Computational Techniques

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

Module No. # 07

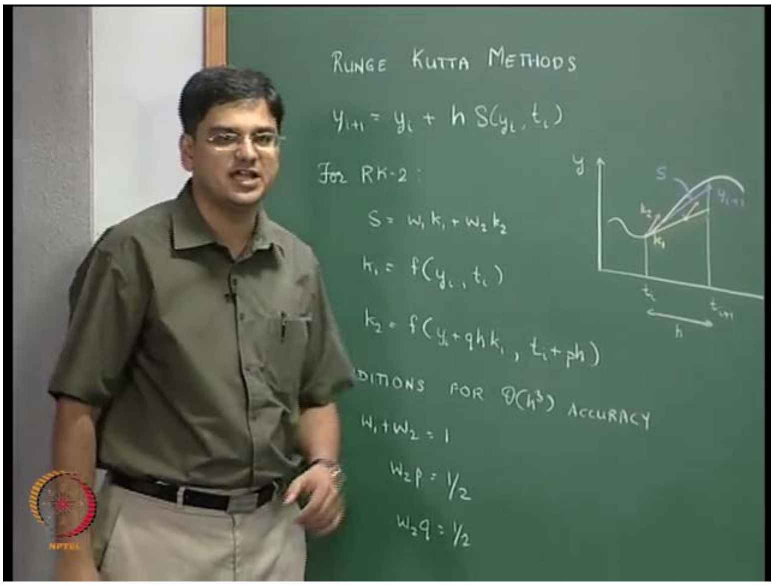
Lecture No. # 03

Ordinary Differential Equations

(Initial Value Problems)

Hi and welcome to lecture 3 of module 7, where we are considering ordinary differential equations initial value problem. So far in the first two lectures, we have looked at what we mean by the numerical solution of ordinary differential equations; we considered Euler's method - Euler's implicit and Euler's explicit method - and then, in the previous lecture 2, we moved onto Runge-kutta methods, specifically we talked about the second order r k method.

(Refer Slide Time: 00:48)



So, let me just go over some of the results of the r k - 2 methods that we derived in the previous lecture. So, the r k - 2 method in we are going to obtain our y i plus 1 is going to be equal to y i plus h multiplied by sum slope s computed explicitly based on the values of y i and t i, that means, we are not going to use the value of y i plus 1 in order to compute this slope S. For r k - 2, we choose the slope s as a weighted sum of the slopes computed at two specific points within the overall interval. So, S we wrote that as equal to w 1 k 1 plus w 2 to k 2, where k 1 was equal to function f computed at (y i, t i) and k 2 was f computed at y i plus sum value q multiplied by h multiplied by k 1, t i plus some value p multiplied by h. So that was our k 1 and k 2.

And the conditions that we derive, We derived certain set of conditions for r k - 2 method and those conditions gave us the order of accuracy as h to the power 3 and those conditions, were w 1 plus w 2 equal to 1; w 2 times p equal to 1 by 2; and w 2 times q equal to also 1 by 2. And based on these two equations, we said that p equal to q is one equation; w 1 plus w 2 is equal to 1 is the other equation; and w 2 p equal to half can be the third equation.

So, p is equal to q is one of the things that we obtained in the Runge-kutta method - second order runge-kutta method - and the geometric interpretation of the second order Runge-kutta method is when you are going to plot y against t and we have any arbitrary curve of this sort and let this be t i and let this be t i plus 1, which with the difference between the two being equal to the step size h.

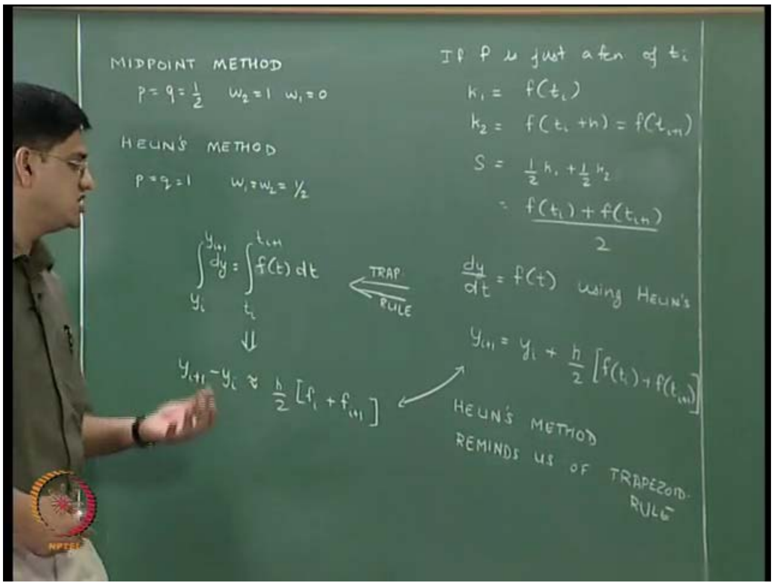
And that time k 1 is nothing but the slope computed at this particular location and that slope is represented by this particular yellow line and that is going to be our k 1. And we take certain point not at an arbitrary location, but… may be this particular line does not exactly represent the slope very well; I will just redraw that line.

