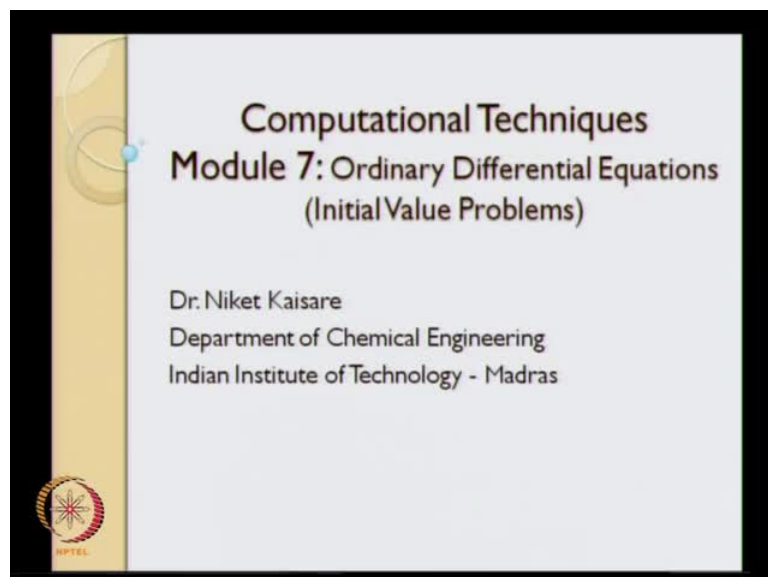


Computational Techniques
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Module No. # 07
Lecture No. # 01
Ordinary Differential Equations
(Initial Value Problems)

Hello and welcome to module 7 of the computational techniques course. In module 7, we are going to discuss ordinary differential equations - the initial value problems. what I am going to do in the next few minutes is, just give an overview of what we mean by ordinary differential equations and specifically what we mean by initial value problem and then go through the outline of the things that we are going to cover in this particular module.

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

- Given: $\frac{dy}{dt} = f(y, t)$
- $y(t_0) = y_0$
- ↓
- $y(t)$

To the right of the equations is a graph with a vertical axis labeled y and a horizontal axis labeled t . A curve is plotted, and a red arrow points to it with the label $f(t)$.

In the bottom left corner of the slide, there is a circular logo with a star-like pattern and the text "NPTEL" below it.

So, the background is given that, we have an equation - a differential equation - of the type $\frac{dy}{dt} = f(y, t)$, keep in mind that, this function f in general, we let it be function of both the dependent variable y that we are interested in finding out and the independent variable t that varies and for which we are interested in finding the particular value of y .

In addition to this particular differential equation, we also need to be given an initial condition an, initial condition would be of the form y at time t_0 is given as certain value y_0 ; and the objective of solving this ODE problem is to obtain y at any time t .

So, this is an example that I am showing graphically, where I have plotted the function y against the time t and this is some arbitrary function y against t . So, let us consider any time t_i , at that point t_i the slope of this curve is going to be the f of t .

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The slide is titled "Compare with Integration" and is divided into two sections. The top section, labeled "Given:", shows the differential equation $\frac{dy}{dt} = f(y, t)$ and the initial condition $y(t_0) = y_0$. A downward arrow points to the solution $y(t)$. To the right is a graph of a curve $y(t)$ on a coordinate system with axes y and t . The bottom section, also labeled "Given:", shows the function $f(t)$ and the definite integral $\int_a^b f(t) dt$. A downward arrow points from $f(t)$ to the integral. To the right is a graph of the function $f(t)$ on a coordinate system with axes $f(t)$ and t . The area under the curve between $t = a$ and $t = b$ is shaded in yellow. In the bottom left corner of the slide, there is a logo for NPTEL.

So, the objective of the ODE all over is given the function $f(y, t)$, that is the slope of the particular curve; we are interested in then finding out the entire curve as a function of y of t ; that is the overall background for this particular problem; **this problem is, if you**, if you can see **this kind of related to the problem of integration**; in some ways, it is related to the problem of integration, is in some other ways, that is actually very different from the problem of integration; in case of integration, what we had is dy by dt as a function of t only, we did not have dy by dt as a function of y and t ; under that condition we can have y equal to integral f of $t dt$ and that is what we had done; in the previous **- module -** module 6, we are considered integration of a function f of $t dt$ between the values a and b ; and in that case, when we plot the function f of t against t , the integral signifies the area under this particular arbitrarily drawn curve and the shaded area over here becomes the integral going from a to b of $t dt$.

Now, in case of an integration problem, the problem is a little bit different, in the sense that, we are now plotting or we are interested in plotting or finding the function y of t given any function f . So, in that sense, this problem are different; in this case, we are interested in finding out this particular curve given this starting point y at some time t_0 equal to y_0 ; **whereas**, whereas, in the integration problem we are interested in finding out this particular f of t curve, the area under that curve between the two limits of integration; so that is the comparison with integration.

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Example: Plug Flow Reactor

- Design Equation for volume of PFR
$$V = F_{A0} \int_0^X \frac{dX}{-r(X)}$$
- Volume of PFR is given by area under the curve $\frac{1}{-r(X)}$
- Conversion from a PFR
$$F \frac{dC_A}{dV} = -r(C_A) \quad \Rightarrow \quad F_{A0} \frac{dX}{dV} = r(X)$$

HPTEL

Now, let us take an example of a plug flow reactor, what we have done in the previous module was to determine the volume of the plug flow reactor, that will give a certain conversion x ; and in that particular case, we had plotted the function negative of 1 by $r x$ as a function of x ; so, what we did was, inverse of the rate of conversion we plotted it all as the y axis and the conversion we plotted it as the x axis, the area under the curve multiplied by the - inlet - inlet flow rate of the reactant a in terms of moles per unit time, that product actually give us gave us the volume of this c s t r.

Now, this particular design equation sorry, the volume of a PFR, this particular design equation of a PFR is obtain from this overall model of the PFR, where the model is initially written based on the mass balance; and based on the mass balance, we will get a model of this form; and then expressing the concentration in terms of conversion variables, we will, we will be able to convert that particular model in this form.

So, what we are going to do in case of an ODE solving is, we are going to solve this particular equation, given that the volume at the, given that the conversion at 0 volume at or conversion at the starting of the reactor is 0; so, with, with that condition we are going to start our ODE solvent.

So, there are some parallels between integration and solving of the ODE, but in general, ODE solutions for chemical engineering problems or in general for engineering problems, go well beyond the - limits a - limitations of an integration method of solving.

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Numerical Method

- To solve: $\frac{dy}{dt} = f(y,t)$

↓

$$\lim_{\Delta t \rightarrow 0} \frac{y_{i+1} - y_i}{\Delta t} = f(y_i, t_i)$$

↓

$$y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$$

Now, let me motivate the means that we are going to use in order to solve numerically the ODE - subject to the initial conditions, we are given the ODE $\frac{dy}{dt} = f(y, t)$; let us say at the current instant, let the say the current instant is given by t equal to t_i - and at t_i - and at t_i we know all the value y_i t_i and everything else that we need to know about the system.

