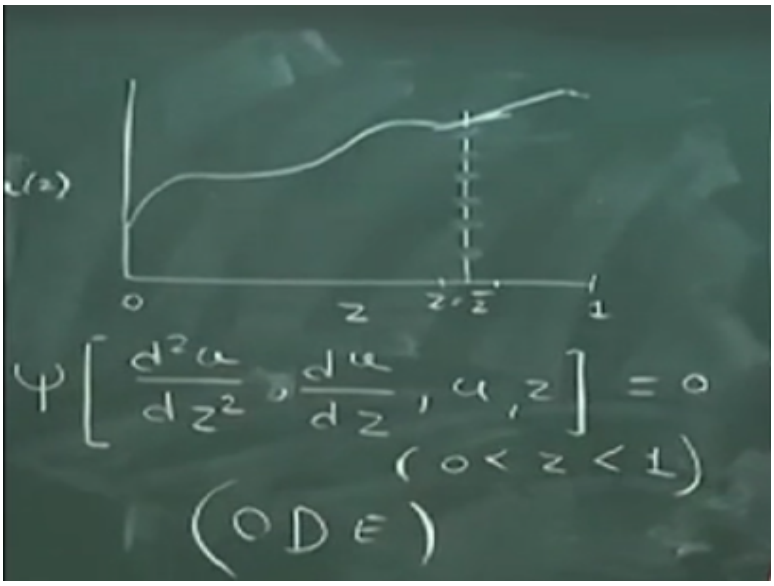

So this is d2u/dz square. So typically we have this second order differential equation, which I am writing it some sign. This could be a linear differential equation, this could be a non-linear differential equation, some differential equation. In different context, we will get different differential equations. Now when you are studying transport, when you are studying your analytical methods, we will encounter many such questions.

When we actually solve problems, we will also come across many such equations. Right now, I am writing in an abstract form, a second order ODE can be written in an abstract form, u is the dependent variable, z is the independent variable, z spans from 0 to 1. So this is my ODE, ordinary differential equation, which holds over 0-1 and at the 2 boundary points, I have 2 boundary conditions.

So by BC1, I am going to write this as F1 dz0 du0/dz u0 0=0, this is my first boundary condition. I am writing it in the abstract form. We will look at specific examples. This is my first boundary condition and this is my second boundary condition. So there are 2 boundary conditions at z=0 and z=1. The differential equation should be satisfied everywhere in the domain 0-1 except at the boundary points. What do you want would happen at the boundary points?

There are 2 boundary conditions. This would arise from the specific nature of the problem, for example if you have a double pipe heat exchanger, we will have some conditions of temperature

at the entry. So we will have some conditions of say rate of change of temperature does not change after fluid leaves the boundary. So those conditions will be given here. The rate of change of temperature does not change after fluid leaves the heat exchange boundary.

That could be a condition in double pipe heat exchanger here, initial temperature of the fluid entering here, that would be a initial condition at z=0 specified. So depending upon whether it is a reactor, whether it is a heat exchanger, or whatever, a distributed parameter system, you will have different boundary conditions and you want to solve this problem. Please remember that this original problem is my y=T(x) equivalent.

X here is uz and y here is 0 function and say alpha 1, alpha 2. Another way of writing these is this is = alpha 1, this is = alpha 2. So I put this, this is my original problem, which I actually want to solve. I am not able to solve this problem exactly except when the operator is linear and boundary conditions are nice, you can actually construct analytical solution, but that you will be looking at when you will be studying that under some theory.

You will be studying all those kind of things, but majority of the problems where the differential equation is non-linear or boundary conditions are not nice and simple, you cannot solve the problem analytically and then you have to construct a numerical solution to this problem. So now I am going to use Taylor series idea to approximate this problem. So I want to use these derivative approximations. Now the problem is where do I use the derivative approximation.

The derivatives are required at the boundary points. The derivatives are also required everywhere inside the domain. How many points this differential equation should hold? At every point, there are infinite points between 0-1 everywhere this differential equation should hold. Now when I am solving it numerically, I cannot afford to formulate this differential equation at every point between 0 and 1. What I am going to do is instead of that, I am going to convert this.

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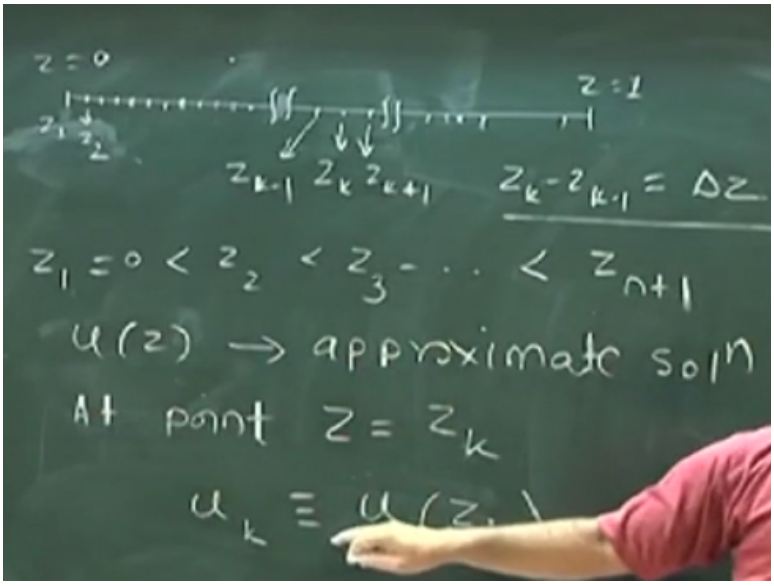

