Computational Techniques
Prof. Dr. Niket Kaisare
Department of Chemical Engineering
Indian Institute of Technology, Madras

Module No. # 07
Ordinary Differential Equations
Lecture No. # 02
(Initial Value Problems)

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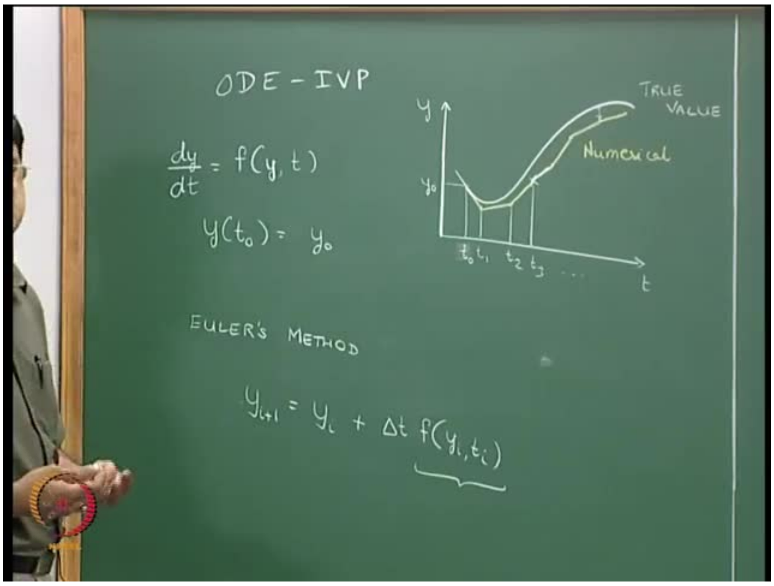

Hello and welcome to lecture 2 of module 7, where we are discussing ordinary differential equations - the initial value problem. What we did in yesterdays lecture is to go over the geometric motivation behind the numerical methods for solving an initial value problem - ODE-IVP, initial value problem - is what we are trying to consider in this particular module.

So, the problem that we are trying to solve is of the form d y by d t equal to some function f(y, t) and given y at - some time - t 0 is equal to a value y 0; and what we are interested in getting is the curve how the value y changes with the time t.

So, let us say, the actual curve looks something like this; and let us say, we are going to start with - say, y 0 value - t 0 value over here and the corresponding value is y 0. So, what we are going to do in the numerical method to solve this ordinary differential equation is, to figure out what the next value of y is going to be as we progress forward in t.

So, perhaps, the way we will progress is will go from this point to this point; so, as the time t progress from t 0 to t 1 to t 2 t 3 and so on, we are going to get the yellow curve - the yellow curve is the numerical solution; and the white curve over here is the true value; and as we have been doing throughout this particular set of lectures, a difference between the true value and the numerical solution is the error. And the objective of the ODE solving technique that, the several ODE solving techniques that we are going to consider in the next - next - few lectures is to, we want to use a method that is going to minimize this particular error - this particular deviation - between the numerical value and the true value of that integral.

So, this was the - the - idea behind using this - this - numerical technique. Then we considered a simplest form of numerical solution to ODE is and that was the Euler's forward difference method. And in Euler's method what we, the expression for Euler's explicit method was written as, y at i plus 1 equal to y i plus delta t multiplied by f(y i, t i).

So, where f is nothing but the slope, that is computed at the point y i t i; so, if we look at or if we look at say any point y i t i at this particular location, we find out the slope of the curve, that is, function f at - y y 3 - y 3 t 3, that is the value of f that we get, that multiplied by the difference - delta a - delta t will give you essentially the next point where we are going to reach. So, that is, what the Euler's methods tries to do is, find out the slope to that particular curve and then move along - that - that slope and that slope is nothing but, some function f - the same function f of y i t i. So, that is the Euler's method; what we said next is that, instead of the function f computed at y i t i, we can find a better way of getting this value of the slope.

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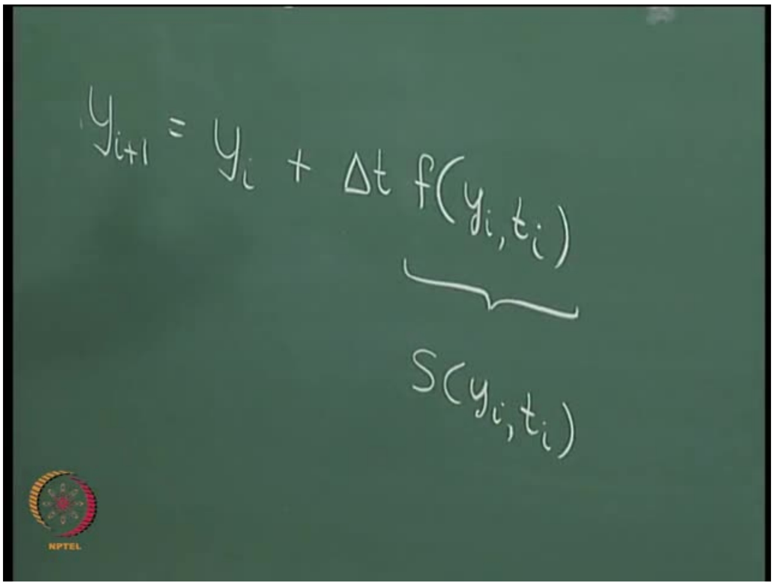