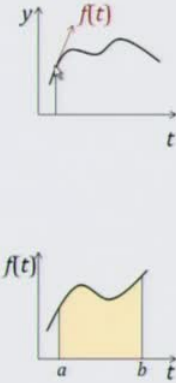
So, τ , $\frac{dy}{dt}$ is nothing but limit as Δt tends to 0 $y_{i+1} - y_i$ divided by Δt , now that is going to be equal to $f(y_i, t_i)$; when we write this particular expression and let Δt be very small, in that particular case, what we will get this as the solution is a means of numerically solving the ODE; and that particular, by a simple rearrangement of this particular equation what we will get is, $y_{i+1} = y_i + \Delta t \cdot f(y_i, t_i)$.

Now, what i have done over here is, replaced $f(y_i, t_i)$ with another function $s(y_i, t_i)$; recall based on our geometric discussion, s is nothing but the slope of the curve y against t ; so, we will go back a couple of slides earlier, this act a point t_i , s is nothing but the slope.

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Compare with Integration

- Given: $\frac{dy}{dt} = f(y,t)$
 $y(t_0) = y_0$
 \Downarrow
 $y(t)$
- Given: $f(t)$
 \Downarrow
 $\int_a^b f(t) dt$

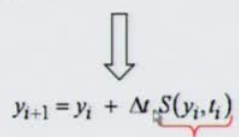


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Numerical Method

- To solve: $\frac{dy}{dt} = f(y,t)$
 \Downarrow
 $\lim_{\Delta t \rightarrow 0} \frac{y_{i+1} - y_i}{\Delta t} = f(y_i, t_i)$
 \Downarrow
 $y_{i+1} = y_i + \Delta t S(y_i, t_i)$

Numerical methods focus on using appropriate value of "slope" $S(y,t)$ to improve accuracy

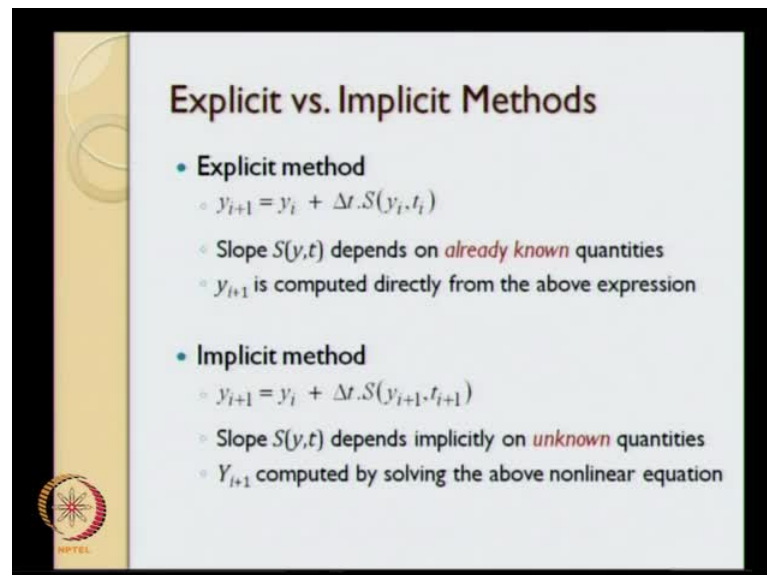


Now, that is slope can be computed at the point (y_i, t_i) or it can be computed using the various different means; and the means that we are going to use in order to compute this particular slope is again going to give us different methods of solving the ODE problem. Some methods are going to be more accurate than certain other methods; some other methods have certain stability properties of interest to us, all these are something that we are going to consider in this particular module; so, the numerical methods are going to focus on using appropriate means to obtain the slope s in order to improve the accuracy

of the solution y_i , that we get as a function of time t ; so, that is what we are going to use that is, how rather we are going to use a numerical method to obtain the ODE solution. So, we start with certain value y_0 and we use a certain small enough Δt and we keep using the numerical method recursively in order to get y at t_1 t_2 t_3 t_4 and for the entire range of t of our interest; that is the recursive method of solving ODE; it is under cursive numerical method for solving the ODE and we will actually be able to get y at discrete times t_0 t_1 t_2 t_3 t_4 and so on.


Now, we can choose our Δt either to be a constant value or we can change the value of Δt depending on how the slope s changes; if the slope s is very steep, we will take small Δt values; or if the slope s is not very steep, we can perhaps take larger Δt values; that is the basis behind what is known as adaptive step size; Δt is the step size of the independent variable and this step size is something for us to choose; and we will see how the choice of step sizes as going to affect the overall quality of the solution, how to choose this particular step size, how the accuracy of the solution depends on the various numerical methods, so on and so forth, or something that what we are going to cover in this particular module.

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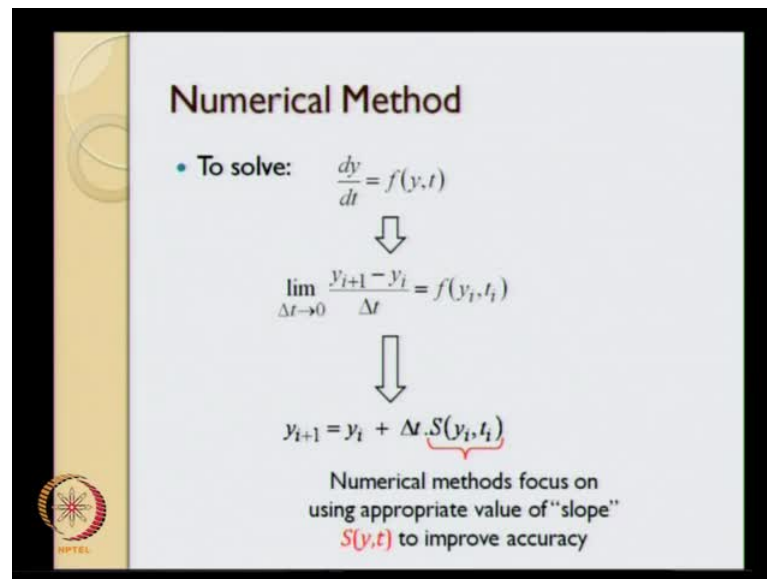


Explicit vs. Implicit Methods

- **Explicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$
 - Slope $S(y, t)$ depends on *already known* quantities
 - y_{i+1} is computed directly from the above expression
- **Implicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_{i+1}, t_{i+1})$
 - Slope $S(y, t)$ depends implicitly on *unknown* quantities
 - Y_{i+1} computed by solving the above nonlinear equation