So, now, we have this particular guy as k 1 and then, what we said is, now we select one point and this particular condition tells us that this particular point is going to be selected somewhere along this line not an arbitrary location in this rectangle, but somewhere around that line, perhaps over here and then, we compute the slope at that particular x that particular point and that slope let us say is this guy and that is going to be our k 2.

And thus the value of S that we are going to consider is going to be a weighted average of k 1 and k 2 and that value might look somewhat like this, and this is going to be point y i plus 1 that we will get, and this the slope of this purple line is going to be nothing but S.

So, this is the geometric interpretation of the r k - 2 method. So, the yellow that I have shown over here is the geometric interpretation of the Euler's method; the purple line that I have shown over here is the geometric interpretation of r k - 2 method.

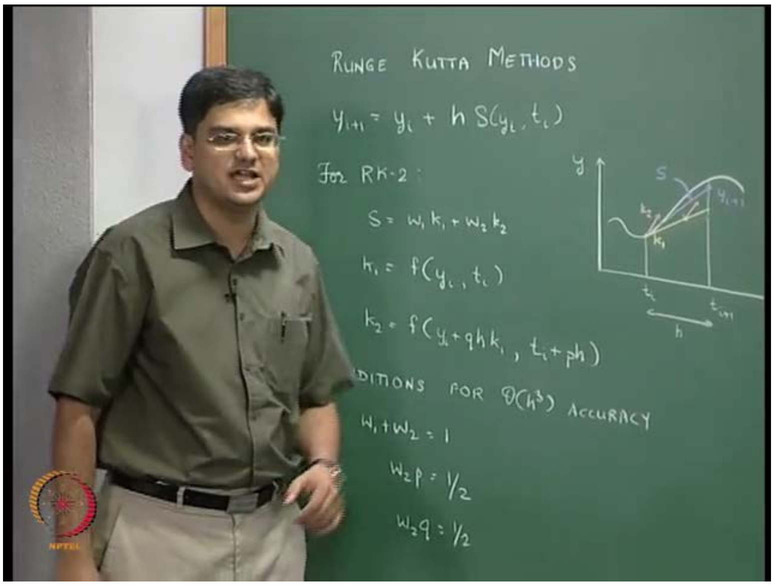
(Refer Slide Time: 06:20)



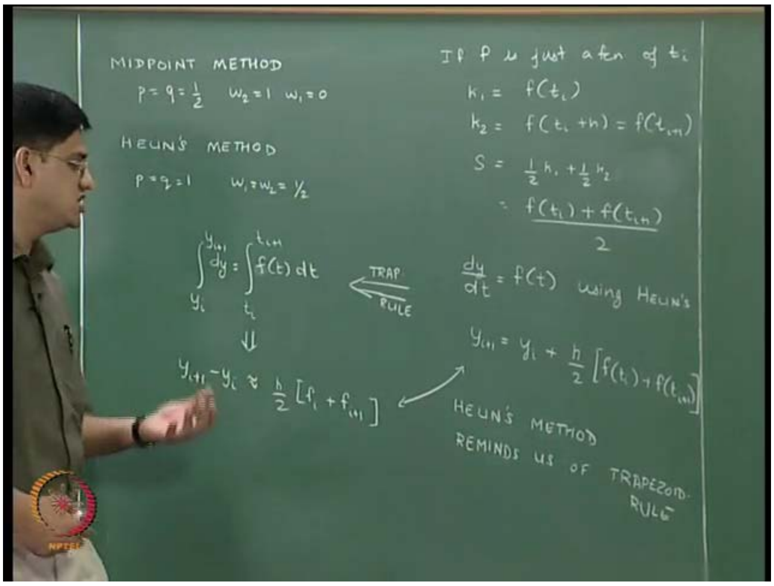
The two specific r k - 2 methods are that of a greater interest to engineers - one is the midpoint method. In midpoint method, we had chosen our p equal to half; so our q also was equal to half ; w 2 was equal to 1, and w 1 was equal to 0.

So, p equal to q equal to half; w 2 equal to 1, w 1 equal to 0 was the midpoint method. And the other method was Heun's method for which we had obtained p equal to q equal to 1, and w 1 equal to w 2 equal to half, this is what we had obtained for Heun's method. In the previous lecture, what I had mentioned, but not really expounded on it was that, in some ways the idea behind Heun's method is kind of collinear or similar to the idea behind the trapezoidal method.

