

Foundation of Scientific Computing

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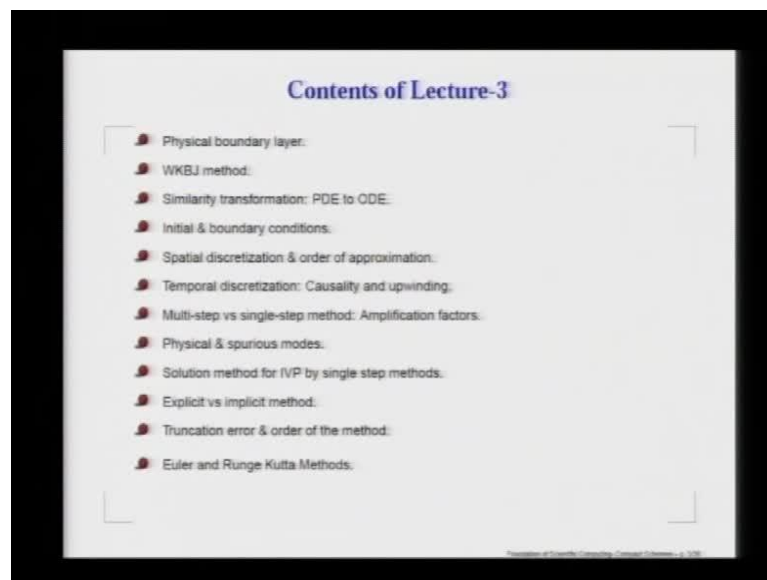
Department of Aerospace Engineering

Indian Institute of Technology, Kanpur

Module No. # 01

Lecture No. # 03

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On this third lecture of our meeting today, we are going to discuss what constitutes physically a boundary layer and we will talk about the various methods that have been used in studying this area. One of it is due to Wentzel-Kramer-Brillouin and Jeffrys method which is again applicable only for linear systems.

So, leaving that aside we will basically talk about similarity transformation, that will allow us to take the PDE directly to an ordinary differential equation and to solve this ordinary differential equation we will require auxiliary conditions; the auxiliary conditions consists of the initial and boundary condition. Having talked about this, we will briefly discuss how we actually use spatial discretization method in solving this ordinary differential equation.

We also touchup on the time discretization and show how it is different from space discretization, because of the requirement of causality, which is distinct from the concept of upwinding that can be used in spatial discretization. When it comes to this solution of ODEs, we classify the solution methods in terms of whether we take one-step at

a time or we take multiple steps and in doing so we actually numerically introduce what is called the amplification factors.

And having set the goal here, we try to distinguish between multi step and single step method: while single step method only gives rise to physical modes, multi step methods have this additional problem of having spurious modes. We will be talking about that.

Having described the requirement of a single step method, we will talk about solution methods for initial value problems and in this particular activity, we distinguish between explicit and implicit methods. In resolving this flow or the problems, we talk about truncation errors, the orders of method which defines these methods and as a follow up we will specifically focus our attention on Euler method to describe what it is; that will be followed by two stage or multi stage two step Runge Kutta methods.

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Physical Boundary Layers

- This singular achievement by Prandtl went unnoticed for almost a decade!
- Computationally, it transformed the equation type and ushered a virtual revolution. This converts a **boundary value problem** to a **marching problem**. (We will discuss classification of PDEs later).
- Blasius further simplified the Boundary Layer Eqn. by introducing the concept of similarity where

$$u(x, y) = u(\eta) \quad (15a)$$

where η is the similarity variable,

$$\eta = \eta(x, y) \quad (15b)$$

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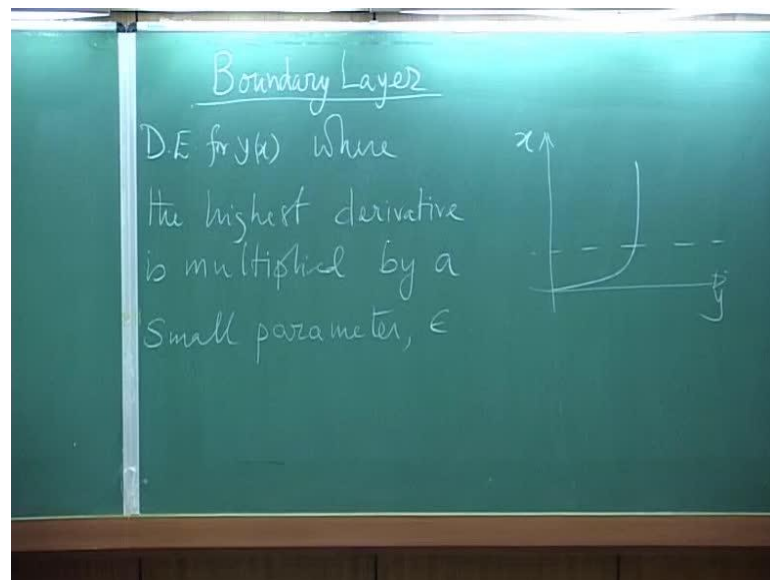
We did talk about boundary layers, right. I think one of you after the class came and asked me that look I have not done any fluid mechanics, is that going to be an

impediment? My answer to you would be not at all; there are various ways of learning subjects.

What I prefer is associative learning. If you have an anchor on a particular subject, you have understanding on some topic, what I wish you to also probably look at the positive aspect of that way. Suppose, I know something then based on that knowledge I go to something which I can build upon.

So, that is why I started with two problems: one was from mechanics and one was from fluid mechanics to give you a glimpse of what boundary layer does.

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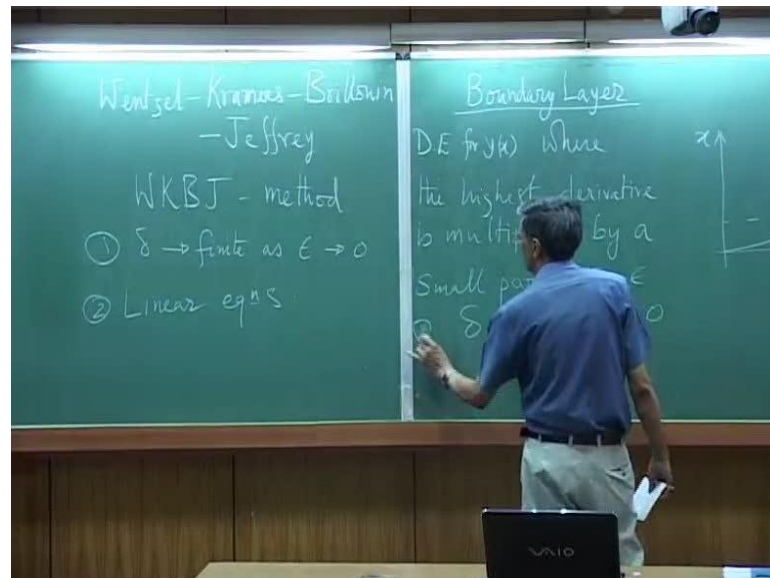


If you want to have a sort of an impersonal mathematical way of stating the same thing, I would say boundary layer is a study of differential equations for say, some variable y of x where the highest derivative is multiplied by a small parameter; that in a sense we noted that a thin layer of pumps in the solutions space. Suppose, if I am plotting say y on this axis and x on this axis like the way we saw the velocity profile. What we found was that we have a thin layer over which you see a rapid growth and a good computing would require you to be able to resolve such rapid variations. So, this is one of the issues that come about in talking about boundary layers.