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Numerical Method

- To solve: $\frac{dy}{dt} = f(y,t)$

↓

$$\lim_{\Delta t \rightarrow 0} \frac{y_{i+1} - y_i}{\Delta t} = f(y_i, t_i)$$

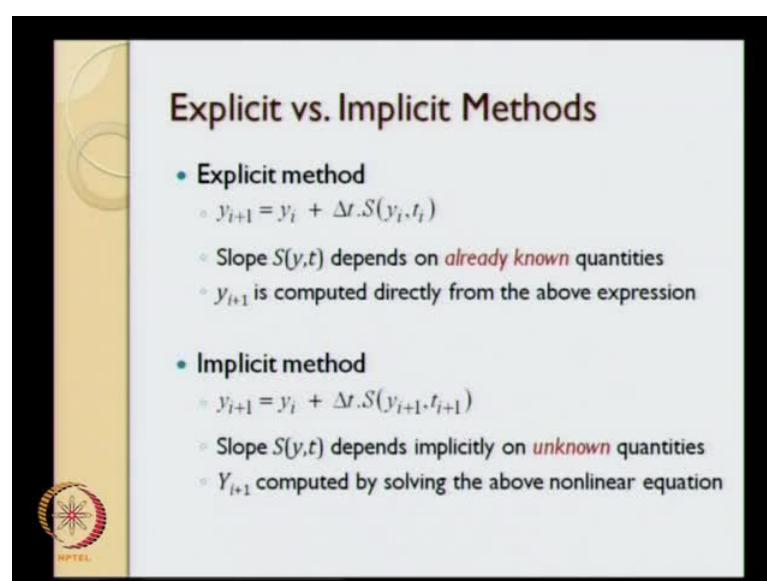
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$$y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$$

Numerical methods focus on using appropriate value of "slope" $S(y,t)$ to improve accuracy

The next important question that we are going to cover in this module is the question of explicit versus implicit method. In the previous slide, we will go back to the previous slide, what we had done is, the differential $\frac{dy}{dt}$ we had represented it as $y_{i+1} - y_i$ divided by Δt ; the other way to represent this particular differential is also to be represented as $y_i - y_{i-1}$ divided by Δt ; and these two different methods are going to lead us to different ways of solving - this - this particular problem.

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Explicit vs. Implicit Methods

- **Explicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$
 - Slope $S(y,t)$ depends on *already known* quantities
 - y_{i+1} is computed directly from the above expression
- **Implicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_{i+1}, t_{i+1})$
 - Slope $S(y,t)$ depends implicitly on *unknown* quantities
 - y_{i+1} computed by solving the above nonlinear equation

This method that I have shown over here is what is known as an implicit method; whereas, if we had represented $\frac{dy}{dt}$ as $\frac{y_i - y_{i-1}}{\Delta t}$, that would be what is known as an explicit method. Now, we can just rearranged the implicit method in a little bit different way and those ways I have shown it over here; this is the explicit method that we have talked about; and this is the implicit method.

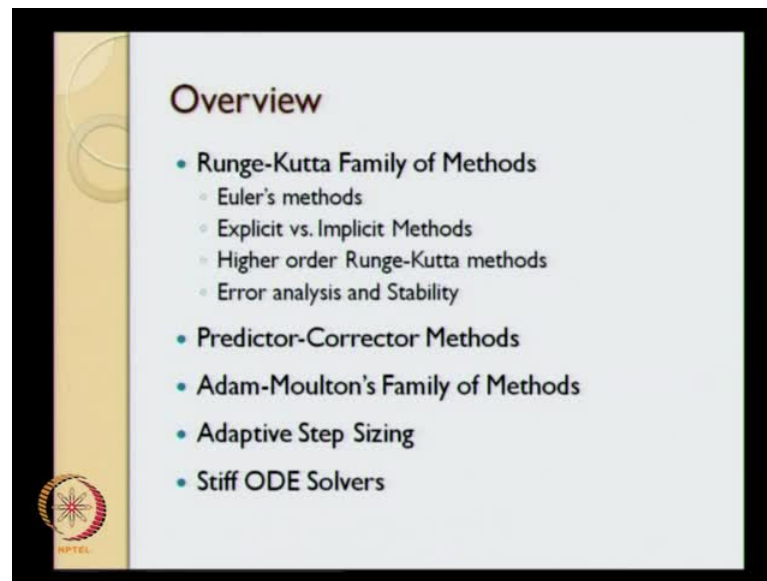
Let us go to the explicit method first, y_{i+1} is $y_i + \Delta t$ multiplied by the slope; the slope depends explicitly on y_i and t_i , y_i and t_i are quantities that are already known at the time t_i .

So, y_{i+1} is computed directly from known quantities, from already known quantity; so, this particular equation is not used as an algebraic equation, but instead its use as an expression, that means, we solve the right hand side, whatever value we get at the right hand side, we just use that value as y_{i+1} and keep proceeding into the future; that is the explicit method. The implicit method with slight rearrangement, we can write implicit method as, y_{i+1} equal to $y_i + \Delta t$ multiplied by the slope computed based on y_{i+1} .

So, what is happening over here is, at time i the value y_{i+1} is not yet known, so the slope $\frac{dy}{dt}$ is computed at a point, **which we are**, which is currently not known; so, it depends implicitly on the unknown quantities; so, y_{i+1} that can be computed using the above non-linear equation.

So, in this particular case, this particular form of equation is used as an explicit expression, that means, we calculate the right hand side and just assigned it to y_{i+1} , whereas this is used as an algebraic equation, which we can perhaps solve using techniques such as newton-raphson's techniques, or fixed-point iteration techniques, so on and so forth; so, y_{i+1} implicitly depends on itself - y_{i+1} - that is the implicit method of solving the equation; and we are going to cover implicit methods and explicit method and what it means from the stability view point of any algebraic equation solver; these are the things that we going to cover in this particular module.

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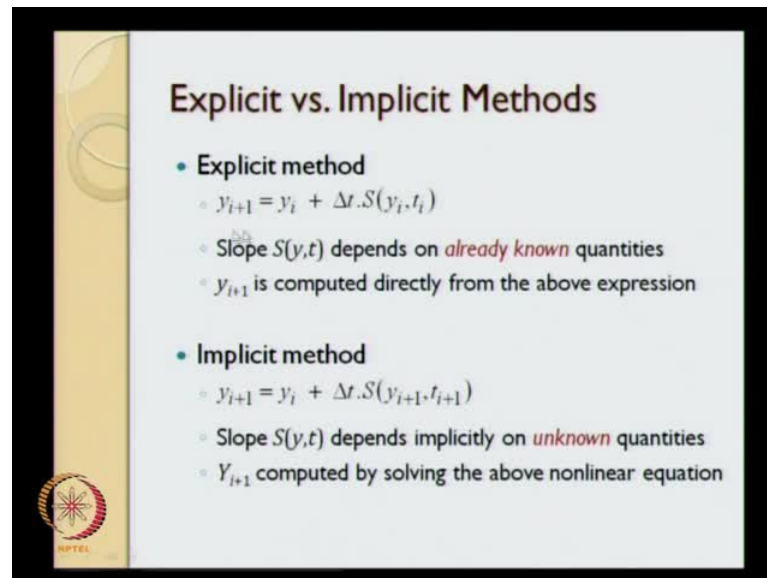
So, finally, to give an overview of this particular module, we will cover what is known as the Euler's methods; Euler's methods are the implicit and the explicit method that we just spoke about couple of slides earlier; those are actually known as the Euler's methods; **then will** in general talk about implicit methods versus explicit methods, **what what**, what do implicit versus explicit actually means, then we will talk about the Runge-Kutta family of methods.