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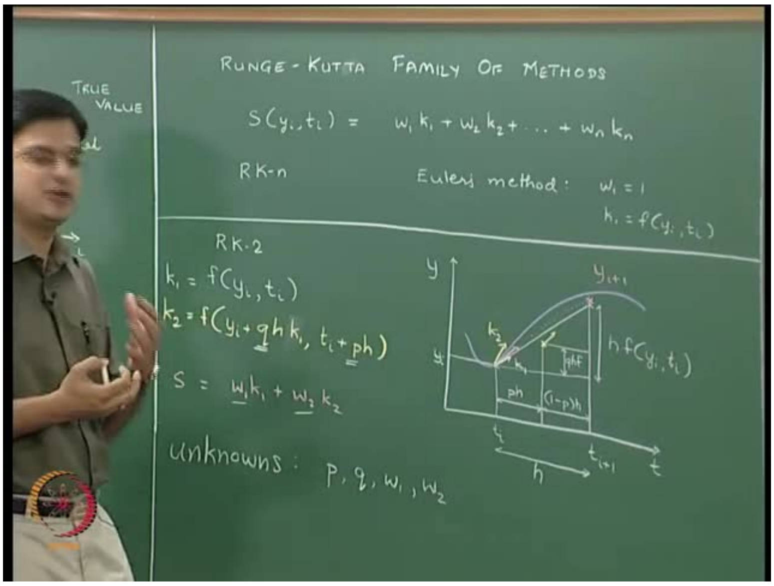

So, instead of f of y i t i, we replace that with s(y i, t i); and then we concluded the previous lecture, lecture 1 of module 7, we concluded by saying that there are several methods which incorporate different ways of finding this particular s; and one family of the methods is known as the Runge-Kutta family of methods.

So, in Runge-Kutta family of methods, what we do is, we express our s(y i, t i) as - some, weighted some or - weighted some of slopes computed at various points in the interval going from t i to t i plus 1; so, we will write that as, w 1 k 1 plus w 2 k 2 and so on up to w n k n; this is going to be the expression - a general expression - for an nth order R K method, Which is, which will represent as R K-n. Euler's method in one way we can call that as the first order Runge-Kutta method, because in Euler's methods we do not - did not - have k 2, k 3, and so on up to k n, we only had w 1 k 1; and for Euler's method, w 1 was equal to 1, and k 1 was equal to nothing but f (y i, t i), that was the Euler's method.

So, when we substitute w equal to 1 and k 1 equal to f, we will get s as - nothing but - equal to f at y i t i and that is really what we see as the Euler's method for solving the ODE - the numerical solution for the ODE.

Next, what I am going to do is, I am going to talk about second order R K methods; that means, we will talk about R K 2 methods, we will look at the geometric interpretation and then we will derive the expression for the - R K - R K 2 method using the Taylor's series expansion.

The reason why I am going to consider R K 2 method is, that it is going to be relatively easier to explain and to understand; I am not going to consider R K 3, R K 4 methods and higher order R K methods, but only give you the final results towards the end of this particular lecture, that is how we are going to progress in this lecture.

So, now the idea behind the R K 2 method, let us look at the geometric interpretation of word R K 2 methods again, again we will draw the curve, the true curve, y against t and this time I will just use a purple chalk to draw that - that - true curve y against t.

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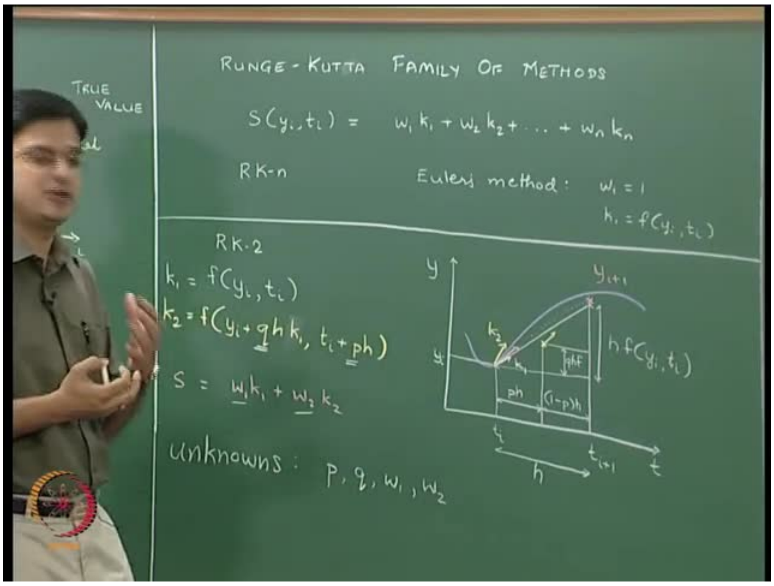

Let us say the curve looks something like this; and let us say, the current value of y i is at this particular location, this is t i, and the corresponding value of the - the - dependent variable y is y i; and now we are interested in using better method in order to find y i plus 1 at another time say t i plus 1, I will, instead of calling the difference between t i and t i plus 1 as delta t, I will just call this h, h is nothing but - but the - the delta t that we have use so far.