This is my domain. Let us put this z=0 here and this is z=1 here. I am going to mark what are called as grid points. I am going to mark grid points in general, when I mark this grid points, they need not be equidistant, but for a problem you could start creating equidistant grids points. So I am going to grid points here. So I am going to label them, this is my z1, this is my z2, and so on. So in general this is grid point zk, this zk+1, this zk-1. These are my grid points.

So I am going to create grid points. So z1=0, which is <z2, which is <z3. How many grid points I am going to create? n+1 So I am going to label them as z1 to zn+1 and then I am going to develop local approximations of the solution at each of the grid points. What is the solution of this equation? The solution of this equation is let us call it u*z. this u*z is a function, which is twice differentiable. It should be otherwise it will not be a solution of this differential equation.

The true solution is a twice differentiable function, continuously differentiable function for the interval 0 to 1. Remember this, this is a true solution. So the solution is a twice differentiable function over domain 0 to 1. I am going to construct a local solution, an approximate solution uz, uz is not going to be u*z, you would realize why it is not going to be u*z very soon. What I am going to do is, I am going to approximate this unknown solution.

Right now, it is unknown to me. I want to solve the problem. I do not know what it is, but I am going to approximate at any point, the first and second order derivatives of uz. So uz, first of all

remember is an approximate solution, which is going to be constructed numerically. Now at point k, at point z=zk, if I want to enforce the differential equation, what do I need. I need the first derivative; I need the second derivative.

I need to enforce, look at this differential equation here, I need to enforce this differential equation at every point in the domain. Instead of that, what I am going to do is, instead of enforcing it at every point in the domain, I am going to enforce this equation at some finite number of points. What are these finite number of points? These finite number of points are listed here z1, z2, if I have the domain marked.

So in general you can mark this in such a way that zk-zk-1=delta z, let us make a simplifying assumption that the gap between any 2 is delta z. It need not be constant, but I am making a simplifying assumption that these equidistant points. So at z=zk, I can say that du, so the first derivative, I am going to approximate as uk. Before that, let me develop a notation and then we proceed to this. So let us develop a simplifying notation that uk it corresponds to u at zk.

The dependent variable u at point zk is going to be called uk. This is just a simplifying notation. This helps us to write this equation in a very, very simple manner, discretize in a simple manner. Now let us look at.

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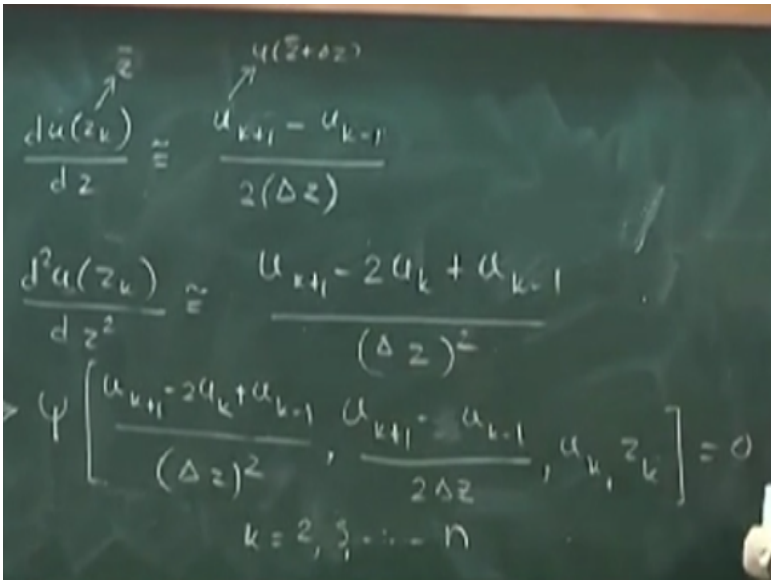

So my du, how do you locally approximate the derivative at, this is my z bar, earlier I talked about a point z bar, this is my z bar, what is this, this is u calculated at z+delta z, this is u calculated at u-delta z, so this is my local derivative. What is my second derivative? So this is going to be approximated as uk+1-2uk+uk-1/delta z square. So with these 2 approximations, this equation here will be transformed to. Where do I want to enforce this differential equation?