As I told you that it got started in the early part of 20th century by the group at Gottingen, but people have been also looking at associated problems notably from the

point of view of the same issue where a differential equation that has derivative term is always multiplied by small parameter.

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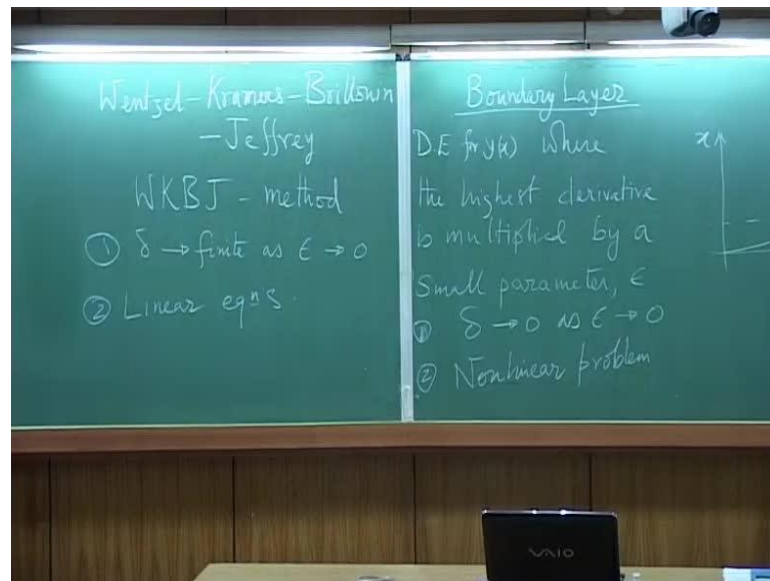


So, in one case you can get boundary layer's theory. There is the other method which has been looked up for a long time which is now known by this name Wentzel-Kramers-Brillouin. Some people also add Jeffrey's name to it; it is called WKBJ method.

This also comes under the same class of problem where the differential equation has this kind of attribute.

The only difference here between these two cases is that in this case delta goes to 0. I call this the thickness of the boundary layer delta goes to 0 as epsilon goes to 0 where as in WKBJ method delta remains finite as epsilon goes to 0. This is the first difference between these two methods; both are global analysis methods.

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The second difference of course, is the very relevant one that this only works for linear equations. You can study linear equations. Well, but here boundary layer theory is little more versatile; it can also tackle non-linear problems. In fact, you noted that the boundary layer equation that we solved was a non-linear PDE and we could tackle it with quite ease.

Despite that, you may note that WKBJ method gets a little more sort of exposure in the literature because those three physicists used it for studying quantum mechanical systems.

So, I do not wish to **[or sadly]** with equations originating from Schrodinger equation and talk about boundary layers and WKBJ method. That is why, that was the reason that I took up something which engineers can visualize a boundary layer growing in a fluid flow or you could see that you have early transient problem in that mechanics problem, the spring mass system we saw that to be able to resolve those early transient you have to be better equipped.

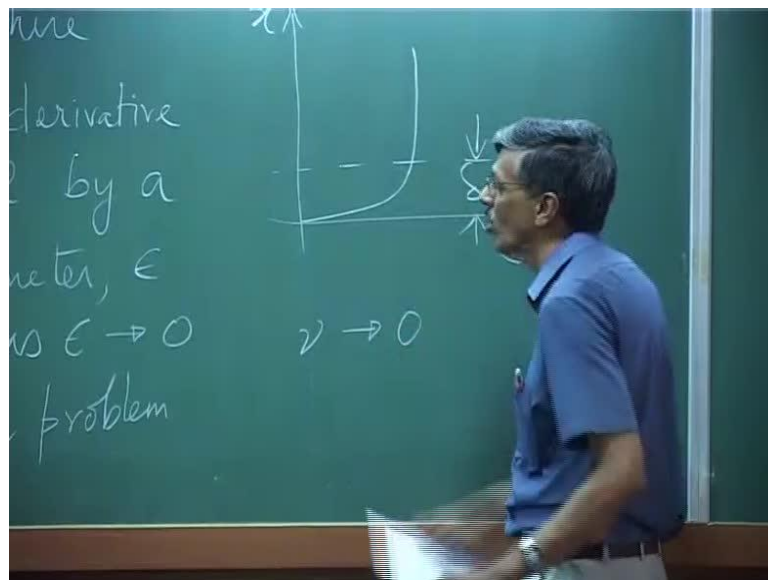
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Auxiliary Conditions of ODEs

- The auxiliary conditions are either at the ends or at one end only.
- For the solution of $f \frac{d^2 f}{d\eta^2} + 2 \frac{d^3 f}{d\eta^3} = 0$; $0 \leq \eta \leq \eta_\infty$ (16)
We need three auxiliary conditions.
- To solve (16), we need to satisfy auxiliary conditions at $\eta = 0$ and at $\eta = \eta_\infty$.
- As stream function is defined by, $\psi = \sqrt{\nu x U_\infty} f(\eta)$, the velocity components are therefore given by,
 $u = \frac{\partial \psi}{\partial y} = U_\infty \frac{df}{d\eta}$
and $v = -\frac{\partial \psi}{\partial x} = \frac{1}{2} \sqrt{\frac{\nu U_\infty}{x}} \left(\eta \frac{df}{d\eta} - f \right)$

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Let us get back to where we stopped. We saw that we could tackle a non-linear problem and we saw this particular attribute that as the parameter ν , kinematic viscosity in that problem played the role of epsilon. So, if ν becomes smaller and smaller or what some of you would know that corresponding non dimensional parameter called the Reynolds numbers goes higher and higher; you get to see this boundary layer shrinking - the thickness shrinking.

We saw that based on that observation, Prandtl and his group including Blasius, they exploited the nature of the solution and Blasius went one step ahead and introduced similarity transformation. Similarity transformation as I pointed out to you is a very versatile technique for converting PDEs into ODEs. (Refer Slide Time: 10:16) That is where we had landed up with this equation 16. So, that was the converted boundary layer equation in terms of that non dimensional stream function f .

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Layer 2

$$\Psi = \sqrt{2\nu U_\infty x} f(\eta)$$

$$\Rightarrow f''' + 2f \frac{d^2 f}{d\eta^2} = 0$$

Initial Condition(s)
Boundary Condition(s)

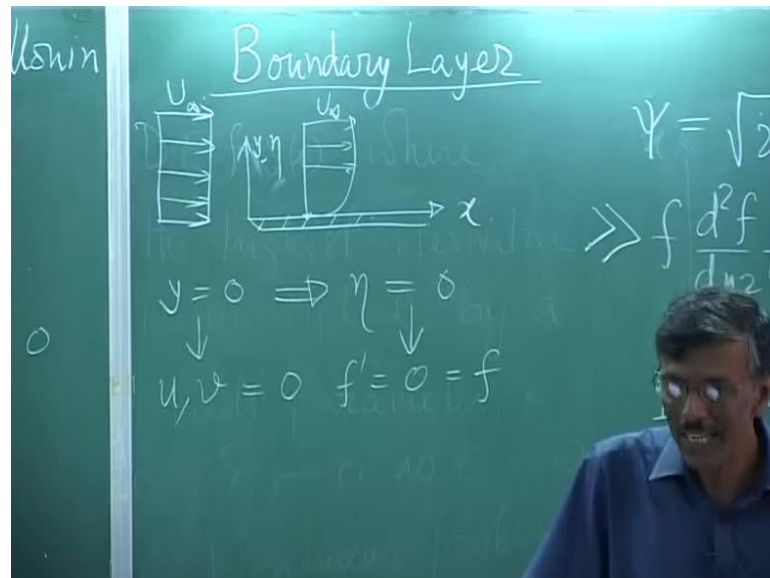
ψ was written down like $\nu U_\infty x f'(\eta)$ and this is your governing equation that you had obtained. $f''' + 2f \frac{d^2 f}{d\eta^2} = 0$ plus 2 times the third derivative of f with respect to η that is equal to 0.