The reason why I am going to use h over here rather than delta t is simply because writing all the expression in terms of delta t, is going to be just a little bit more tire some job with h, it is actually which is going to be a little bit simpler with from notational point of view. But for all practical purposes, there is absolutely no difference between h and the delta t that we had used in the previous lecture and also in this particular lecture so far.

So, now, what we did with respect to the Euler's method was, we found the function f (t i, y i) and that function was nothing but this particular slope. So, let us just draw this particular line as the slope that has been computed at (y i, t i); so, what we did in Euler's method was, just use that slope projected up to the point at the time t i plus 1 and this particular guy we said was, nothing but, our y i plus 1 and then we progressed.

What happens is, that particular way of solving ODE is not accurate enough; as we will see later on in this particular lecture that gives us h to the power 2 accuracy whereas the Runge-Kutta methods tend to give us a - much - much more accurate way of solving this problem.

So, now, if we look at the overall geometry, what we will do is will just complete this particular triangle over here, this distance is nothing but y i plus 1 minus y i; and y i plus 1 minus y i was nothing but f (y i, t i) multiplied by delta t; in this case, instead of delta t we are using the term h.

So, this distance is nothing but h multiplied by f (y i, t i); now, what we do in Runge-Kutta method is that, you we consider a virtual box over here, where a virtual rectangle over here, where this is the - the - lower edge of the rectangle and this is the right edge of the rectangle and you can just consider - you know - a rectangle, that is formed from right over here; and then we choose a point with in that particular rectangle.

We can…, we are free to choose the point anywhere in - in - that rectangle for now and then we will try to figure out a better - a numerically better - way in order to figure out exactly where we are going to locate that point. So, let us say, we are going to locate a point somewhere over here, the x, the t coordinate for this - this - particular point, let us say, is going to be p multiplied by h.

So, we will just drop this particular vertical line over here and we will call this…, this is distance is nothing but p multiplied by h and this distance is, of course, going to be 1 minus p multiplied by h. Likewise, the vertical distances, we will call them as q multiplied by h multiplied by f and 1 minus q multiplied by h multiplied by f.

So, now, what we have is, we used the function f (y i, t i) in order to find the projection along this particular line, there is a white line represents the projection on t i plus 1 along the line or which has a slope f (y i, t i).

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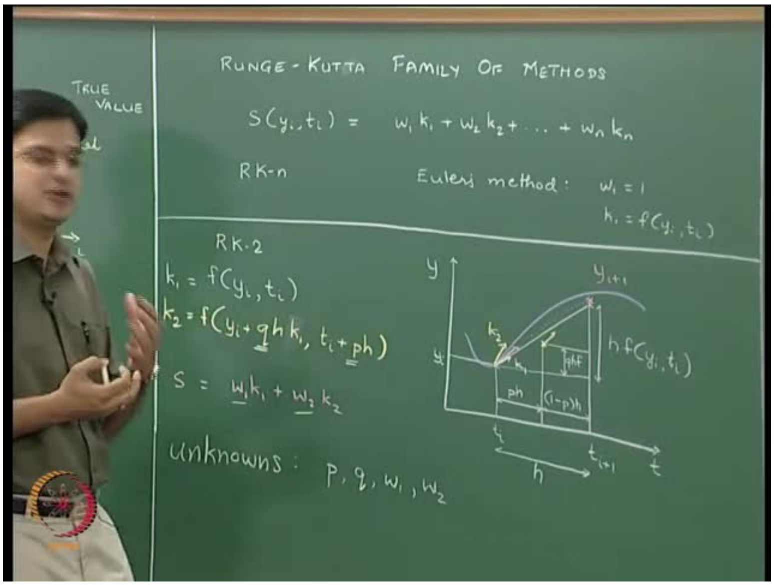

Then we got this particular virtual rectangle and in that virtual rectangle we randomly choose a point which is shown by…, I have just converted into a yellow x over here. So, we randomly choose this particular point; now, this point is at - at - a fractional distance of p from t i and a fractional distance q from y i. So, that is where this point is located. Now, what we are going to do is, we are going to find the function value f computed at this particular point.

So, that function value is going to be f computed at y i - y i plus q multiplied by h multiplied by f - plus q multiplied by h multiplied by f, that is the y coordinate for the computing the function; the t coordinate for computing the function is going to be t i plus p times h. So, this is t i plus p times h, that is the t component; and y i plus q h f is going to be the y component; so, this is the slope that is computed at this yellow point.

So, the slope computed at this yellow point, perhaps, is going to look somewhat like this; so, the slope computed at the point y i t i is this white arrow over here; the slope that is computed at this yellow x, we are going to just show that, as this yellow arrow; and what Runge-Kutta method is - Runge-Kutta second order method is - going to do is to find some kind of a weighted sum of this slope multiplied by w 1 plus this slope multiplied by w 2; and that weighted slope is what the R K 2 method, is going to use in order to project the point in the future; and the point that i am representing by the red x is going to be our y i plus 1.

So, that is thing going to be the geometric interpretation of the Runge-Kutta method. The red arrow that i have shown over here is a weighted sum of the white arrow, w 1 multiplied by the white arrow plus w 2 multiplied by the yellow arrow. So, the white arrow we are going to represent as k 1; and the yellow arrow we are going to represent as k 2; so, I am going to say k 2 is going to be equal to f of this guy and am going to write k 1 is going to be equal to f (y i, t i).