At the internal points in the domain. So what are the internal points here, if you go back here, what are the boundary points. Z1 and z n+1. So I should enforce the differential equation at all the internal grid points. So I am enforcing this differential equation at all the internal grid points. How many equations I will get here, n-1 equations I will get. In how many variables, what are the number of variables? What are the unknowns, just look here.

My unknown is u1, u2, u3 in general uk, uk-1, uk+1, how many unknowns are there n+1. So unknowns are u1, u2, u3, u4, u5 up to un+1. So this equation, which actually was supposed to be enforced over the entire domain, now I am enforcing only at a finite number of points. I have discretized my original problem. This is original problem was differential equation. What do I get here when I substitute this, non-linear or linear.

Depending upon what the differential equation is, I will get either linear algebraic equations or I will get non-linear algebraic equations. So original problem which was a differential equation got transformed into set of non-linear or linear algebraic equations depending upon how the original differential equation is. So we end up solving this problem instead of the original problem. Now there are 2 more equations required. How do you get the 2 more equations?

Boundary conditions, at boundary I have a choice, what kind of approximation I use, I could use an approximation which is forward difference, backward difference, or Coulomb approximation, because at a boundary point, here this derivative at a point requires a point before and point afterwards. So if I want to use central difference here, I will need a point on this side and a point on this side. So there are 2 approaches, right now I just talk about 1.

The second 1, we will talk later. So just to end this lecture, I will say there are 2 more equations required to solve this problem.

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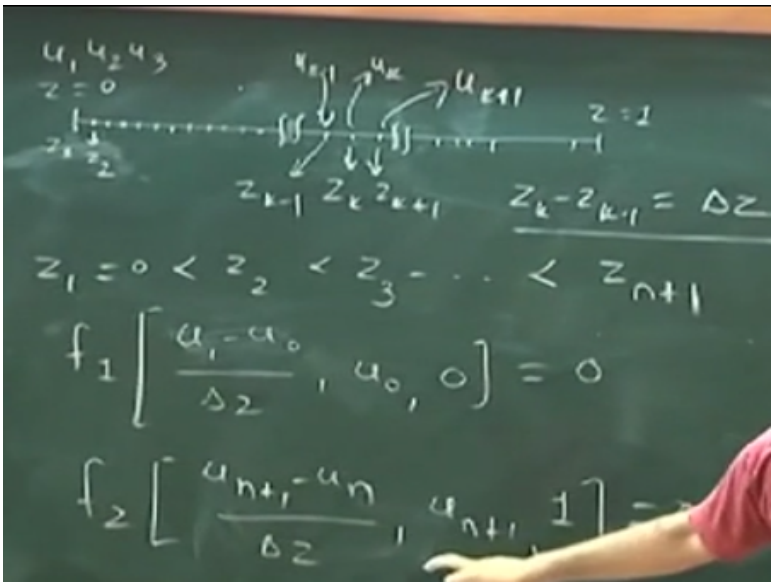

So we generate this u1-u0/delta z, so I am using the forward difference here, u0=0 and f2, I am going to use backward difference here un+1-un/delta z un+1, 1=0. So these 2 equations together with these n-1 equations when they are solved simultaneously, I will get an approximately solution of my boundary value problem. Original problem, which is a boundary value problem ordinary differential equation boundary value problem, get transformed to set of algebraic equations, linear or non-linear depending upon what kind of differential equation you have at hand.

This is discretization. You realize this. we started the original problem in some space and then you actually solved the problem in the finite dimensional space, are we working with finite dimensional spaces now, u is actually discretized, uz is actually a continuous function for my infinite dimensional space. The approximate solution has been constructed by discretizing at finite points. This is a function at finite points.

So this problem has been converted from infinite dimensional space problem to a finite dimensional space problem, why it is computable. How do you get a better and better approximation? You take more and more points, whatever you do, you will still have finite

number of points. Somebody might say I take 100 points, somebody might say no, no I take 1000 points, but remember, now when you take 1000 points, you have to solve 1000 equations in 1000 unknowns simultaneously.

We will be doing these kind of things in this course. The next assignment is going to be solving at least 100 equations and 100 unknowns. That is what you should get this confidence that you can solve as many equations, but these are finite number of equations, non-linear equations. How do I use this, how do I solve this problem? If it is non-linear, how do I solve this problem. Newton's method. I talked about Newton's method, yesterday's lecture.

In the programming assignment, we are using Newton Raphson method. Once I get this, I still cannot solve it, so I have to further approximate. So it is a cascade of approximations, not just because finally we know how to solve Ax=B. We are using Ax=B to solve this non-linear set of equations, but this non-linear set of equations is arising from discretization of a boundary value problem, so you can see the levels of approximations.

You have an approximation, then again you approximate because the approximate problem cannot be solved exactly. So let us continue with tomorrows class, we will see some concrete examples of boundary value problems where we will take some differential equation discretize it and see what happens. Remember these equations are coupled equations. You cannot solve them separately. Because for any point, k+1 and k-1 appear in the equation.

So these are all tightly coupled and you have to solve them together. You cannot solve them separately.