(Refer Slide Time: 07:29)



(Refer Slide Time: 07:39)



And let us see why I made that particular statement. So, let us consider the case, where this particular function f of (y i, t i) was not a function of y i explicitly, but it was only a function of t i. If that is the case, f is just going to be a function of t i, then k 1 is just going to be equal to f of t i. For Heun's method, we are talking about. k 2 is going to be nothing but f of t i plus p h, and p for Heun’s method is equal to is equal to 1 and so that is going to be t i plus h.

So, f is going to be t i plus h, which is nothing but f of t i plus 1. So, our S is going to be half multiplied by k 1 plus half multiplied by k 2, which is f of t i, which is equal to f of t i plus f of t i plus 1 divided by 2.

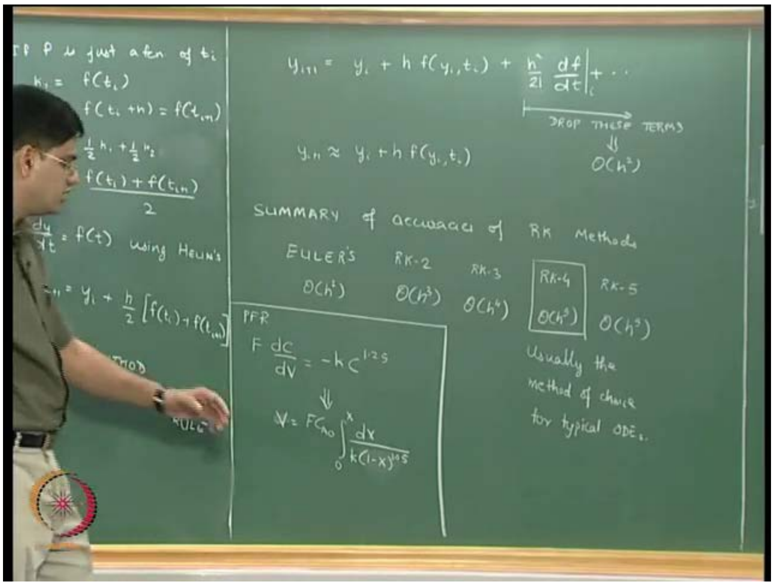
So, now, if we had to solve d y by d t equal to f of t using Heun's method, the expression that we are we are going to get from Heun's method is y i plus 1 is going to be equal to y i plus h multiplied by S, and h multiplied by S is nothing but h by 2 multiplied by f of t i plus f of t i plus 1.

And this particular term for us is reminiscent of nothing but the trapezoidal rule. trapezoidal rule was for the trapezoidal rule we obtained the trapezoidal rule we had we had obtained as follows: d y d y is going to be f of t d t and then, we integrate this from t i to t i plus 1 and this is going to go from y i to y i plus 1 and the trapezoidal rule would give us y i plus 1 minus y i is approximately equal to h by 2 multiplied by f of t i plus 1 plus f of t i, which is same as the expression that we get from the Heun's rule.

So, for this reason, I had made a statement that Heun's method reminds us of trapezoidal rule. And recall from what we did in module 6, is trapezoidal rule also gave us order of h cube accuracy. It's actually not really that Heun's method reminds us of trapezoidal rule, originally the Heun's method was developed as a predictor character method and we are going to talk about that later on in this particular lecture in a few minutes from now, what were that predictor character forms of the Heun's method.

But to go over what we have in Heun's method what we do is, we find a slope at this point, the slope at the projected point and true slope S that we are going to use for moving forward with the O D E solving is going to be just a way just an average of those two slopes that is about the Heun's method.

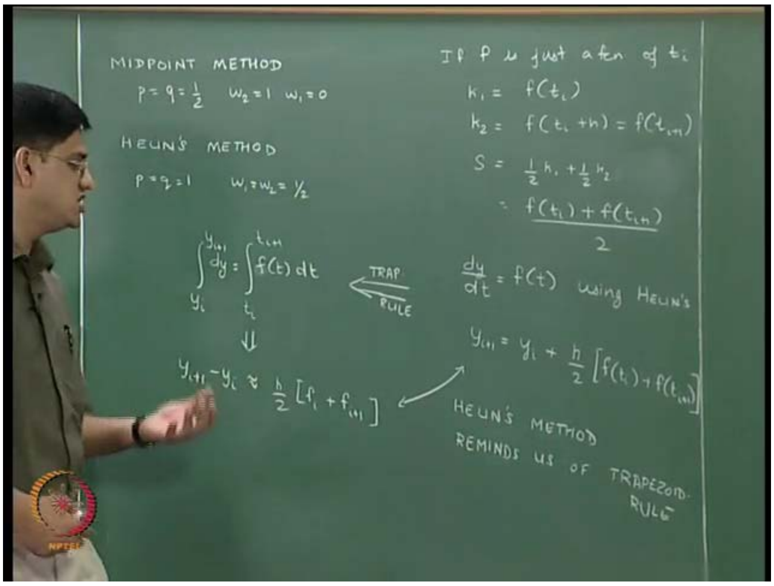
(Refer Slide Time: 12:23)