So, f is nothing but k 1 is nothing but the slope computed at (y i, t i); keep in mind that, what we are doing over here is, we are using y i plus q times h times f, I computed at (y i, t i), f computed at (y i, t i), is nothing but k 1. So, am going to erase this f that i had written over here and write this as k 1; now, this becomes the Runge-Kutta, the 2 slopes required in using the Runge-Kutta second order method and the actual s is going to be equal to nothing but weight w 1 multiplied by k 1 plus a weight w 2 multiplied by k 2.

So, now, let us look at the unknown quantities that are there in the R K 2 method, which we need to now figure out how to find these unknown quantities. The unknown quantities, of course, are the two weights w 1 and w 2 as well as this particular fractional distances p and q.

So, these are the four unknown quantities; and we need to figure out a way how to find these unknown quantities. When it comes to numerical techniques or computational techniques course, one of the things that i use to joke with my students was - was - essentially that, whenever we need to find out ways to get these unknown quantities, if you do not know anything else just use the Taylor series expansion, this perhaps most of the approximations are based on the Taylor series expansion for - for - most of the things that - we we have - we are going to look into in this computational techniques course.

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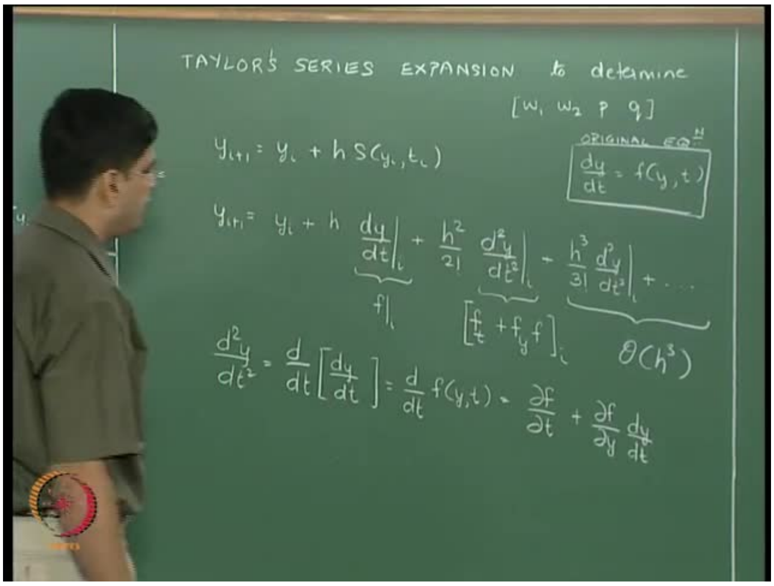

So, again will resort to the same Taylor series expansion; so, again we are going to resort to the Taylor series expansion in order to determine what values this should w 1 w 2 p and q take for the R K 2 - the second order R K method. So, the - the - formula that - we are - we are interested in getting is y i plus 1 equal to y i plus h times s (y i, p i); that is the formula we are interested in getting. So, one obvious thing that we are going to do is, expand or get a Taylor series expansion for y i plus 1 around the value at - y - y i.

So, y i plus 1 is going to be equal to y i plus delta multiplied by d y i by d t plus delta squared multiplied by - d y i - d y i squared by d t squared and so on and so forth; what that delta is, the delta is nothing but our h. So, y i plus 1 is going to be equal to y i plus h multiplied by d y by d t computed at y i plus h square by 2 factorial d square y by d t squared computed at i plus h cube by 3 factorial d 3 y by d t 3 at i plus so on and so forth.

Now, d y by d t computed at i is nothing but f (y i, t i); recollect that what the equation that we are trying to solve, use the ODE that we are going to trying to solve is nothing but f (y, t).

So, this is the original - equation - problem that we are trying to solve; so, d y by d t computed at i is nothing but the value f computed at the location I, the f computed at y i, t i. Now, the next question is, what is d square y by d t square that is something that we need to find - use - using integration, using the differentiation by parts.

So, we will have d square y by d t square, the chain rule that will implement is going to be, d by d t of d y by d t or that is going to be d by d t of f (y, t), which is, which is going to be nothing but dou f by dou t multiplied by d t by d t and d t by d t is 1 plus dou f by dou y d y by d t. The chain rule is going to be, d by d t of f is dou f by dou t d t by d t plus dou f by dou y d y by d t and d y by d t as nothing but our function f.

So, d square y by d t squared is nothing but partial f by partial t, I will - write that - the write that down as f t plus partial f by partial y, I will write that as f y, multiplied by f computed at (y i, t i). So, that is going to be d 2 i by d t squared and so on and so forth. For R K 2 method, we do not need to expand this particular term; so, this particular term, all these terms I will just write them as o h cube.

So, if we discard all this terms, the order of accuracy that we are going to get is the accuracy of h to the power 3; what - what - we will show in a few minutes from now is that indeed, these are terms that we are going to discard, these are the terms that we are going to retain, and therefore, the R K 2 method has an accuracy of order of h cube.