We started talking about auxiliary conditions. Auxiliary conditions refer to both initial conditions. Well, it could be a single condition or could be multiple and then you could have boundary conditions. The appellation really tells you that initial condition relates to time variation. We talk about a problem; what are the conditions at t equal to 0. That is why we relate it to the initial conditions.

However, you could also use with equal felicity, if you have the ability to solve the initial value problems using multiple initial conditions. For example, this equation that we are noticing here has the order very clearly visible here. It is a third order equation;

so, we will require three conditions and those are the ones we are calling as auxiliary conditions.

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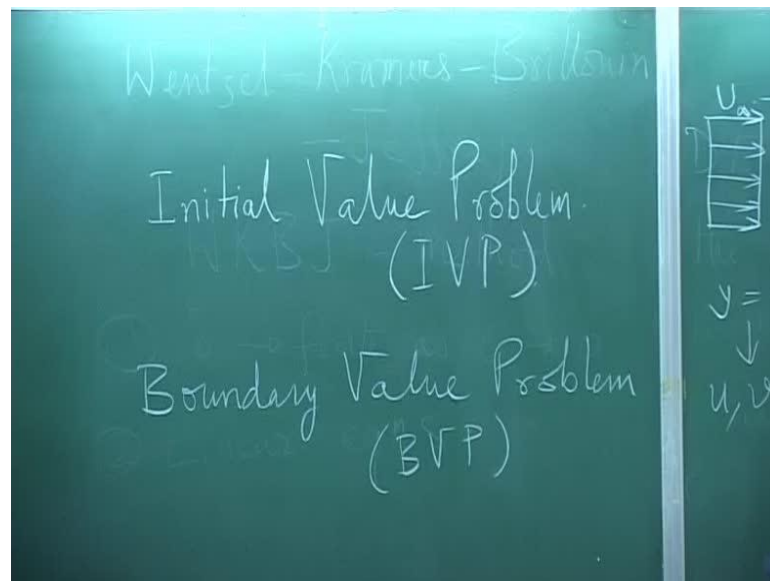


If the stream function is given by psi here then of course, we need to know what we are studying. If you recall that we were looking at this problem. We have a simple geometry sharp leading edge flat plate exposed to a uniform flow which is indicated like this and that forms the boundary layer like this at a [later stations]. If this is U_{∞} , on the outside you have U_{∞} and on the surface you have no slip condition 0 velocity.

That is what you are noticing that u and v are the velocity components given here. and these velocity components If I call this axis as y or η and this as the x , the similarity solution allows us to do away with the x and y variation separately. Instead we look at it in terms of η and what we notice that y equal to 0 essentially corresponds to η equal to 0 and at y equal to 0, we require velocity to be 0. This in turn will tell you that if u is 0, the first derivative of f that should be equal to 0. What about the other condition? If v is 0 of course, you can see that f also has to be equal to 0.

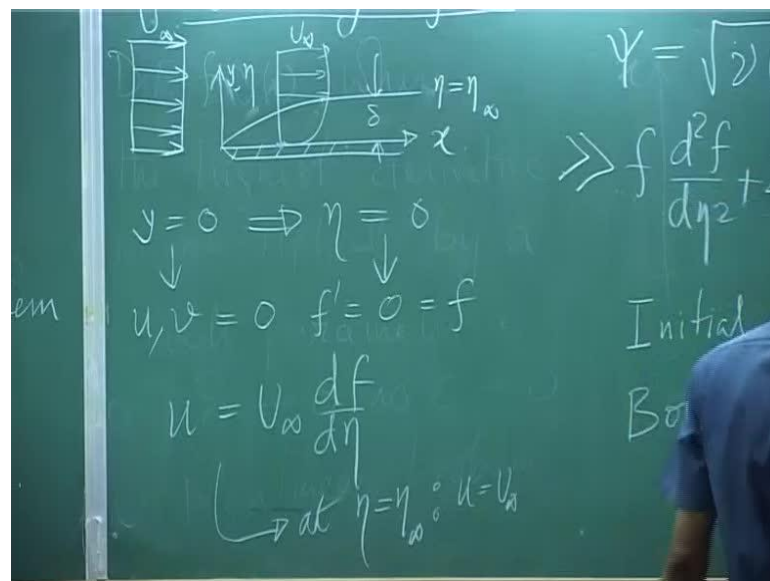
So, this is the usual easier way to visualize that two conditions are fixed here. Unfortunately, you cannot have more conditions at this point. If we would have been able to generate all the three conditions here then we would have obtained what we call as an initial value problem.

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You can now distinguish how ODEs are viewed in terms of initial value problem. We will call them as IVP and we have complementary to it what we will call as boundary value problem. In essence, I just now told you that this Blasius's equation that we have written here will not be classified as IVP because you do not have the all the three conditions available at one of the end of the domain.

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So, the domain that we will have to be looking at as I told you the shear layer forms like this. What we do is this delta, the boundary layer thickness that we talk about has been

stretched out by the η coordinate. That was the whole thing that we telescope it to a larger distance. Then what happens is we have two conditions here; we do not have any idea of any other condition that we could generate from this.

However, we also note one of the properties is that the solution actually smoothly blends to the outer velocity.

So, u starts off from 0. We do not know what is inside it; that is what we are trying to obtain, but we surely know that it smoothly blends into the outside velocity. That is what we say here that the third requisite boundary conditions for solving the Blasius equation is readily obtained from the observation that the boundary layer smoothly merges with the outer flow.

Recall, we talked about inner and the outer variation - inner solution and outer solution. The boundary layer is the inner part and anything that is outside of course, we call it the outer flow. That could be obtained by some other equation by other means which we will not talk about in this course.

(Refer Slide Time: 17:06) Since we noted also the u velocity was obtained as this at the edge of shear layer. So, we need to fix it arbitrarily at some large value of η , the edge of shear layer while we may actually solve this equation not necessarily at the edge of the shear layer δ , but may be 3δ 5δ 10δ . That is what we would be doing. We will be solving this equation over a larger value of δ and that edge of the solution domain we are calling as η infinity.

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Auxiliary Conditions (cont.)

- Boundary conditions at $y = 0$ are: $u, v = 0$ i.e.

$$f, \frac{df}{d\eta} = 0 \text{ at } \eta = 0 \quad (19a)$$

- The third requisite boundary condition for solving (16) is obtained from the observation that the boundary layer smoothly merges with the outer flow i.e. at the edge of the boundary layer,

$$u \rightarrow U_{\infty} \text{ at } \eta = \eta_{\infty} \text{ i.e.,}$$

$$\frac{df}{d\eta} = 1 \text{ at } \eta = \eta_{\infty} \quad (19b)$$

From here you can see that at η equal to η infinity, we have u is equal to u infinity and that gives you this condition – $df/d\eta$ equal to 1 as shown in the slide. So, basically this here is the third condition. Here is an example of a boundary value problem - two conditions given at η equal to 0 and one condition given at η equal to η infinity.