Before going on to the predictor character idea of Heun’s method, let us very quickly go over the Euler’s method and derive the expression for accuracy of Euler’s method. So, y i plus 1 is, if we do a Taylor's series expansion of for y i plus 1 that is going to be equal to y i plus h multiplied by f of (y i, t i) plus h square by 2 factorial multiplied by d f by d t plus dot dot dot. We actually have d square y by d t square, and d y by d t is nothing but f; these are the derivation that we had actually done in the previous lecture.

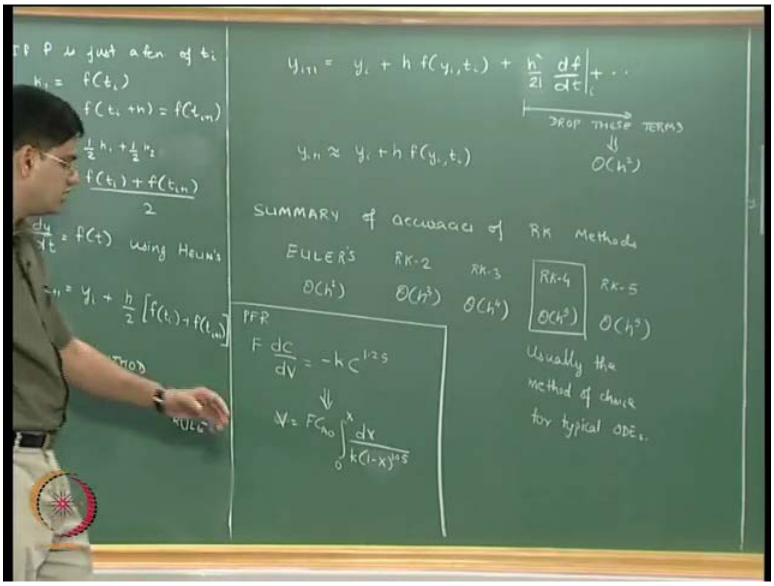
So, I am just using short hand over here; now, if we drop these terms, we will get accuracy of order of h squared, and our y i plus 1 is going to be approximately equal to y i plus h of f (y i, t i). And we have dropped these terms; so the accuracy of the Euler’s explicit method is of the order of x squared.

(Refer Slide Time: 13:57)



So, the Euler's explicit method is x squared accurate, whereas the r k 2 method is h cubed accurate that we had derived in the previous lecture. Like, trapezoidal rule our Heun's method also is h cubed accurate.

(Refer Slide Time: 14:07)

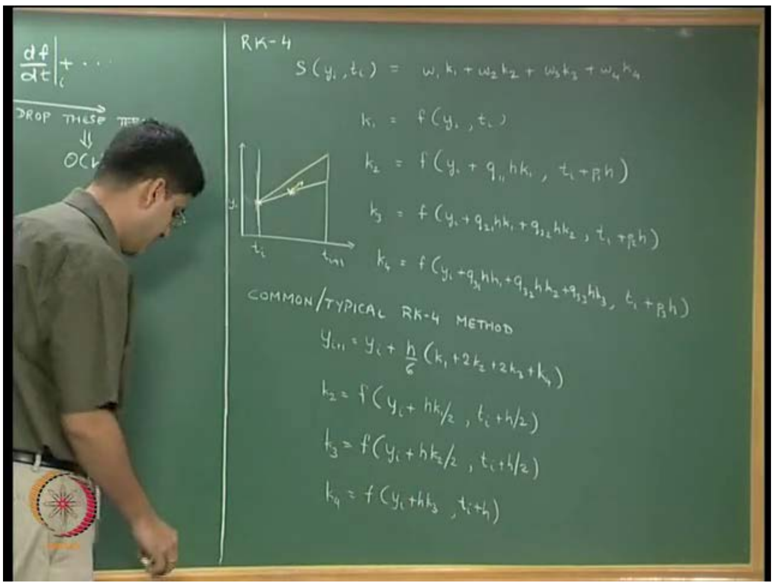


So, to summarize the accuracies - Euler's method that we just derived is accurate to the order of h squared; r k - 2 that we derived in the previous lecture is accurate to the order of h cube; the best r k - 3 method is accurate to the order of h to the power 4; r k - 4 method, the best one is accurate to the order of h to the power 5; and now, this is where the fun starts is r k - 5 method is also accurate to the order 5.