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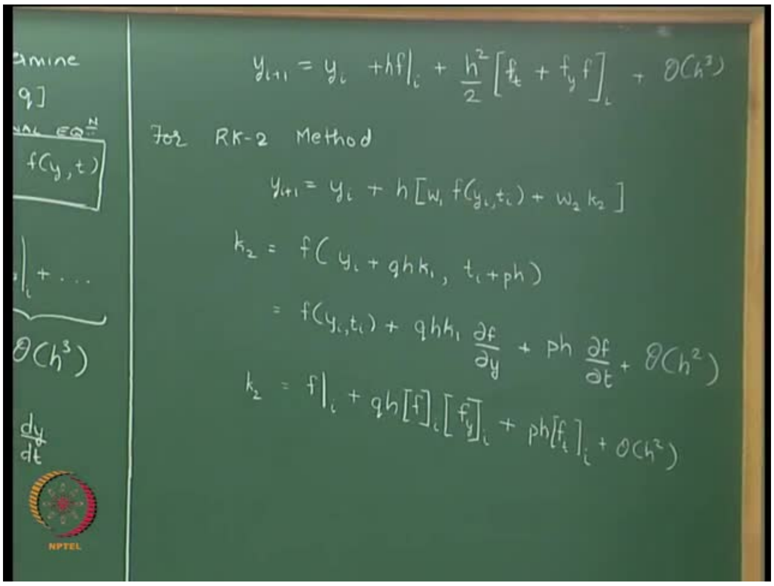

So, this is the equation, one equation - that - that we have obtained; and that - we will – I will just write that down over here, y i plus 1 is going to be equal to y i plus f computed at (y i, t i) f computed at i multiplied by h plus h square by 2 factorial or h square by 2 multiplied by f of t multiplied by f of t plus f of y multiplied by f computed at (y i, t i) plus order h cube; what i have done is, I have just written down this particular expression over here - all over again.

So, this is the Taylor series expansion for the true value - at y i - at y i plus 1. Now, let us go back to the type of problem that we are trying to solve using the Runge-Kutta method; the problem that we are - going to - trying to solve with the runge-gutta method is, y i plus 1 equal to y i plus h times s, where s is w 1 k 1 plus w 2 k 2; so, we will write that down for R K two method, for R K two method y i plus 1 is y i plus h times w 1 k 1 and k one was nothing but f computed at (y i, t i).

So, I will just write that down f computed at (y i, t i) plus w 2 k 2; so, this is what - what - we have; now, k 2, we will also write down the expression for k 2, we go back over here and we find that the expression for k 2 is f at y i plus q h k 1, t plus p h. So, in a time, we have t i plus p multiplied by the delta t and in space - in sorry - in y - in in - the dependent variable we have y i plus q multiplied by delta y and delta y is nothing but h multiplied by k 1.

So, k 2 is going to be f computed at y i plus q h k 1, t i plus p h; now, for this, again we can use our Taylor series expansion, and of course, the Taylor series expansion is going to be around f (y i, t i). So, this - we - can be written as f (y i, t i) plus we have q h k 1 multiplied by partial f by partial y plus p h multiplied by partial f by partial t.

So, this is the 0th order term, these are the first order term in y and in t respectively, and we have the second order term; for now, we are going to ignore the second order term and we will just write them down as the error term; and the error is of the order h squared. We will have h squared multiplied by d square f by d y square h h square multiplied by d f d y d square f by d y d t; and then will have a term in d square f by d t square; all those three terms will be there that would be the second order term, then we will have third order term, fourth order term, so on and so forth; all those we have club them as order of h square.

So, now, what we can do f (y i, t i), we will just write this as f computed at i plus q multiplied by h multiplied by k 1; remember k 1 was nothing but f (y i, t i). So, we will write this as, f computed at i multiplied by f y, that is partial f by partial y, computed again at (y i, t i); so, this is what we get. For this particular term and for this term, we will have p multiplied by h multiplied by f of t computed at i. So, that is what k 2 is going to be; so, what now I will do is, I will take this k 2 and substituted over here and then we will do the further expansion.

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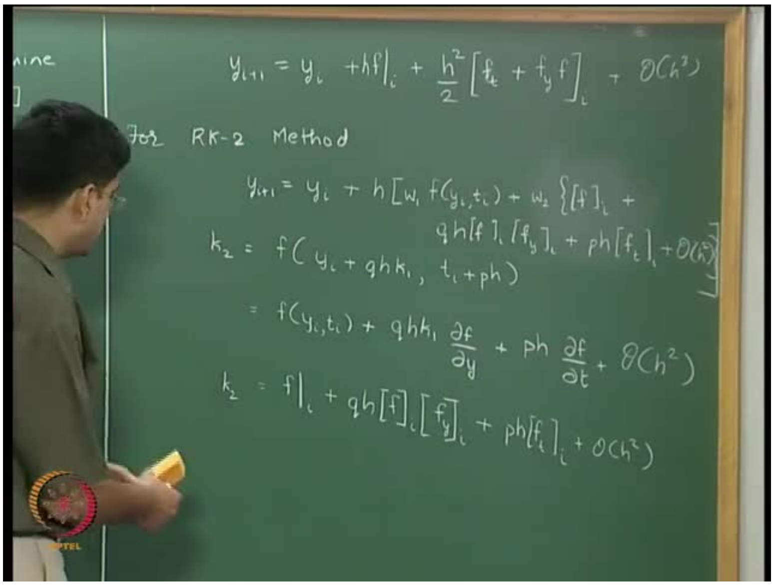

So, I am going to replace this k 2 by this particular Taylor series expansion; so, it is going to be w 2 multiplied by f computed at i plus q h multiplied by f and multiplied by f y plus p h multiplied by f t at i plus o of x squared. So, this is what we will get for our R K two method as y i plus 1 as y i plus h multiplied by the first slope plus the w 2 multiplied by the second slope; in the second slope, again we have use the Taylor series expansion.