We look at the error analysis as usual; **we will**, we will talk about how the error propagates as the i changes as we go from y_0 to y_1 , y_1 to y_2 , y_2 to y_3 , so on and so forth. How is our numerical solution going to compare **- with -** with our analytical solution; we will also talk about stability, which basically means that, given y_0 when we are going to compute y_1 y_2 y_3 y_4 so on and so forth, as i tends to infinity does **our for the solution thus** our numerical solution remains stable or does the numerical solution go to plus or minus infinity; that is the problem that we are going to tackle with respect to the stability **- of our -** of these methods.

So, all these become one class of methods, where we are going to use sum means in order to compute the slope s ; then another class of methods are what is known as predictor-corrector methods; in predictor-corrector methods what we are going to do is, we are going to use a method to compute the slope s , that is called a predictor method;

and then we are going to use certain set of equations known as corrector equations in order to improve the accuracy of the approximation.

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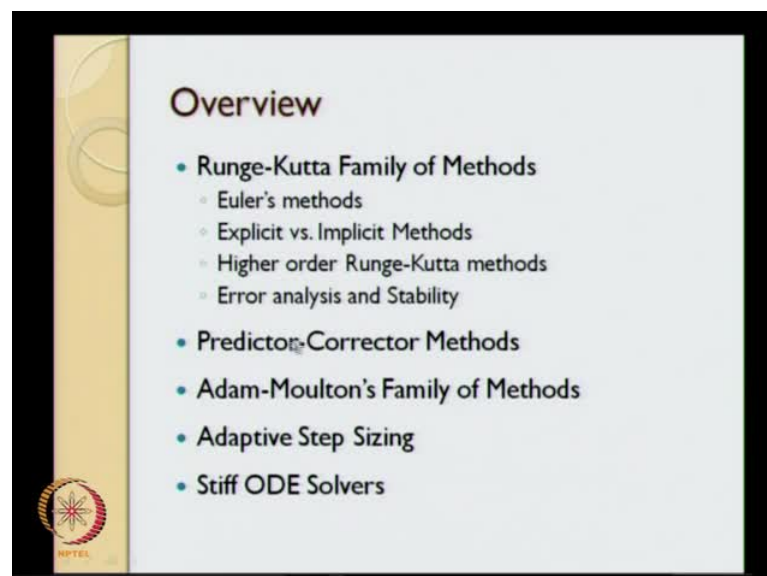


Explicit vs. Implicit Methods

- **Explicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$
 - Slope $S(y, t)$ depends on *already known* quantities
 - y_{i+1} is computed directly from the above expression
- **Implicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_{i+1}, t_{i+1})$
 - Slope $S(y, t)$ depends implicitly on *unknown* quantities
 - y_{i+1} computed by solving the above nonlinear equation

What that means is that, there will be an equation written in this particular form which will be a predictor equation that will help us to compute y_{i+1} . Now, we have the value of y_i and an approximate solution not y_{i+1} , recursively this value y_i and the approximate solution y_{i+1} , we will be used to correct the value of y_{i+1} in order to - **give** - get the higher order accurate formula.

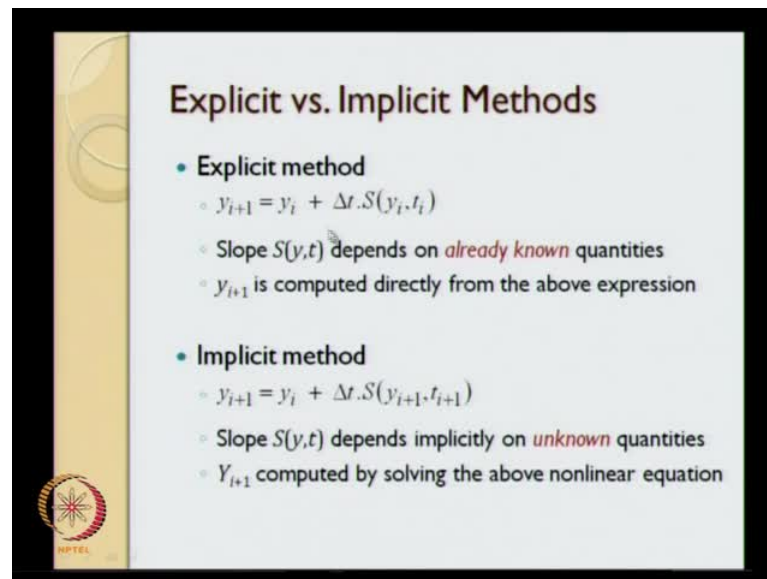
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Overview

- **Runge-Kutta Family of Methods**
 - Euler's methods
 - Explicit vs. Implicit Methods
 - Higher order Runge-Kutta methods
 - Error analysis and Stability
- **Predictor-Corrector Methods**
- **Adam-Moulton's Family of Methods**
- **Adaptive Step Sizing**
- **Stiff ODE Solvers**

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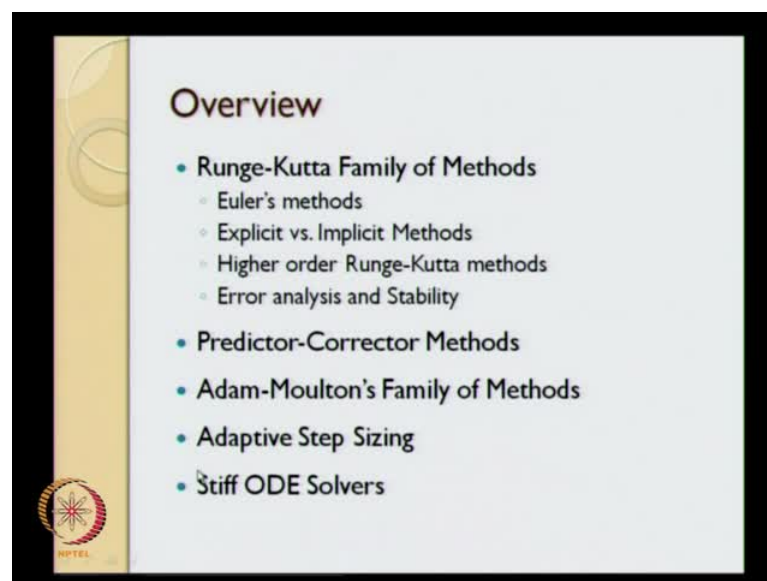


Explicit vs. Implicit Methods

- **Explicit method**
 - $y_{i+1} = y_i + \Delta t \cdot S(y_i, t_i)$
 - Slope $S(y, t)$ depends on *already known* quantities
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 - y_{i+1} computed by solving the above nonlinear equation

The next set of methods is known as the Adam-Moulton's family of methods; and finally, we will cover two slightly advanced topics in **- in in -** this particular module; first is the adaptive step sizing had I mentioned a few couple of first slides earlier, that this delta t need not be constant, the value of delta t we can change based on how the value of slope changes in order to get higher order accuracy formulae.