H squared, h cubed, h to the power 4, h to the power 5 and we go for a more number of terms in the Runge-kutta method, but the order of accuracy does not increase. So, there is not a big jump in accuracy that we get by going to more computationally complex r k - 5 method. As a result of this particular observation, r k – 4 method is usually the method of choice for solving O D E’s. In fact, in various packages such as Matlab and Mathematica and so on, as well as a lot of codes that you will get for download at various different sources for initial value problems of non-stiff nature and I will come to come to explain what the term stiffness and non-stiffness means, perhaps two lectures from now.

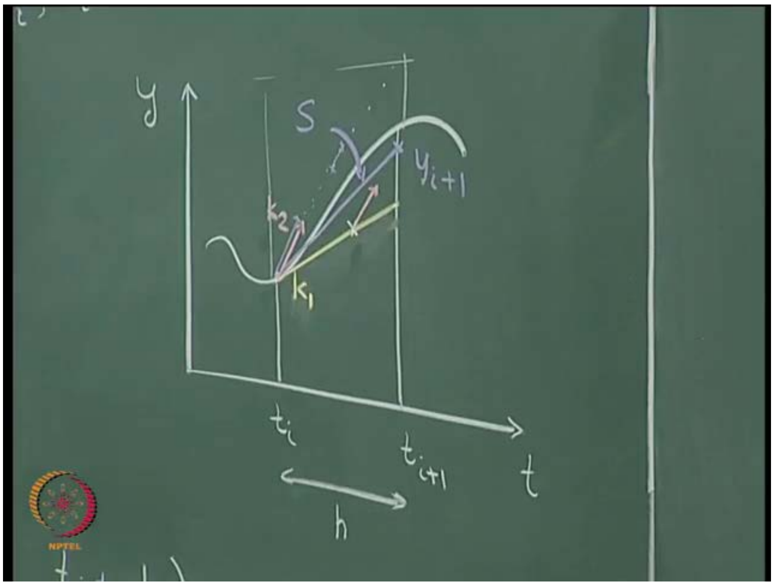
But for a typical o d e i v p you will find that the r k - 4 method is perhaps the most popular method that is used, and r k - 4 has an accuracy of the order h to the power 5. so its its Since it is an r k - 4 or a 4 order r k method, our S is going to be written as w 1 k 1 plus w 2 k 2 plus w 3 k 3 plus w 4 k 4, where k 1 is going to be written as f of (y i , t i); k 2 as we had before, is going to be written as f of y i plus q and now, we will put subscripts for q, we will write this as q 1 1 h multiplied by k 1 , t i plus p 1 multiplied by h. Our k 3 is going to be f of y i plus q 2 1 h k 1 plus q 2 2 h k 2, t i plus p 2 h; and k 4 is going to be f of y i plus q 3 1 h k 1 plus q 3 2 h k 2 plus q 3 3 h k 3 p 3 h.

(Refer Slide Time: 16:50)



So, what we do is, we compute slope at four different locations within t i and t i plus 1. So, if we go back to this particular figure that we have drawn, we will compute k 1 at this particular point, then we choose a point in this rectangle - an arbitrary point in this rectangle- find the slope k 2, based on the slope k 1 and based on the slope k 2. We find out another slope k 3 at another arbitrary point and that arbitrary point will lie in this particular rectangle.

(Refer Slide Time: 19:42)



So, the third point will lie in that particular rectangle and find the slope at that particular point k 3. And another point - fourth point - will also lie in that another rectangle so constructed and that slope will be k 4, and the final S that we are going to use in order to compute the term y i plus 1 is going to be a weighted sum of k 1, k 2, k 3 and k 4. The most typical r k - 4 method that is often used has w 1 equal to 1 by 6; w 2 and w 3 equal to 1 third; and w 4 equal to 1 by 6 again.

So, common slash typical common or typical r k - 4 method has k 1 plus 2 k 2 plus 2 k 3 plus k 4, k 1 of course is f of (y i , t i); k 2 just like the midpoint method, k 2 is going to be f computed at y i plus h k 1 by 2 t i plus h by 2; k 3 is f computed at y i plus h k 2 by 2 , t i plus h by 2; and k 4 is going to be f computed at y i plus h k 3 and t i plus h.