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Classification of ODEs

- If all the auxiliary conditions are given at $\eta = 0$, then we have an Initial Value Problem (IVP).
- If the conditions are distributed between the two boundaries, then we have a Boundary Value Problem (BVP).
- All time dependent problems are inherently IVPs.

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This kind of through an example demonstrates the distinction between the initial value problem and the boundary value problem stated like this: that all the auxiliary conditions are given at one end then we have initial value problem; if the conditions are distributed between the two boundaries then we have a boundary value problem. All time dependent problems are inherently initial value problems because we have to give some initial conditions for time dependence.

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Introduction to Spatial Discretization

- We represent a function at $x + h$ in terms of its value and derivatives at x via the Taylor series expansion:

$$y(x + h) = y(x) + h \frac{dy}{dx} + \frac{h^2}{2!} \frac{d^2y}{dx^2} + \frac{h^3}{3!} \frac{d^3y}{dx^3} + \dots \quad (20a)$$

- Same way, the function at $x - h$ can be represented as

$$y(x - h) = y(x) - h \frac{dy}{dx} + \frac{h^2}{2!} \frac{d^2y}{dx^2} - \frac{h^3}{3!} \frac{d^3y}{dx^3} + \dots \quad (20b)$$

- Expansions as given above can be used to numerically obtain the derivatives appearing on the r.h.s. with the help of nodal values $y(x)$ and $y(x \pm nh)$.

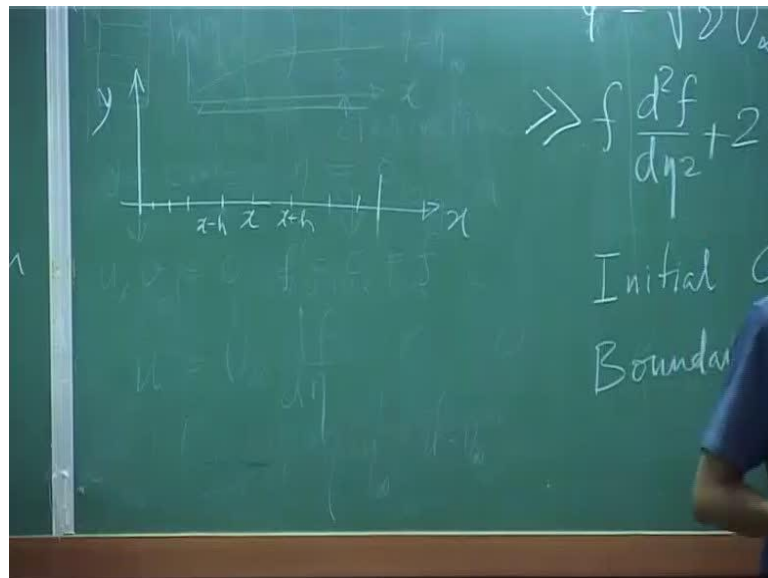
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Now having obtained an equation like this, next thing of interest would be for us to be able to solve this equation. To be able to solve a differential equation, we have to be able to replace these derivatives by some simpler information of the dependent variable and one of the easiest ways to do is use Taylor series expansion.

Say for example, what we are showing here is if we have the knowledge of the function at y equal to x and its derivatives then of course, we can obtain a solution at a neighbouring point which is h apart. If it is in the plus direction then of course, we have a simple look of it like this and if it is on the other side, we will get the odd derivatives with a minus sign; this is quite straight forward.

You all realize that computer does not allow you to directly use these differential or integral operators. So, we will have to do something and that is what we do - discretize the problem. Instead of having the problem in terms of the derivative we convert it in terms of functions at different nodes and that is where Taylor series expansion comes into picture.

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What we have shown here for a point at plus h or minus h , we can do it at points which are at different distance from the point of interest. Basically, what we are talking about is if we are looking at y , this is x and let us say this is our domain of interest. We discretize the domain into a network of points like this and then if I am calling this point as x then

this could be say x plus h . We are talking about uniform spacing, let us say and this could be x minus h and we can similarly get information at x minus $2h$, x plus $2h$ etcetera.

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Introduction to Spatial Discretization (cont.)

- For example, we can approximate the first derivatives by

$$\frac{dy}{dx} = \frac{y(x+h) - y(x)}{h} \text{ or } \frac{y(x) - y(x-h)}{h} \quad (21)$$

- Alternately, we can obtain it as

$$\frac{dy}{dx} = \frac{y(x+h) - y(x-h)}{2h} \quad (22)$$

- While the number of ways to evaluate derivatives are far too many, there are strict rationales for choosing some of them only.

Then with the help of those series representation, we can write the first derivative simply like this. I am sure most of you are familiar with it I am just giving a quick recap of the same.

The first derivative could be written in terms of the function at x and its right neighbour or the function with its left neighbour or we could write it like this. We could write it in terms of the right neighbour and left neighbour divided by twice the gap between these two successive points. Now of course, you can visualize there would be many ways of evaluating derivatives - even these first derivatives.

They would be far too many. How do you choose? Of course, we need to come out with some kind of rational, some kind of a guideline as to how to choose that. One thing you can clearly see in either of these relations if you look up here, I have gotten this first derivative relation by truncating the series beyond this term, second derivative onwards and then of course, pulling this on this side and dividing this by h , I got the expression for dy by dx . This tells you that the Taylor series has been truncated at the first order itself. So, this is called a first order method.

Same thing if I pull this to the right and get this $h \frac{dy}{dx}$ to the left and then of course, ignore these set of terms I get the other expression that also happens to be a first order accurately. (Refer Slide Time: 22:51) Whereas, this expression that you are seeing here taken from these neighbours on either side I subtract the second from the first then of course, $y \times$ cancels out and I get $2 h \frac{dy}{dx}$.

Then you also notice one interesting thing happens that these even derivatives all cancel out. In the process, what you get is this expression in which you have been able to raise your order of approximation from first to second order. So, it is quite obvious that if you get a higher order representation, you have a higher accuracy; this is a legitimate expectation.

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Introduction to Temporal Discretization

- Temporal discretization is different from spatial discretizations due to **causality** i.e. the events at t^{n+1} cannot be influenced by events at t^{n+2} etc.
- For spatial discretization this is done routinely to stabilize numerical methods by upwind schemes.
- However, events at t^{n+1} can depend upon t^n , t^{n-1} , t^{n-2} etc. We will see that this procedure is fraught with danger- as this invokes **spurious modes**. Such methods are called **multistep method**.
- The best method to use are those, where events at t^{n+1} are evaluated in terms of events at t^n only. This retains only the **physical mode**. These methods are called **singlestep methods**.

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So, that could be one of the rational that let me also tell you people have overplayed this obsession with order. We will see that there are better ways of characterizing various operations and we will learn as we go along.

That was about spatial derivative discretization. When we have time derivatives then we have to think afresh. The reason is here – causality. Well, this is something which we all accept at the back of our mind; we assume it to be valid. As I keep telling whenever I get an opportunity that this is more of a philosophic view point than a mathematical statement.