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Overview

- Runge-Kutta Family of Methods
 - Euler's methods
 - Explicit vs. Implicit Methods
 - Higher order Runge-Kutta methods
 - Error analysis and Stability
- Predictor-Corrector Methods
- Adam-Moulton's Family of Methods
- Adaptive Step Sizing
- Stiff ODE Solvers

So, we will try to talk about how to change the step size adaptively based on the current solution of the ODE that we are trying to solve; and finally we will come to what is

known as stiff ODE is, I will motivate what we mean by stiff ODE is, and look at the solvers that solve this stiff ODE problem; and while talking about stiff ODE then adaptive step sizing I will take up a couple of examples that are of interest to chemical engineers and try to motivate what the stiff ODE is actually mean; in - additions - addition to that, all these methods we are going to cover only from the point of view of a single variable problem, we will stick to single variable for most of this module; for a simple reason that single variable problems are relatively easier to tackle, but I will also cover, I will perhaps spend - half to - half to one lecture on extension of these methods to multivariable problems.

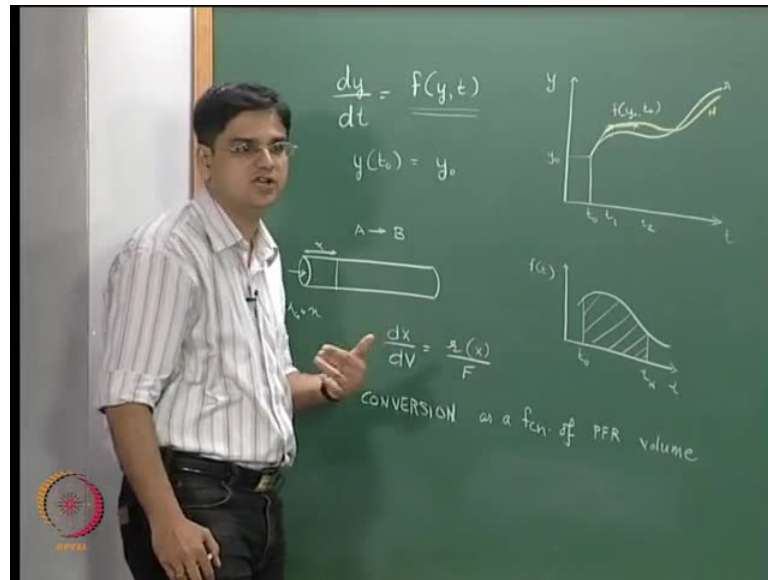
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Compare with Integration

- Given: $\frac{dy}{dt} = f(y,t)$
 $y(t_0) = y_0$
 \Downarrow
 $y(t)$
- Given: $f(t)$
 \Downarrow
 $\int_a^b f(t) dt$

So, that is the overview of ODE solving techniques; what I am going to do in this particular lecture is, go over the geometric interpretation once more, go over the comparison with integration and then talks specifically about the two methods; the two methods that I will - going - going to talk about are the Euler's method and improved Euler's method, that will lead us into the Runge-Kutta family of methods.

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So, what I will - first - first do is, take up the geometrical interpretation once again and try to again distinguish between what we were we were trying to do in the numerical integration versus what we are trying to do in the ODE solving; the specific problem that we are going to solve in the ODE solving techniques is, $\frac{dy}{dt} = f(y, t)$ with y given at time t_0 equal to y_0 .

So, what we are interested in doing in case of ODE solving is, we want to find out the value y as a function of t starting with some value of y_0 given at time t_0 . So, we start with this particular value y_0 and then try to get the overall curve y of t as a function of t ; and **this is**, let us say that, if we have an analytical solution for this particular problem, let us say that, that analytical solution that means looks - like - like this particular curve.

So, what we are going to do is, the function $f(y, t)$ at time **at time** t_0 and at the value of y_0 is going to be nothing but this particular slope that we have; this slope is going to be $f(y_0, t_0)$; so, what we are going to do in an ODE solving is, use this particular value of slope in order to predict or in order to move on to the next point, which is going to be (y_1, t_1) .

Now, this particular next point - can either be - can either lie exactly on the actual curve, but usually there are errors that are associated with any numerical technique; so, what is going to happen is that, the next point is not going to be the white point that I have

shown and I am you going to use white curves in order to show the actual curves and I am going to use yellow dots in order to show the numerical solution; so, what will happen in the ODE solver, based on the ODE solver is, we will reach the point which is shown by the yellow x over here; so, over here then the function value $f(y_1, t_1)$ is going to then represent the slope of the numerically computed curve; and based on the slope that we compute over here - from - from time t_1 , we will then move on to time t_2 and - we might - the slope - might - might be like this and then we might end up at this particular yellow point; and we will keep continuing this over and over again and perhaps finally, the curve that will get essentially is perhaps for argument sake looks something like this.

So, this is in the numerical solution; and this is the actual solution to the problem; so, what we are interested in doing when we try to solve an ODE problem is, we are interested in getting the curve y as a function of t . Now, when we are actually solving the integration problem, we are not interested in getting - this - this curve y as a function of t , but instead what we are actually plotting is, we are plotting the function f of t against t .

So, what this function f of t represents is nothing but the slope of this particular curve at various points; and let us say that particular curve there are the slope f of t represents something like this; in that case, the integral from a to b or integral from y_0 to integral from t_0 to t_1 , or rather than same t_1 , let we call it t_n , that integral is going to be the area under this particular curve.

Now, the first difference that we find is that, for the ODE solver we have this function f which can be a function of both y and t ; in case of an integration, it is going to be just a function of t ; that is going to be one difference; the second difference is that, the integral is an area under the curve, whereas in solving the ODE we are actually trying to trace the curve y of t rather than looking at the curve f of t ; that is the other difference between ODE and higher integration; the third difference is that, because this function dy/dt is in general going to be a function of both y and t , the ODE solving method is going to be a more general way of solving these problems, rather than an integration method; that is going to be a third difference between this.