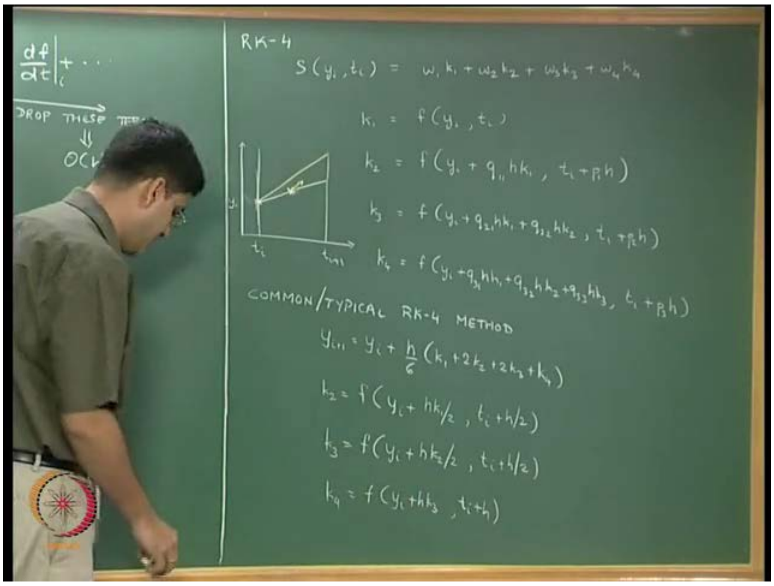
So, this is the most typical r k - 4 method. What r k - 4 method actually will do is, I am not going to draw the true curve over here; this is t i ; this is t i plus 1 and let us say this is our y i. So, our first slope is nothing but slope of that curve, let say that curve is somewhat like this; then our first k 1 is going to be just f of (y i , t i). So, let us say k 1 is actually shown by this particular white line.

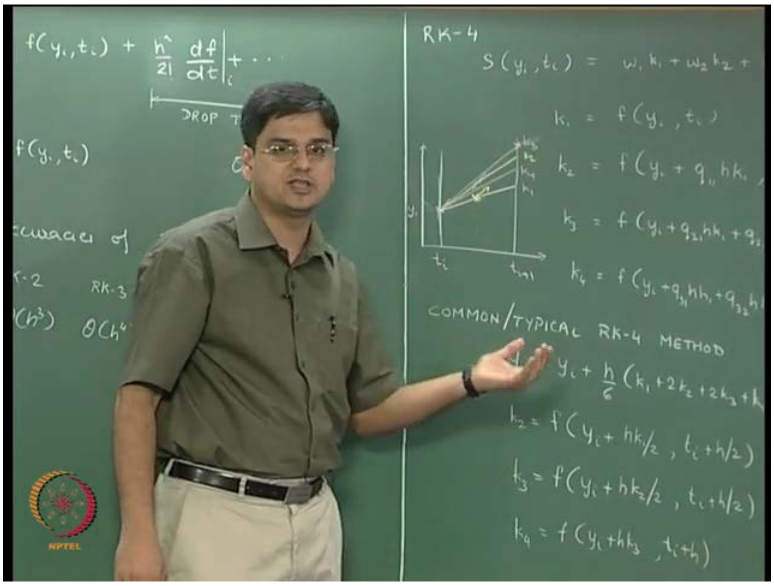
So, now, k 2 is going to lie, because our q 1 1 and p 1 are both equal. Our k 2 is actually going to lie on this particular line itself and k 2 is lying actually on the midpoint. So, k 2 is computed actually on at the midpoint; so k 2 is actually computed at this at the central point the over here.

And k 2 is going to give us a slope at this particular central point; so let us say k 2 is given by this yellow line. So, what we do is, then we go back and then we project that yellow line over here and we will get that that particular yellow line looking somewhat like this; k 3 is going to be a point computed again at the midpoint, but this midpoint is now computed using the slope k 2.

So, the k 3 is computed on the same vertical line over here, but at this particular location and that is going to be the value k 3 and let us say for argument sake, k 3 looks somewhat like this.

(Refer Slide Time: 19:41)



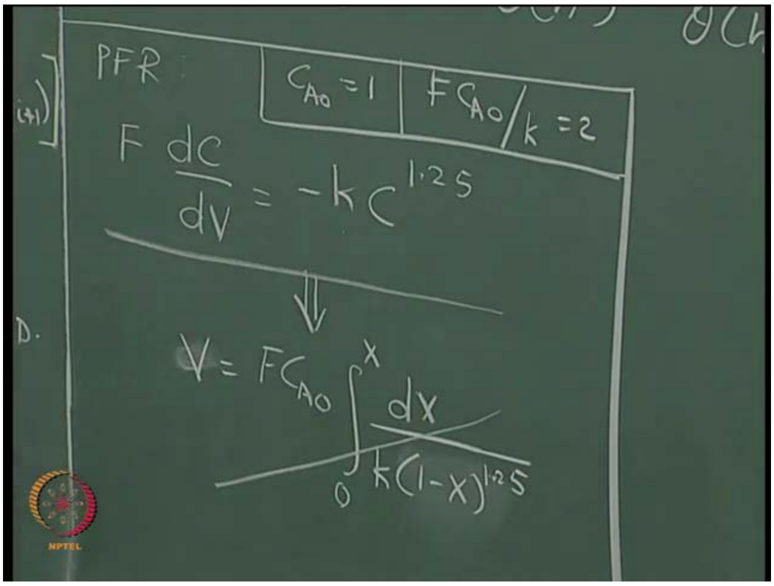


So, we go back to this particular point and then project k 3 again, and k 4 is then computed at the final point and that I am going to show with a pink color. So, k 4 is going to be computed at this particular point and let us say that the slope at that point is over here and so that is that red line is going to be the fourth slope.