Nobody has proven causality, but nobody has seen it violated too. There you have it. It basically tells you that if you are trying to look at events at t at advance level which we did by index n plus 1 from the knowledge of the system, from the values that we have up to t_n that would be legitimate, but we should not be hoping that somehow future can influence present that only happens in Hollywood films anyway, but this is a rock solid statement we have never seen it to be violated.

Basically, we need to be aware of this and let me also tell you that for spatial discretization we have seen that if I am marching from left to right then I could take a point forward to the right. Fine, that is some kind of an analogy of going beyond than where we are now. So, that is routinely done for spatial discretization, but for time discretization you are not allowed to.

However, what you could do is you could write down the expression for the variable associated with the events at t equal to n plus 1th level to be dependent on what happened in the past at the n th level, n minus 1th level, n minus second level and so on and so forth.

What happens then that is a very interesting aspect and this is often been overlooked and this is one of the issue that we are going to talk about in greater detail in future.

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$$\frac{f}{\Delta t} = \frac{L(u^n)}{u^n} \quad (1)$$

$$g = 1 + \frac{\Delta t}{u^n} L(u^n)$$

$$\frac{u^{n+1} - u^n}{\Delta t} = L(u^n)$$

Amplification factor

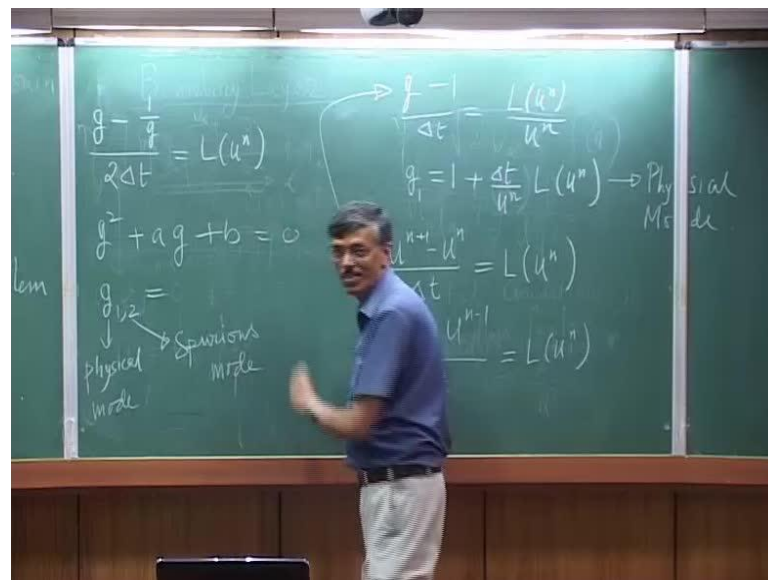
$$g(t^n) = \frac{u^{n+1}}{u^n}$$

Say, give a simple example, if I have a simple equation like this with a first order time derivative written here. What we could do is we could approximate this first derivative in the left end side by its approximation at n plus 1th level. **As I have told you** I could do it in the simplest possible way would be to relate it to the events that had occurred at just the immediate predecessor time.

If I do that then I could define an amplification factor which I call it say g of x because I could be looking at a space time dependent problem. This u could be simultaneously a function of space and time. I could evaluate it at some point. We will not worry about this. What we will do is we will say that g of t **I will write it like t** of n , I will write as u n plus 1 by u n . So, how much the function has gained over one time step; that is the measure of this amplification factor.

Now, you can very clearly see that this equation if I look at it and divide the equation by u of n then what I am getting, u n plus 1 by u n that will be g and 1 by Δt will be L of u n by u n . So, what I find that for a first order equation like this du/dt equal to $L u$, g happens to be $1 + \Delta t$ by u of n L of u n , that is what I get.

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Now, for a moment think of if we would have done it slightly differently. We do not do this; instead, let us do it like this - u n plus 1 minus u n minus 1 by $2 \Delta t$. Remember the central difference formula that we just now saw for the spatial operator. We can do

the same thing and this does not violate causality because we are drawing information from $n - 1$ and we are going from n to $n + 1$. So, this is legitimate; there is not any problem.

Now what happens? If I go through the same exercise, divide this equation on both side by u_n then what am I going to get? Help me. What I am going to get is u_{n+1} by u_n will be g . So, I will get g then I have u_{n-1} by u_n that is 1 upon g . So, what happens?

Yes, tell me.

Sir, the two will not would not be the same g s.

Why not?

One is a t_n and one is t_{n-1}

Depends on how the $L u_n$ is. You will see in most of the cases if you are not seeing what we. We will come to that - distinguish system which are called autonomous which are non autonomous. If you are looking at autonomous system, it will not matter.

We will go in much greater detail. This is just an introductory stage. So, please bear with me. Consider that all g s are same; these are called stationary processes where events are same at all time step. They are called stationary processes and you will be seeing in most of the mathematical physics problem you will come across stationary processes.

It is very rarely you talk about non stationary processes. I might even actually give you an assignment since you provoked me. We will find out that even for a stationary system, careless handling of that system numerically can actually get you to what you are dreading. It will happen and it does happen.

So, what we are essentially getting here is a kind of a quadratic equation. I will just simply write this. What it actually means that here I just simply add g of 1 ; only one amplification factor, here I am going to get 1 and 2 . I could write it down. I am not bothered about this for a moment.

(Refer Slide Time: 32:06) This is what we have noted here that trying to relate events with multiple time steps not necessarily at one time step, but more than two levels are involved. See in this case of course, on the right hand side we have introduced only two time step; here we are talking about three time steps method. These go on from n minus 1 to n plus 1 and as a consequence instead of getting 1 g , we are getting 2. Now, which is correct?

Should we have 1 or should we have 2? Suppose, I would have gone on; instead of three time levels if I would have incorporated four time levels I would have a cubic for g now. So, I would end up with 3 values of g .

Yes.

Sir, I could not see that we are deliberate discretization in terms of time, sir because u_{n-1} and u_{n+1} are the discretization in terms of the space.

No, it is not space; it is time. We are talking about time; that is a time derivative du/dt .

So, I have not written; for a moment forgot about space. Let us say this is a node e and time is the independent variable and n is the time index. I posed a question to you that more than two time level method gives rise to multiple values of g and this seems to be somewhat dependent upon what is the number of levels that we invoke.

So, can someone tell me I mean what is the correct thing? I have already written it down; you have read it. All that I am saying is that this two time level method is the correct one, the real one. Why? It is because whatever you are doing your differential equations are limit processes - Δt going to 0. So, you should involve as a kind of a local or instantaneous representation of the derivative.

More defused your information is, you start involving more time step from farther and farther backward. That is the artifice of your numerical method; that cannot be physics. That is why this one, g_1 , I will call it as the physical mode. Here I may have one physical mode, we will see we will go much deeper into it as we go along and in this case mode will be basically numerical mode and no doubt about it that this is spurious.

So, please be attentive to whenever you are doing temporal discretization that when you involve more than two time levels, those methods are called multi step methods. They come with the baggage of generating spurious modes. If you are not careful, these spurious modes can play havoc. In fact, the subject of chaos dynamics is probably built around, fooling around wrong numerical method.

In many of the cases, you will see that if you are not careful about chaotic dynamical system and if you do discretization mindlessly then you might see totally a different dynamics than what you would like to see.