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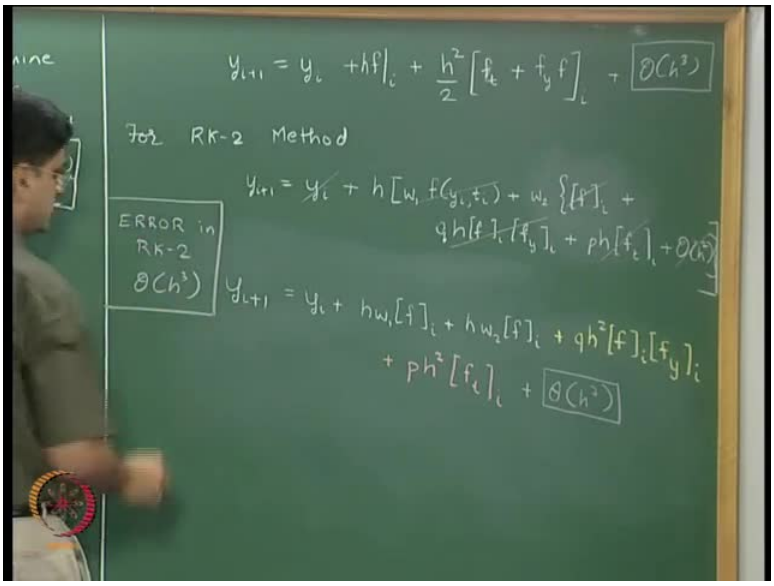

What I will do is, I will erase this, this part that i have written over here and I will continue with the derivation; so, this can be written as, now we will have this term y I, the next term is going to be in terms of f of i. So, what we will do is, collect all the terms involving f i only, not d f by d t, not d f by d y, but only the term containing f computed at (y i, t i).

So, we have h multiplied by w 1 multiplied by f computed by at (y i, t i); so, we will have this h multiplied by w 1 multiplied by f computed at i plus the other term that is computed by i is h multiplied by w 2 multiplied by f computed at i h w 2 multiplied by f computed at i.

So, what I will do is, I will just strike out these two term, so that we know that we have taken care of those terms in this particular equation, then i will collect the terms in f i multiplied by f y i, that means, function f computed at (y i, t i) multiplied by dou f by dou y computed at (y i, t i) and I will write that with yellow color chalk.

So, this is h multiplied by q multiplied by h multiplied by f multiplied by f y; so, that is q h squared f I and f y i not f t f y i; so, I will just again with thin with a thin yellow strike i will just cut this particular value of as well.

Now, i have the terms that are remaining are these two terms, I will write down these two terms with red and purple color chalks, so this is going to be h multiplied by p multiplied by h multiplied by f t. So, that is p h squared multiplied by f t computed at (y i, t i); that is the - red - red guy over there and I will just strike of that red guy. And the final term is going to be h multiplied by order of h squared and that we are going to write as order of h cubed; what does order of h square means, that the leading error term has h square multiplied by some other quantities.

Now, h squared multiplied by h multiplied by some other quantities leads us to h cubed multiplied by the same other quantities; so, the order of h cube represents that, is the leading term that we are going to throw away if we do not incorporate; if we only incorporate the terms in white yellow and pink in our final expression will just strike this out as well.

So, y i plus 1 for the R K 2 approximation is going to be of the form y i plus, this guy plus this guy plus this plus this and the terms that we are going to throw away; the Taylor series expansion for y i plus 1 is this plus this plus this, and this is the term that we are going to throw away.

So, the term that we are going to throw away - keep in mind - is order of h cubed; so, I will write this down, write now, now what we see over here is that the term that we are.., the terms that we are going to throw away the leading term in that is of order of h cube, the leading term in the term that we are going to throw away here also is of the order of h cube.

So, I will write down this information right away and I will say that error in R K 2 is order of h cube, so we will keep this information for future; and right now we are not going to worry about this particular term. So, I will just erase this slightly so that it is not very visible to us, so it is there on the board, but we do not have to worry too much about it.

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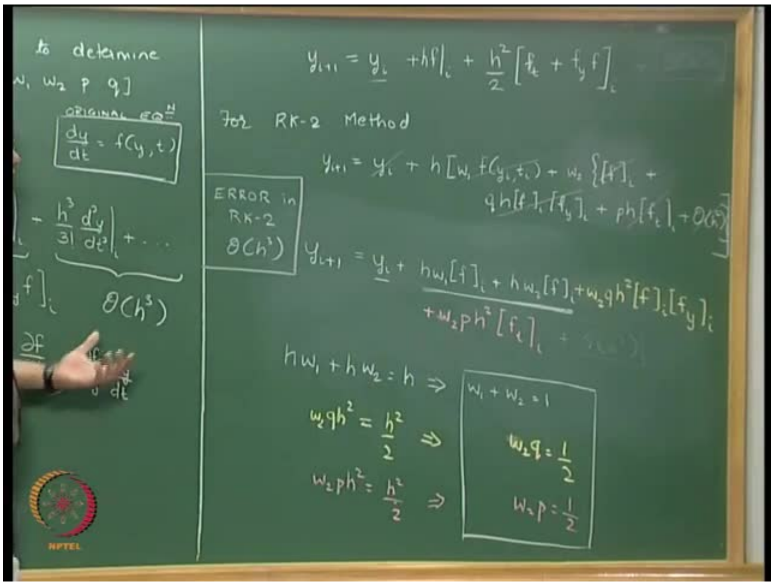

Now, we are going to compare the individual terms in this expression and in this expression; now, these terms are the same we do not have to worry about it; now, there is a term in h multiplied by f I, and the terms in h f i are basically these terms over - over - here. So, for this expression, to represent closely the approximation that we get using the Taylor series expansion, the coefficients over here have to be the same as the coefficient over there.