So, the white line represents the slope k 1; yellow line represents the slope k 2; the purple line represents the slope k 3; and the red line represents the slope k 4. And the final S that we are going to use in order to compute y i plus 1 is going to be k 1 plus 2 times k 2 plus 2 time k 3 plus k 4 the whole thing divided by 6.

So that is the geometric interpretation of the simplest of r k - 4 methods. In one of the summary lectures, I will go over the various different types of r k - 4 methods that people have actually come up with over the last sixty, seventy years.

(Refer Slide Time: 25:06)

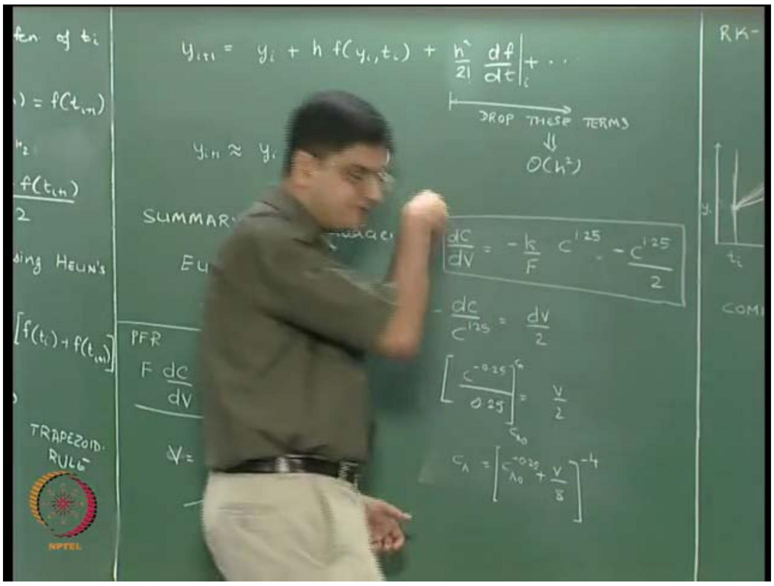


So, now, what I will do is, I will go on to Microsoft excel and solve the specific problem of the p f r. The p f r problem, the design equation that we had solved; we had obtained the design equation based on the overall equation d c by f multiplied by d c by d v, where f is the flow rate - volumetric flow rate - that is going to be minus k c to the power 1.2 5.

So that was the overall expression and then, we converted that through straight forward techniques. We had converted that to get give ourselves the design equation V equal to F times C A0, which we had called F A0 multiplied by integral from 0 to x d x divided by minus r of x, where minus r of x was nothing but k multiplied by 1 minus x to the power 1. 25.

And then, we had plotted F C A naught divided by k multiplied by 1 minus x to the power 1.2 5; we plotted that against x and the area under that curve that we calculated was equal to V. So, instead of solving this particular problem, we are actually going to be interested in solving this particular problem. And if you recall in the previous module, the value of F C A naught divided by k, we had taken that equal to 2.

(Refer Slide Time: 27:32)



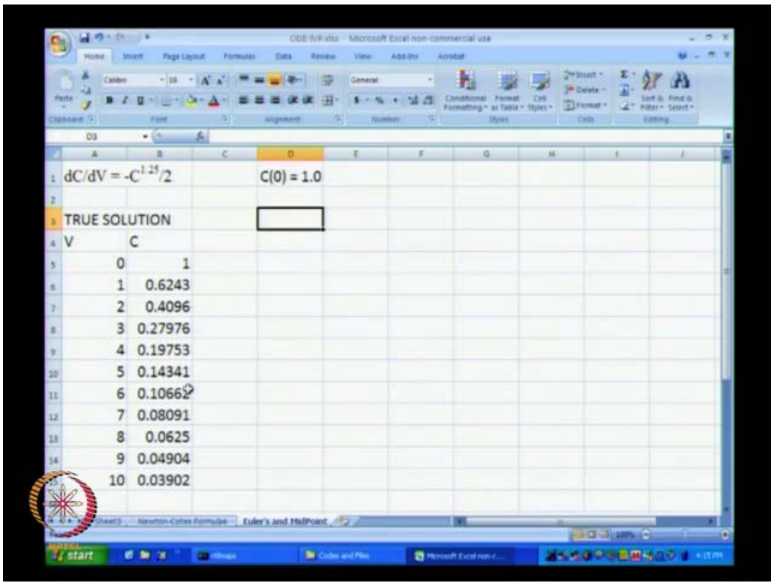
And C A naught was equal to 1. so what we had we had So, for these conditions, we had tried to solve this P F R problem using the integration method. Using the design equation of the P F R, we can rearrange this and we can get an analytical solution and k by f k by f for C A naught equal to 1 k by f is nothing but 1 by 2.