Now, let us look at the PFR problem, now what we physically mean by the plug flow reactor problem is, let us consider that we have a tube of this sort, let a b the area of tube

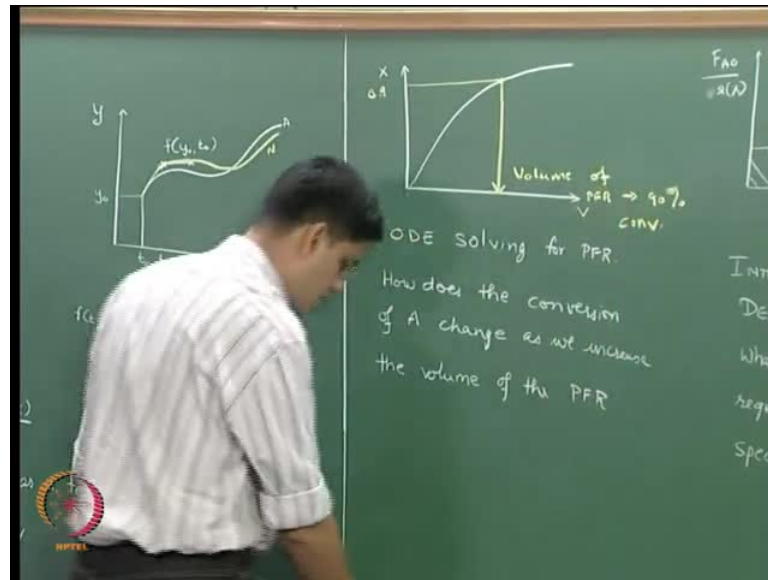
at the inlet, what we have is, **we have the system flowing in...**, we have solution of any particular compound, let us call that compound a and the reaction, let us say, we have the reaction going from a to b and $A_c s$, let us say, is the area of cross section of the tube.

So, the volume is going to be nothing but $A_c s$ multiplied by x , where x is any distance from the inlet. So, what happens is that, **the a where**, the species a keeps getting converted to species b, because of any reaction that takes place within this this particular system; and the overall equation for this system can be represented in the form of $d x$ by $d v$ equal to the rate of reaction r , which is as given as a function of x **divided by** divided by f , so this is what we get as **$d x$** $d x$ by $d v$.

So, now, in the ODE solver, what we are going to do is, we are going to find the conversion, so we are going to find the conversion as a function of the volume of the PFR; if some of you have covered or who have already gone through reaction engineering courses will perhaps recognized, **what**, what I mean by this, if you are not gone through a reaction engineering course, basically I will just give you an overview of what happens as the species a enters into the reactor **- into the reactor -** into the plug flow reactor, it gets converted because of the reaction to the species b; and this particular equation represents how this species a or how quickly this particular species a is going to get converted within the reactor.

So, x represents conversion, that means, how many how much percentage of species a has been converted to species b. So, what we get if we are going to plot conversion against volume; initially, when the concentration of a is high, that means, closer to the inlet, where the concentration of the species a is high the rate of reaction is faster; so, a gets converted very quickly as we move towards the end of the reactor; so, at the inlet, the volume of the reactor is 0, we are starting right at this; as we keep going towards the right, the volume keeps increasing, that is what is happening, that is what this represent.

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Now, as the volume increases, the amount of A that is converted increases; the rate of conversion of A is going to be very fast right in the beginning that is, because there is a lot of A that is available for reactions to take place; as we go towards the other end of the reactor, as the amount of A depletes, the rate of reaction reduces; as a result of this, the conversion curve that we are going to get as a function of volume is perhaps going to look somewhat like this; the rate of reaction is high in the beginning and then it starts to taper off.

Maximum conversion is going to be hundred percent; the conversion cannot exceed hundred percent at any given time. So, in an ODE solving, in ODE solving for a plug flow reactor, the question that we are trying to ask is, how does the conversion of A change as we increase the volume of the reactor. So, this is the question that an ODE solver or while ODE solving we are trying to ask.

Now, the same equation, the same equation we will rewrite it in a different form; what we will do is, we will take dv on this side and f by r will take on to the left hand side and we will write this in the form dx divided by r of x multiplied by f - actually I missed f_{A0} over here - to keep it consistent with the notation that we have used in the previous lecture, f_{A0} multiplied by dx divided by r of x is going to be equal to dv .

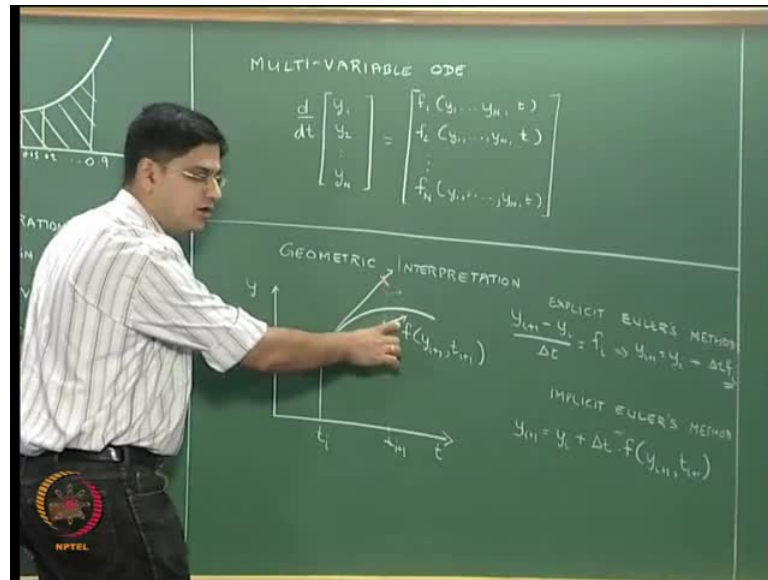
Now, if we are going to plot the $1/r$ as a function of x , in that case the volume that is required to meet a certain conversion is going to be the area under the curve. So, **what we are plotting**, so what we are plotting is $f(x)$ divided by r , **let us**, let us not worry about the negative signs over here as a function of x ; so, what we plot is how the value $f(x)$ divided by r changes as the conversion changes and let us say that particular value changes like this.

So, now, the question is, what is the volume of the PFR that is required in order to meet a certain conversion; **in the**, in the previous module, what we said is, we wanted to get ninety percent conversion, that means, x equal to zero point nine. So, what is the volume that gives you ninety percent conversion; so, the volume that gave us ninety percent conversion was the area under the curve.

So, integration for solving design equation; so, in this case ODE is for solving the PFR equation; integration is also **use can be** used for solving the design equation of the PFR, but the question that we are going to ask is going to put in a slightly different context; and the question that we are going to ask in case of solving the design equation is what volume of PFR required to achieve a specific conversion value.

So, we have now recast the same question in a slightly different way and in that we are asking, what is the volume of PFR that is required to achieve a certain conversion. Now, the question is, how can we use an ODE solver in order to answer the same question; the way we can use the ODE solver in order to answer the same question is, let us look at the point at which conversion is ninety percent.

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So, the point at which conversion is ninety percent and draw the horizontal line over here; the value of the volume that you get over here is the volume of PFR, that gives you ninety percent conversion and I will call this multi-variable ODE; and if we have the equation of the form $\frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} f_1(y_1, y_2, \dots, y_n, t) \\ f_2(y_1, y_2, \dots, y_n, t) \\ \vdots \\ f_n(y_1, y_2, \dots, y_n, t) \end{bmatrix}$ and so on up to y_n equal to f_n of y_1, y_2, \dots, y_n, t .