So, for the white color guy that we have over here, the coefficient is going to be h multiplied by w 1 plus h multiplied by w 2 and that is going to be equal to h; so, that is the first equation, w 1 plus w 2 equal to 1. Now, let look at the yellow color term, the yellow term over here is q multiplied by h squared, the corresponding term in the Taylor series expansion should have f multiplied by f y at a both computed at i.

So, we have f multiplied by f y computed at i, the coefficient for that term is h squared; so, we will write q h squared equal to h squared divided by 2 factorial and that would give us…, I think I missed out the w factor over here; so, the w 2 factor i have missed out, I will just write that down right now; and likewise, i have miss the w 2 factor over here also, w 2 multiplied by p h square multiplied by f of t.

So, what we get? The next equation that we are going to get over here is going to be w 2 q will be equal to 1 by 2; and the third expression that we are going to get is, w 2 p h squared is going to be equal to h squared by 2. So, the three equations that we get for the R K two method are these expressions; and when we ensure w 1 w 2 p and q satisfy these equations, the are, the method that we are going to get is - has an is - going to have an error of the order of h cube.

So, that is the whole idea behind R K 2. Now, one thing that you will notice in R K 2 is that, we have four unknowns w 1, w 2, p, and q but we only have three equations; what that means is that, we are now free to choose any one of the parameters according to our choice and based on that particular choice will have various different R K 2 methods.

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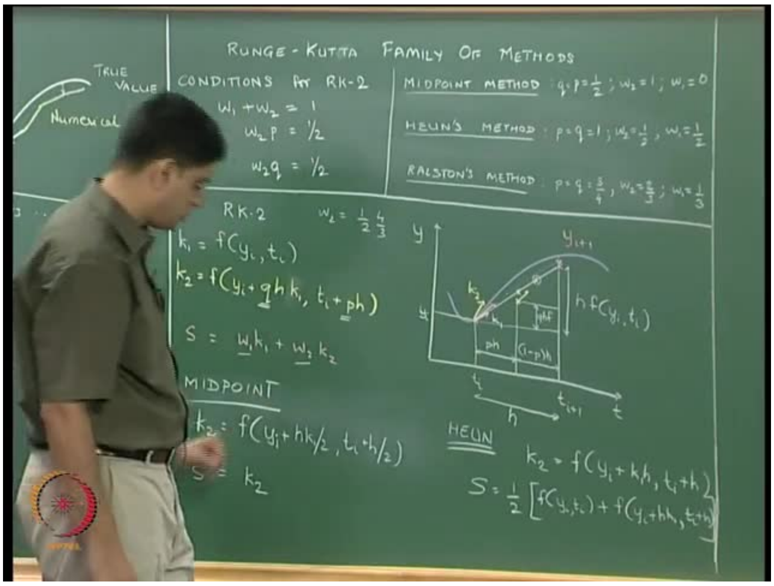

So, let us now go back to our geometric interpretation and see the various different R K 2 methods that we are going to get; so, what I have done is, all these conditions w 1 plus w 2 equal to 1 w 2 q equal to half and w 2 p equal to half, I have written it down over here; and let us look at the various different methods - that - that can come out - of of this - of this particular scheme.

The first method is what we had considered towards the end of the previous lecture and that method was the midpoint method; so, in midpoint method, if you recollect what we did in the previous lecture is, we said that this point is going to be mid-way between t i and t i plus 1, we took this point as t i plus half.

What that means is that, p is going to be equal to half, 1 minus p is also going to be equal to half; for midpoint method, what we choose was, we choose p equal to half, when we choose p equal to half; our w 2 is going to be equal to 1; and our w 1 is going to be equal to 0 from this particular equation; and our q is also going to be equal to half.

So, q is going to be equal to p is going to be equal to half; so, the midpoint method that we talked about yesterday was that, we discard the k 1 completely, we only use k 2 and we have…, we are calculating k 2 at the midpoint between t i and t i plus 1, that was the midpoint method that we obtained.

So, I will write down the expression for midpoint method, y i plus h k 1 by 2, t i plus h by 2 and s is going to be equal to k 2. So, the slope that we will use for midpoint method is nothing but the slope that is computed at the midpoint; and since p is going to be equal to q, these points are going to lie on this particular line always; that is one thing that we will see from the R K 2 methods, is that, if we look at these two equations, p is always going to be equal to q; what it geometrically means, when we say p equal to q is that the yellow cross that we had shown at an arbitrarily location in this particular rectangle.