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Solution methods for IVPs

- For the model time-dependent equation,

$$\frac{du}{dt} = f(t, u); \quad t_0 \leq t \leq t_f \quad (23)$$

- The initial condition is given by,

$$u(t_0) = u_0 \quad (24)$$

- The methods described here are equally applicable for spatial IVPs also.

Whereas, whenever you use only two time level methods, we will call them as single step methods. Let us keep this in mind and then we will go along. Let us get to a very simple task of solving initial value problems.

The initial value problem is of course, given by $\frac{du}{dt}$ is equal to some forcing term f which could be a function of t as well as the dependent variable. Now, this we would require. This is a first order in time equation; so, we require an initial condition. That is the whole idea. That initial value problem, the first derivative tells you that you need only one condition and that is provided to you.

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Solution of IVPs by singlestep methods

- Numerical solution of (23), subject to (24) by singlestep method is represented by,

$$u^{n+1} = u^n + h\varphi(t^{n+1}, t^n, u^{n+1}, u^n, h) \quad (25)$$

where h is the time step and φ - dependent on f , u and times t^n and t^{n+1} - is called the increment function.

Singlestep methods are subdivided into

- **Explicit method:** Here, the r.h.s. of (25) is independent of u^{n+1} & φ is directly evaluated to take u^n to u^{n+1} .
- **Implicit method:** Here, the r.h.s. of (25) is a function of u^{n+1} and it cannot be explicitly evaluated. Such methods are compute-intensive and they are complex to code.

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Well, this method that we are talking about you can also use it for spatial initial value problems. There is not much to worry about as I told you that multi step methods are dangerous. We will keep away for the time being. We will focus simply on single step methods; they help you in avoiding trouble.

So, if I am trying to solve that equation $du/dt = f$. This is the generic equation by which we will be solving it. u at n plus one is equal to the predecessor at u of n plus h , h is the time step. Time is a function. This function we will have to work upon. That function will depend on the time levels which are involved here for the single step method. They are t^n and t^{n+1} , the function at the n plus 1th level, the function at the predecessor level and the time step level itself.

This φ or variable φ - var φ , what you call this? It is called the increment function. So, all numerical methods revolves around figuring out this increment function and we can see that this single step method which has a generic appearance as given here can be further sub divided into two.

If the right hand side is independent of u^{n+1} that means we have a what we call as an explicit method because you can explicitly calculate the right hand side and then you can march from u^n to u^{n+1} .

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Solution of IVPs by singlestep methods

- Explicit methods are simple, but with h restricted to smaller values.
- Implicit methods allow much larger time steps and provide incentive to adopt them.
- In the following, we will restrict ourselves to explicit time integration methods given by,

$$u^{n+1} = u^n + h\varphi(t^n, u^n, h) \quad (26)$$

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In contrast, if the right hand side is also a function of u^{n+1} then you have to worry about solving an implicit coupled equation that involves both the left and right hand side. What happens is explicit methods are simple to execute computationally; implicit methods are difficult. Why should we bargain for difficulty? The reason is the explicit method comes with severe restrictions whereas, implicit method allows you to circumvent these restrictions.

For example, one of the restrictions for explicit method is the time step h ; you have to take it very small. We will see whereas, implicit method would allow you to take much larger time step and when we are talking much larger means we are talking about order of magnitude improvement. So, that is the kind of payback that you can have that should give you enough incentive to really probe into implicit methods.

However, let us keep our attention focused to explicit time integration methods because we are also going to show as we go along that while numerical restrictions are relaxed for implicit method, when it comes to the genuine accuracy of the solution explicit methods are better.

So, you pay for it by large number of time steps, but you get better quality result. That is why I would tell you about explicit method first, later on we will go to implicit method.

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Characterizing Singlestep Methods

- Truncation/ discretization error:

The exact value $u(t^n)$ satisfies the equation

$$u(t^{n+1}) = u(t^n) + h\varphi(t^{n+1}, t^n, u(t^{n+1}), u(t^n), h) + T^{n+1} \quad (27)$$

where T^{n+1} is the truncation/discretization error.

- The truncation error can be written as

$$T^{n+1} = u(t^{n+1}) - u(t^n) - h\varphi(t^{n+1}, t^n, u(t^{n+1}), u(t^n), h) \quad (28)$$

- Order of a method:

is defined by the largest integer p for which

$$\left| \frac{1}{h} T^{n+1} \right| = \mathcal{O}(h^p) \quad (29)$$

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So, this is the way that we write numerically. If I represent the exact value with time indicated inside the bracket with indices like t^n and t^{n+1} , this is representation of the exact value of u .

What we have written is that we could evaluate that at t^{n+1} in terms of t^n and then with this increment function and of course, we have in the process left some terms behind which we will be calling as the truncation error.

So, truncation error is nothing, but pulling this first term on the left hand side, that is $u(t^n)$. What happens is we talked about order of the method when we were talking about spatial derivative. We saw first order method; we saw second order method. So, generic expression for the order of the method is you look at the truncation error term. For this first derivative, you divide it by $1/h$ and then you will see what is the order of the polynomial that you are getting - the terms that you have left behind.

If that is the leading term h to the power p then I will call that method as p th order method. This is what we do.

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Different Singlestep Methods

- Unknown at t^{n+1} is represented by it and its derivatives at t^n :

$$u(t^{n+1}) = u(t^n) + hu'(t^n) + \frac{h^2}{2!}u''(t^n) + \dots + \frac{h^p}{p!}u^{(p)}(t^n) + \frac{h^{p+1}}{(p+1)!}u^{(p+1)}(t^n + \theta h) \quad (30)$$

where $0 \leq \theta \leq 1$ and for the explicit method,

$$h\varphi(t^n, u(t^n), h) = hu'(t^n) + \frac{h^2}{2!}u''(t^n) + \dots + \frac{h^p}{p!}u^{(p)}(t^n) \quad (31)$$

Now, we wrote the numerical equivalent and in terms of Taylor series this is the story. u of $t_n + 1$ written in terms u of t_n plus $h u'$ at k . Everything is evaluated at t_n and this is the Taylor series. We are stopping at the p th time. So, it is a p th order method.

Anything that is left behind, we can use mean value theorem and club it all in the $p + 1$ th order time. Please note the argument. This is somewhere in between t_n and $t_n + 1$. That is what that θ is doing; θ is restricting you to remain in between the current time and the next time level $t_n + 1$.

If I now compare with the previous page then I can simply see for a p th order method, this increment function is given in terms of this set of terms. It is almost like a Taylor series, but note that u of t_n is missing. Anything beyond that, u of t_n comes under that increment function term.

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Different Singlestep Methods (cont.)

- Thus (30) can also be written as,

$$u(t^{n+1}) = u(t^n) + h\varphi(t^n, u(t^n), h) + \frac{h^{p+1}}{(p+1)!} u^{(p+1)}(t^n + \theta h) \quad (32)$$

- Numerical implementation of (30) and (32) is simply to neglect the error term and write

$$u^{n+1} = u^n + h\varphi(t^n, u^n, h) \quad (33)$$

- With the truncation error given by,

$$T^{n+1} = \frac{h^{p+1}}{(p+1)!} u^{(p+1)}(t^n + \theta h) \quad (34)$$

- So the method is of order p .

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So, we have now an estimate for writing the exact solution at n plus 1th level in terms of the value at n th time level and increment function and plus the truncation error term. The truncation error term is readily identified by this.