So, when we have n equations of ODE - of the - of that n differential equations and we want to solve them given n initial conditions $y_1(0), y_2(0), \dots, y_n(0)$ at time $t = 0$; and that particular case, we can easily extend the ODE solving techniques in order to obtain the values of y_1, y_2, \dots, y_n as a function of time t ; so, let this - white - white curve represents the true curve y against t ; and the problem that we are trying to solve is, $\frac{dy}{dt} = \sum f_i$; let t_i be the current time; and y_i is the current value of y .

Now, the slope at this particular point is nothing but the tangent to this curve; so, I am just going to draw the slope over here, so this is the point t_i , let this be the point $t_i + \Delta t$. Now, if we are going to use the slope computed at (y_i, t_i) in order to obtain the solution of y at the point $t_i + \Delta t$, that is going to give us the Euler's explicit method. So, the Euler's explicit method is going to lead us to the point represented by this Red Cross over - over - here.

So, what Euler's explicit method does is, we will write $\frac{dy}{dt}$ as nothing but $y_{i+1} - y_i$ divided by Δt equal to f , I will just write it at this short hand notation f_i , which means, f computed at (y_i, t_i) ; and therefore, from this, we will have $y_{i+1} - y_i = \Delta t \cdot f_i$, where f_i is the slope of the curve computed at (y_i, t_i) .

Now, this leads us to an explicit Euler's method; the next method that we can talk about is an implicit Euler's method; and the implicit Euler's method, we will write it as, $y_{i+1} - y_i = \Delta t \cdot f(y_{i+1}, t_{i+1})$.

So, what **we are** we are doing is, we are trying to find the solution y_{i+1} , such that, the slope that is computed at y_{i+1} is going to be actually the slope that was going to be used over here in order to get the projection. So, what I will do is, I will just guess a particular slope over at this particular point, let us say, I am going to quick guess the slope at over here and see where this particular slope leads me.

Now, this particular slope is going to lead me to a different point over here. So, that is not a solution, so I will then use, let us say, a Newton-Raphson's method in order to again try to solve this particular implicit expression and go on; so, let us say, I will try a slope now, because this point is much higher than this particular point. So, I am going to try a slope which is slightly higher with a slope with of this particular form I perhaps I am going to reach this point.

Now, the slope at this point is, let us say is, going to point in again in this particular direction, so the slope that I have used is this one, where as the slope that is pointing over here is in this particular directions.

So, what I am going to do is, I am going to tend try to project this point over here and I will keep doing the recursively perhaps using a fix point iteration method perhaps using a newton-raphson's method until I get the final solution; at that final solution, let us assume that, final solution is shown by a yellow cross, let us say, this becomes the final solution.

Now, this final solution is, such that, the slope at that point is $f(y_{i+1}, t_{i+1})$ is the slope that we have used in order to reach that point itself; so, what we are seeing over

here is, this particular slope is actually the slope that will be computed at this particular point right over here.

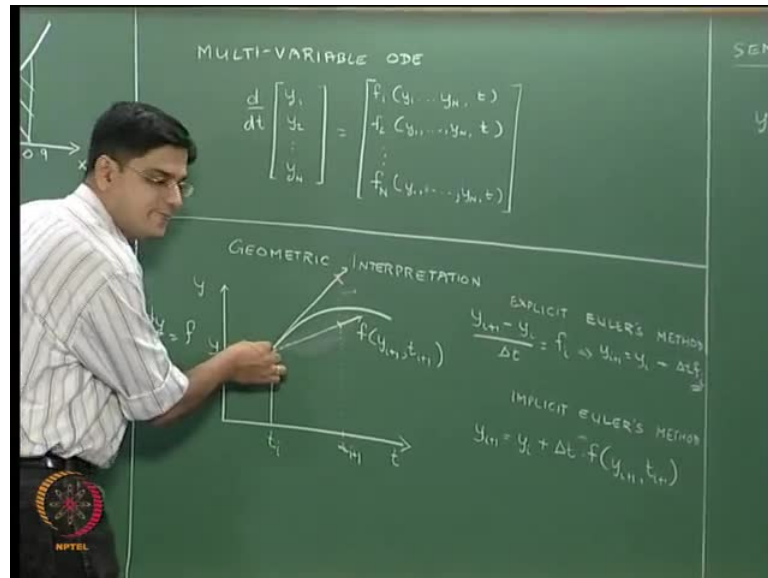
So, this yellow cross is the cross that we get using the Euler's implicit method; the red cross is the cross that we are going to get using the Euler's explicit method. Now, what we can perhaps think of is, we can think of a method which is a semi-implicit method.

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The image shows a chalkboard with three sections of handwritten text. The top section is titled "SEMI-IMPLICIT METHOD" and contains the formula
$$y_{i+1} = y_i + \Delta t \left[\frac{f(y_i, t_i) + f(y_{i+1}, t_{i+1})}{2} \right]$$
. The middle section is titled "EXPLICIT EULER'S METHOD" and contains the formula
$$y_{i+1} = y_i + \Delta t f(y_i, t_i)$$
. The bottom section is titled "IMPLICIT EULER'S METHOD" and contains the formula
$$y_{i+1} = y_i + \Delta t f(y_{i+1}, t_{i+1})$$
. There is a small NPTEL logo in the bottom left corner of the chalkboard.

Now, the semi-implicit method in this particular case is going to be y_{i+1} equal to y_i plus Δt multiplied by $f(y_i, t_i)$ plus $f(y_{i+1}, t_{i+1})$ divided by 2; so you see what I have done over here, what I have done essentially is, taken the slope at the initial time (y_i, t_i) taken, the slope at the solution point y_{i+1}, t_{i+1} taken an average of these slopes; this average is the slope that I am going to use in order to compute the next value y_{i+1} .

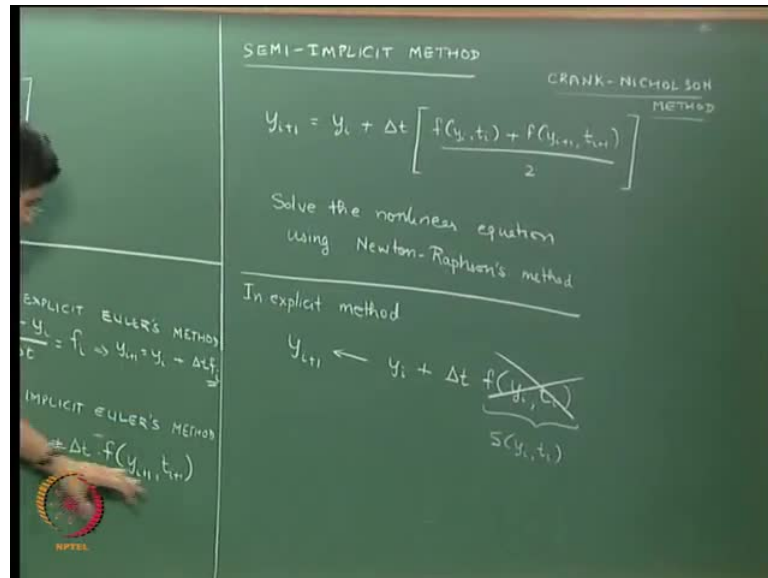
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So, again if we go back over here, slope at (y_i, t_i) is already known to us; this particular quantity is already known to us, this quantities something that is unknown to us currently. So, what we are going to do is, we are going to solve this particular non-linear equation together in order to get the value of y_{i+1} ; and let us say the that, we will use a purple chalk in order and a purple x in order to represent this particular solution; and this particular solution is reached by this purple dotted line now; this purple dotted line if you if you see over here, if that one should be the average of the slope, that is computed at this - excuse me - the slope that is computed over here and the slope that is computed at this point.