For R K 2 method does not appear at an arbitrary location with it always appears on this particular line segment, that joins y i plus 1 (y i, t i) and has a slope equal to f (y i, t i). So, this point is always going to lie on this particular curve; that is one of the things that we get out of the derivation for the R K 2 method. The second possibility is, what is known as Heun's method; this Heun's method we will show later; this - kind of similar in a in some the idea is - kind of similar to our trapezoidal method for doing the integration.

In Heun's method, what is, what we do is, we choose our p equal to 1; that means, the slope first k 1 is of course computed at this point; the slope k 2 is computed at the projected point, which is going to be f of y i plus h k 1, t i plus h. So, for the Heun's method, our k 2 is going to be equal to f of y i plus k 1 h, t i plus h, that is what the value of k 2 is going to be; so, the p is going to be equal to q is going to be equal to 1.

If p is 1, our w 2 is going to be equal to half; and if w 2 is half, our w 1 is going to be equal to half as well.

So, w 2 is half and w 1 is also half; so, Heun's method that we are going to get is going to be s is going to be half of f (y i, t i) plus f of y i plus h k 1, t i plus h; why i said that is, it is kind of equivalent to the trapezoidal method, because the slope at this particular…, the red slope that we compute over here is nothing but an average of the slope k 1 that is computed at this point and slope k 2 that is computed at this particular point.

So, that is going to be our Heun's method. There is another method called Ralston's method; and in Ralston's method p and q are chosen as equal to 3 by 4; and when p is going to be equal to 3 by 4, our w 2… So, w 2 is going to be 1 by 2 multiplied by 4 by 3, which is going to be 2 by 3; so, w 2 will be 2 by 3, and w 1 is going to be 1 by 3.

So, in Ralston's method, what - what - we do is, we take the slope, the white slope over here, the point that is projected is going to lie three quarters of its way towards ah this particular - vertical - vertical line, that is where this particular guy is going to lie; then we will find out the slope at this particular point; and the red slope is going to be an - average - weighted average of k 1 and k 2; the weight for k 1 is going to be one third, and the weight for k 2 is going to be two third; so, this is essentially what I wanted to cover with respect to R K 2 method.

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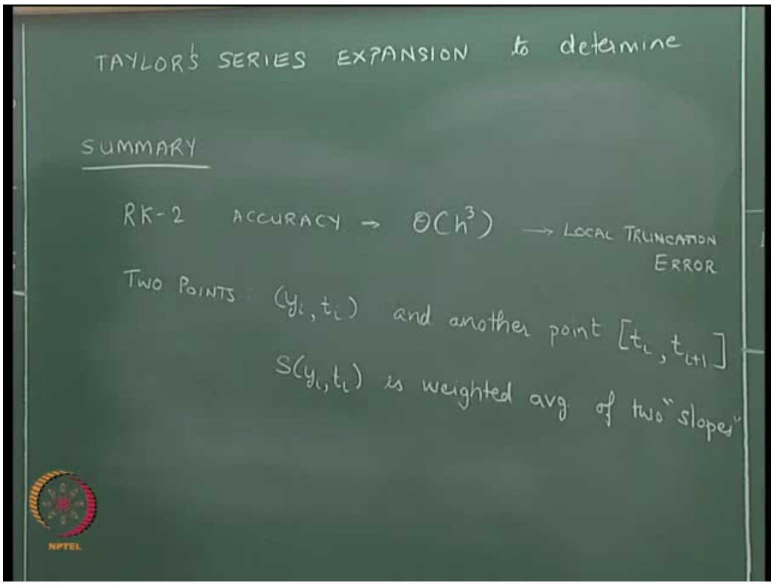

The R K 2 methods have an accuracy of order of h cube and this is nothing but the truncation error, we are not talked about the round off errors. There are two types of errors that we have always been saying in this entire series of lectures - the first one is the truncation error and the second one is the round off error. In case of ODE numerical solutions of ODE, there are actually two types of truncation errors; and this particular truncation error is known as local truncation error.

The other type of error is known as the global truncation error; we would not talk about the global and truncation error is in this lecture, we will come…, we will cover them in in subsequent lectures. So, the R K 2, the accuracy is of order of h cube, it uses two points, (y i, t i) and another point between t i and t i plus 1 in order to compute the slope; so, the slope is computed as the weighted average of the two slopes; the first slope computed at (y i, t i); and the second slope computed at an appropriate location between t i and t i plus 1 lying on the straight line with a slope equal to k 1 connecting t i to the curve point in t i plus 1; so, the second point lies along this particular line - line – itself; and the three expressions that the R K 2 conditions are going to satisfy or w 1 plus w 2 equal to 1, w 1 w 2 multiplied by p equal to half and p equal to q, so - that - those are the method, those are the things, that R K 2 method are is going to satisfy; so, that finishes today's lecture. In - the in - lecture 3 in this particular module, what we are going to cover? We are going to consider is now that, we have derived the overall expressions for R K 2 method, I will quickly derive the expression for the Euler's method and show that the Euler's method is less accurate than the R K 2 method.

I will then talk about higher order R K methods and describe, how to get, how to derive these higher order R K methods; and I will talk about why an a fourth order R K method is actually the most popular method and after that we will go on to Microsoft excel and pick up the example, the plug flow reactor example, that we had done during the six module; I will take up that particular example and solve it using the Euler's method and using the R K 2 method; and we will see the effect of changing the steps size h on the accuracy of the solution that we are going to get. Thanks.