When I say I have a p th order term, the leading truncation error term will be p plus 1th term; that is h to the power. See this is where the order actually fools us because we are simply obsessed with the order of h , but who gives you a guarantee about this derivative of the dependent variable. See this is the p plus 1th derivative of u .

There is no way we could guarantee that successive derivatives are going to become smaller and smaller. In fact in many physical systems you will see that it just happens the other way. **I don't know about** Quite a few of you must have taken this other course on numerical methods in the second year level.

There you must have come across a topic called interpolation and you must have also been told that you are trying to interpolate a function. It is always better to restrict yourself to a lower order than to higher order. Am I making sense? No, then we will come back to it in future.

Well, you have a noisy data and you are trying to fit it with some polynomial. It is always better to stay as low an ordered system as possible because any small difference

between the physical state and the measurement actually amplifies more, if you try to fit it with the higher order polynomial.

Because This error if it is localized, actually excites the higher wave number or higher frequency and that is the reason that you should be well advised to not only pay attention to what this order of h is, but what the associated derivative is.

In fact, we will figure out a method; we have developed a theory over here over the last 5-6 years. We look at in the case space, the wave number circular frequency space. We will talk about it as we go along and then that would all make sense. We will come back to it again and again.

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Different Singlestep Methods (cont.)

- If we set $p = 1$ in Eqn. (31), then Eqn. (33) reduces to the **Euler method**- a first order method given by,

$$u(t^{n+1}) = u(t^n) + hu'(t^n) \quad (35)$$

- To implement higher order methods, we evaluate higher order derivatives in (31) analytically, using the definition of $u' = f(t, u)$ as

$$\begin{aligned} u'' &= f_t + f f_u \\ u''' &= f_{tt} + 2f f_{tu} + f^2 f_{uu} + f_u(f_t + f f_u) \end{aligned}$$

Let us look at few single step methods. The easiest one is in fact, what I have written it out here p equal to 1 and then what you get u at t_n plus 1. I am just simply relating with u of t_n and the right hand side function has been evaluated here like this.

So, that is what we call as Euler method. Of course, suggested by Euler and you would note that Euler method looks easy, but very nasty method. Many times it will lead to numerical problems and you practically will be advised to stay away from it, if you are just simply looking at solving ordinary differential equation.

So, what happens? You can raise the order of your method. You notice that here we needed the first derivative in Euler method. If I want to go to higher order method, say second order method then I will recall u double prime and since u prime is f, I could differentiate it and I could get u double prime which is f of t plus f into f u. If I want to go to a third order method, I will have to do a little extra work and if I want to go fourth order method, I will have to be looking at more details.

So, this is what you have to do at the coding level. You will have to be evaluating them and you will have to be plugging them in, write your code and you have high order methods.

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Different Singlestep Methods (cont.)

- Practical methods to fix the order of the method (p) and time step (h) for a prescribed error tolerance (ϵ) is obtained from the estimate of T^{n+1} in (34) by,

$$h^{p+1} \left| u^{(p+1)}(t^n + \theta h) \right| < (p+1)! \epsilon \quad (36)$$

$$\text{or, } h^{p+1} \left| f^{(p)}(t^n + \theta h) \right| < (p+1)! \epsilon$$

- As $(t^n + \theta h)$ is not known a priori, maximum value of $f^{(p)}(t^n + \theta h)$ is estimated in full time range.
- Euler method is a restrictive method although not prohibitive and that will be discussed while solving a model space-time dependent problem.

Now, there could be a practical method to fix the order of the method. If I look at the truncation error term and I say, look I am stopping at the pth order and I do not wish to cross this threshold, the error tolerance epsilon then what happens? This is your leading truncation error term that should be bounded by epsilon.

If I do, I have to estimate this quantity within this modular sign - mod sign. What happens? After all, I do not know what this theta is; so, it becomes a difficult task. Instead, what you would be doing? You would be looking at the right hand side function, its pth derivative and you find out in that range from t_n to $t_n + 1$. What is the

maximum of that function? Well easily said than done, but you would be happy to note that solving ODE is quite common place, quite routine.

So, if you go to [CCE] and look at any of You may have already used it. Say, go to any of these packaged routines available - libraries they would all have that and they would without asking you, do this exercise for yourself, but we are not talking about how to use packages; we try to find out why the packages work the way they are designed.

I make an observation here that Euler method is a restrictive method all though not completely prohibitive. Will again spend some time talking about what exactly you mean by it. Every sentence is loaded; it would come with lot of explanation as we go along. We will be talking about it when we come to space time dependent problem later.

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Singlestep Multistage Methods

- One disadvantage of using higher order methods is in obtaining partial derivatives analytically and this is avoided in Runge-Kutta methods.
- Advancing Eqn. (23) by one time step leads to,

$$\int_{t^n}^{t^{n+1}} \frac{du}{dt} dt = \int_{t^n}^{t^{n+1}} f(t, u) dt$$

- Applying Mean value theorem to the r.h.s. of the above leads to:

$$u(t^{n+1}) = u(t^n) + h f(t^n + \theta h, u(t^n + \theta h)) ; 0 < \theta < 1 \quad (37)$$

- Different values of θ and evaluation methods for $f(t^n + \theta h, u(t^n + \theta h))$ yield different numerical schemes.

Now, we noted our restriction that we would not like to go beyond single step method, but then we find that the rudimentary method - the Euler method, is difficult to handle. Higher order methods have the disadvantage that you will have to evaluate all these partial derivatives not only in terms of coding difficulty, but computing time also will increase because you will have to be evaluating all those derivatives - high derivative terms, numerically and they would involve lot of extra work.

What happens is these two mathematicians Runge and Kutta developed simultaneously what is called as single step method, but within that single step you break the domain further into smaller stages.

That is why the word multi stage comes in here. So, we are talking about single step, but within that single step we will be stopping by at various stations and different stages.

This was a very brilliant way of conceiving how we can address this issue of accuracy and not bringing in spurious modes. You can see that right. We are still keeping ourselves routed to single step method, but by adopting multi staging we should be able to improve the accuracy; that is the whole idea about this method.

If I am trying to evaluate this equation advanced by one time step, this is what we do applying mean value theorem we write the expression like this.

This f , I need to know at some intermediate state which I identify with θ . There are various possibilities of choosing the value of θ . After having chosen the value of θ , I could also evaluate this quantity f by multiple options and that is where you have the whole basket of different methods.

So, it is not that you would be talking about a unique method here. You would have all kinds of freedom to look around and shop around.

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Singlestep Multistage Methods (cont.)

- Case-1: If we chose $\theta = 0$, then (37) simplifies to

$$u(t^{n+1}) = u(t^n) + hf(t^n, u(t^n)) \quad (38)$$

which is the **Euler method** obtained earlier. The increment function is evaluated at the starting gate!