Now, the slope computed at this point might be - might - look in this particular way; so, we have, we have the slope computed at y_{i+1} as thus this purple color slope, the slope the slope computed at y_i as this white color slope and the average of the two is the slope, that is shown by the dotted line by by this particular line.

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So, what we do in implicit or semi implicit method is, use this particular equation that I have written over here is as us non-linear equation; and we will solve the non-linear equation using an appropriate means such as the newton-raphson's method, whereas in the explicit method, for example, an explicit method of this type, the right hand side term is use as an expression and y i plus 1 gets that value, that is computed using the right hand side expression.

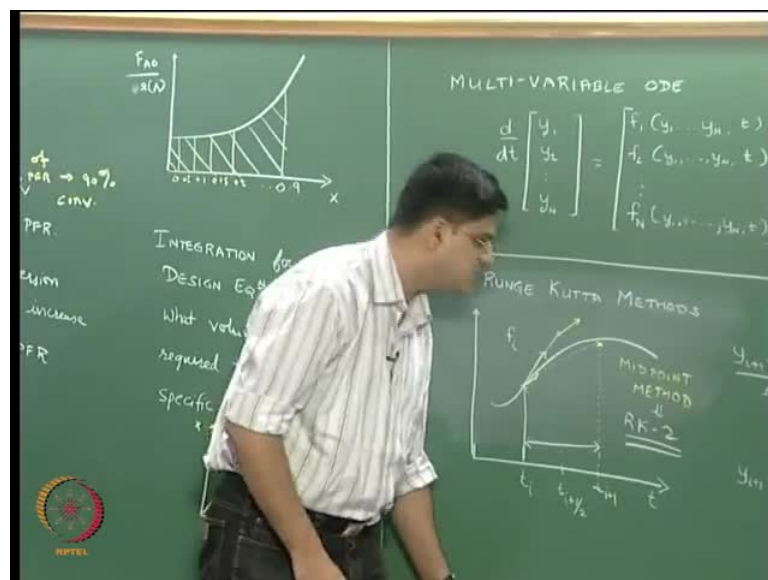
So, I will write y i plus 1 given by y i plus delta t multiplied by f (y i, t i); so, this is the Euler's explicit method; and instead of Euler's explicit method, we will use instead of f (y i, t i); we will use a certain improved slope s (y i, t i); and this improved slope s(y i, t i) can be computed in various ways; one set of ways will give us what is known as Runge-Kutta family of methods and that is what we are going to cover essentially in the next lecture of this particular module.

So, if this particular slope is computed explicitly based on the value of y i and certain other computation and does not depend on the final value y i plus 1, then what we get are explicit methods; if it depends on the final value, y i plus 1 as well as the initial value, y i then we get semi implicit method; and if it depends only on the final value y i plus 1, then we get implicit method; in both implicit and the semi implicit methods, we are going we are going to use non-linear equation solver such as a newton-raphson's method.

The name for this particular semi implicit method is crank-nicholson method; and what we are going to do in either crank-nicholson method or in the implicit Euler's method is to solve the non-linear equation. So, the question is, where does crank-nicholson hide us crank-nicholson method is better than the implicit Euler's method; the reason why crank-nicholson method is better is, it has a greater accuracy than the implicit Euler's method; in the next lecture, we will see that both the explicit Euler's method as well as the implicit Euler's method have an accuracy of delta t to the power 2, whereas the crank-nicholson method, we will see has an accuracy of delta t to the power 3, we will look at various different Runge-Kutta methods; the Runge-Kutta method, that the second order Runge-Kutta method has an accuracy delta t to the power three fourth order; Runge-Kutta method, which is perhaps the most popular Runge-Kutta method has an accuracy of delta t to the power 5; all these things we are going to cover - in the next - in the next lecture.

Now, what is common in the Runge-Kutta family of methods is, something that I will just talk about for a couple of minutes before ending this particular lecture; so, what we did in the - explicit - Euler's explicit method is just computed the slope at y i and use that as the slope s.

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That is not the best that we can do in crank-nicholson method; what we did is, we found out to the slope of y I, we found out the slope at the final point y i plus 1 and then took

an average of the slope; now, this was an implicit method, because we needed to know this, the point y_{i+1} in order to get the slope - slope - at y_i .

Instead of that, we have Runge-Kutta family of methods and I will again draw the curves that I had earlier and this is our slope that is f_i , so what we do in the Runge-Kutta family of methods is that, we choose various different points in this particular interval t_i to t_{i+1} .

In that particular interval, we project the various points based on the slope f_i ; at the projected points not at the final solution, but at the projected points we calculate the new slope and the final $s(y_i, t_i)$ is going to be sum average of the slopes that are computed at this projected points. So, for example, what we will do is based on this particular x , this particular cross f_i computed at this cross we will project the point, let say at the midpoint let us call this as $t_{i+1/2}$.

So, based on this particular curve, we have computed, we have reached, let say this point which I have shown with a circle and an x now, keep in mind that, this particular point with a circle and an x is not the solution $y_{i+1/2}$. This is just a projected point at $y_{i+1/2}$, now what we do is, compute the slope at this particular projected point and let us say that particular slope is shown by the - yellow - yellow line over here.

So, this is the slope computed at the projected point not at the real point; so instead of using this particular white slope, if we were to use this particular yellow slope over here and then go on to point y_{i+1} , we will reach this yellow x ; this particular method is what is known as midpoint method; and this particular technique of finding the slope s as some kind of a weighted average of the initial slope; and the slope at the projected points is known as a Runge-Kutta family of methods; this midpoint methods uses two points in order to - calculate - calculate the slope, the first point is this point (y_i, t_i) .

The second point is the projected value at the time $t_{i+1/2}$; so, we are using these two slopes in order to compute the value of $s(y_i, t_i)$ and that is the reason why the midpoint method is a falls under Runge-Kutta second order method.

So, what we have covered so far is an overview of a numerical method to solve an ODE initial value problem; we gave geometric interpretation of the Euler's implicit method

and Euler's explicit method and then the specifically covered two second order methods. One is an explicit second order method, which is the Runge-Kutta method, specifically we covered the midpoint method and we covered a semi implicit second order method, which is known as the crank-nicholson the methods.