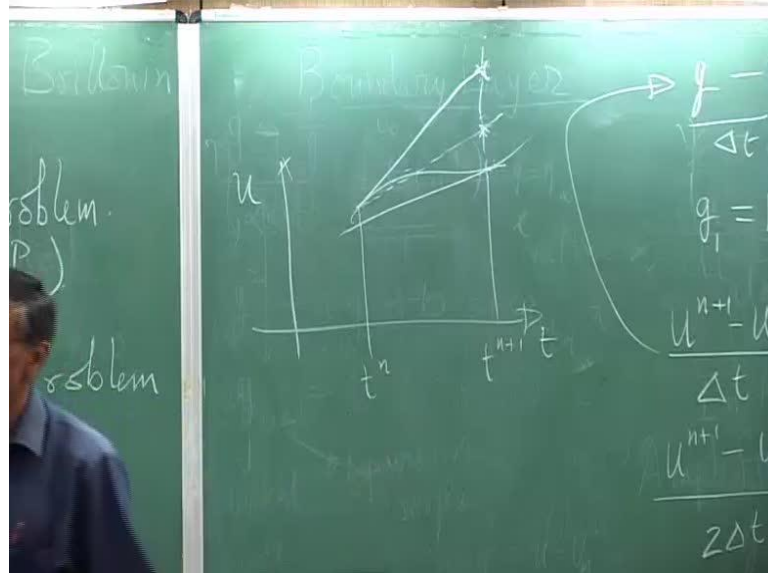
- Case-2: If we chose $\theta = 1$, then the **Backward Euler method** is obtained given by,

$$u(t^{n+1}) = u(t^n) + hf(t^n + h, u(t^{n+1})) \quad (39)$$

Here, the increment function is evaluated at the exit gate of the time step! Hence this is an implicit method.

For example, we have already seen that if we choose theta equal to 0 that is your Euler method. Basically, what we have done. Let us try to look at the solution and try to see what we are aiming actually.

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Let us say I am plotting here u versus t and I have a solution at t_n and I am trying to go t_{n+1} and this is say the exact solution. What we did if you can see here this increment function that we have evaluated is nothing but, the slope of the curve, is not it? Where have we evaluated the slope? At the starting gate. At this point if I draw a slope, Euler method basically gives me the solution here and that is where we have so much of problem, so much of error if the function is rapidly varying and the slope is not truly representative of what the function is doing. In the single time step, you will always end up with a distant point from the exact solution and that is one of the issues.

Now, Euler also came out with this method that instead of calculating the slope at t_n , you calculate the slope at t_{n+1} . What happens? I could draw a slope here. I will start from here; so, what I am doing is I am drawing a parallel to this line which is the basically the tangent here. What I am going to get is something like this.

So, this line is parallel to this. Well, my drawing is not at all good, but I should be mindful of that and let us say we do that. That is your solution. So, if this is your basic

Euler method, backward Euler method would get you there, but this just happens to be the way we have drawn the variation.

In another case, this may not be as good as what it has been seen here. So, you can see that these two possibilities are not really at all that good that you also notice that the right hand side involves $t_n + 1$. That means, you will have to know the solution to evaluate the slope. If the function descriptor is tough then you will have a tough implicit method at hand because u_{n+1} is involved on both sides.

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Singlestep Multistage Methods (cont.)

- Case-3: If we choose $\theta = \frac{1}{2}$, then

$$u(t^{n+1}) = u(t^n) + hf(t^n + h/2, u(t^n + h/2)) \quad (40)$$

- Since, $(t^n + h/2)$ is not a node, various approximations are possible:

- Subcase-3a: If $u(t^n + h/2)$ is evaluated by the Euler method, then

$$u(t^n + h/2) = u(t^n) + \frac{h}{2}f(t^n)$$

$$u(t^{n+1}) = u(t^n) + hf\left(t^n + \frac{h}{2}, u(t^n) + \frac{h}{2}f(t^n)\right) \quad (41)$$

- If we set $K_1 = hf(t^n)$; $K_2 = hf(t^n + \frac{h}{2}, u(t^n) + \frac{h}{2}K_1)$, then, $u(t^{n+1}) = u(t^n) + K_2$ (42)

So, the other possibility is suppose [a query] we fix the mid stage at half way. I choose theta equal to half then you evaluate at $t_n + 1$ and it would be obtained like this. Now, you notice that this is not a node and we could again have the possibility of choosing our self.

For example, for this we can look at the followings of subcase. If this is evaluated by the Euler method, that means what I am saying is I have to work out what this u at $t_n + h/2$ is. What I would do? I will evaluate it as u of $t_n + h/2$ into f evaluated at t_n .

Then what happens is wherever I have this function, I will write down as u of $t_n + h/2$ f of t_n .

In an algorithmic sense, what I would do? I would first evaluate K_1 ; K_1 is nothing, but h times f evaluated at t_n . Then having obtained K_1 , I will evaluate the right hand side with the help of the knowledge that the mid station, the solution is obtained as u of t_n plus h by 2 K_1 . Once I have the K_2 evaluated in this fashion, I will just simply add that K_2 to the previous time level to get the new solution.

So, this is a very simple demonstration of how a multi stage method works, if we decide to clean our information from midpoint of the stage.

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Singlestep Multistage Methods (cont.)

- Subcase-3b: Here, $u(t^n + h/2)$ is evaluated by averaging i.e., $u'(t^n + \frac{h}{2}) = \frac{1}{2} [u'(t^n) + u'(t^n + h)]$
- Similarly, the r.h.s. is evaluated from, $u'(t^n + \frac{h}{2}) = \frac{1}{2} [f(t^n) + f(t^{n+1}, u(t^n) + hf(t^n))]$
- We obtain from (40),

$$u(t^{n+1}) = u(t^n) + \frac{h}{2} [f(t^n, u(t^n)) + f(t^{n+1}, u(t^n) + hf(t^n))] \quad (43)$$

- Define $K_1 = hf(t^n)$; $K_2 = hf(t^{n+1}, u(t^n) + K_1)$
- Then, we obtain the **Euler-Cauchy method** given by:

$$u(t^{n+1}) = u(t^n) + \frac{h}{2} [K_1 + K_2] \quad (44)$$

Now, we could also do various other things. For example, I could have suggested that look this quantity that we have, we could wherever we need to have obtained this average, we will just take it as a half of what we have at t_n and what we have [at the end of the...]

Basically, then this will be written in terms of f of t_n plus this and eventually plug that information in there and there you have it. Then we will be evaluating K_1 in this case again the same way, but K_2 has been evaluated in this fashion and the difference comes from the previous method is the final step here. I just simply take the average of K_1 and K_2 .

In the previous case, I just simply obtained it in terms of K_2 remember $u(t_n)$ plus K_2 , but in this case what you are doing you are taking an average of K_1 and K_2 . That is a method attributed to Euler and Cauchy. So, call that as Euler-Cauchy method.

Yes.

(()) what is the (()) second order equation

Yes. so I have Starting point was a first order method we are trying to get it better. So, second order method is a better method than first order method; that is the whole approach.

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Singlestep Multistage Methods (cont.)

- It is imperative to evaluate the suitability/applicability of the methods from a plethora of possibilities.
- A natural way to address this is to develop analyses tools which study standard benchmark problems that mimic the most important physical processes.
- We will address these issues in the later part of the course.
- We next discuss an important class of methods for solving ODEs: The Runge-Kutta Methods.

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Let us try to recap what we just now looked at. If we have to evaluate then we have to see the suitability, applicability of the method from many possibilities. A natural way of course, would be to develop some analysis tools with the help of some standard benchmark problems.

That really mimics the most physical processes involved in the differential equation. We hope to we will of course, we will address this issues as we go along.

Let us now look at solution methods as given by Runge and Kutta and that is where we will begin from next Monday.

Thank you.