So, this we can write as C to the power 1. 2 5 divided by 2 and we can just rearrange that and we can write d c and I forgot the minus sign over there, d c negative of d c divided by C to the power 1.2 5 is going to be equal to d v by 2 and then, we are going to integrate this; we are going to get c to the power minus 0. 2 5 divided by 0. 2 5, there will be a minus sign over here and there is a minus sign over here; that is going to be equal to be equal to v by 2 and C going from C A 0 to the value C A.

And then, if we rearrange this entire thing, we will get C A; C A to the power minus 0. 2 5 minus C A naught to the power minus 0. 2 5 is going to be equal to 0. 2 5 multiplied by V by 2 that is going to be v by eight plus C A 0 to the power minus 0. 25. So, C A to the power minus 0. 2 5 is going to be equal to this term and then, we will divide by minus 0. 2 5 in the exponent over there and we will get this as C A equal to C A naught to the power minus 0.2 5 plus v by 8, where v is the volume of the P F R whole raise to the power of minus 4.

So that is the analytical solution and this is the problem that we will try to solve numerically, and using the Euler's method, using the Runge-kutta second order method and then, we will compare the results that we have obtained from the two methods.

(Refer Slide Time: 30:03)



So, now, we will go on to Microsoft excel and we will try to solve this this particular problem. Now, the problem that we are going to solve is the is d c by d v was equal to minus c to the power 1. 2 5 divided by 2.

That is the expression that we have just derived a few minutes ago on on the board. So, I will write that down, d C divided by d V is going to be equal to minus C to the power 1. 2 5 divided by 2. so by d C by d V equal to minus C to the power 1. 2 5 divided by 2.

And I will just format cells and make that superscript. So, this is the problem that we are trying to solve with C 0 equal to 1.0. So, that is the problem that we are trying to solve and let us get the true solution. So, we will have V and the corresponding C concentration. As we had obtained earlier, the true solution is actually going to be equal equal to to the concentration C A 0 to the power minus 0. 2 5; C A 0 is 1, so 1 to the power anything is also going to be equal to 1 plus volume multiplied volume divided by 8; the volume is given over here, this guy divided by 8, the whole raise to the power of minus 4.

So that was the value that we had we had obtained. So, let us look at the volume of the reactor going from 0 1 2 let us say up to10, and let us find out the concentration that we get from this particular figure.

Now, let us try to see what values we had derived in in the lecture on integration. At that particular case, what we had said is, we need to find out the volume that gives the conversion of ninety percent; ninety percent conversion means that the exit concentration C that we get from the reactor is going to be equal to 0. 10.

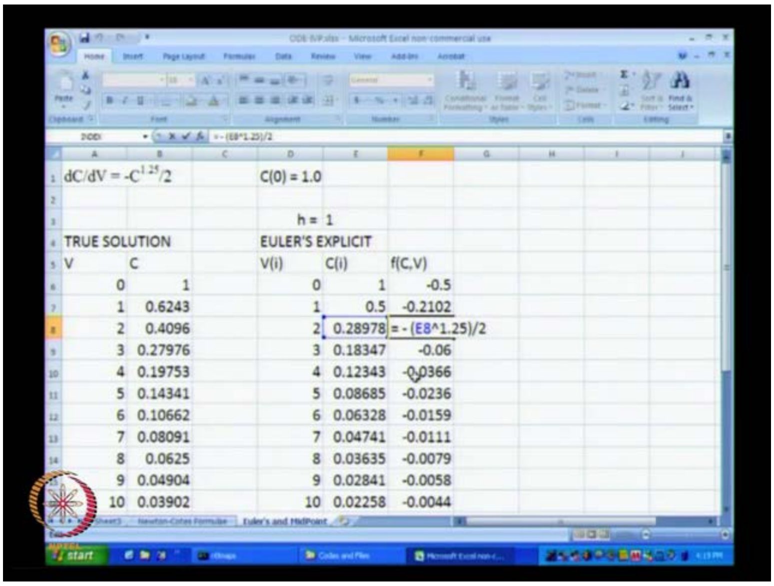
So, the solution - the actual solution - is going to lie close to 6; so the volume is going to be close to 6. So, what I will do is, between 6 and 6. say 6.1, 6.2 and so on. I will just plot a few more values and 6. 3 as well and let us see what value we will get over here.

So, between 6.2 and 6.25, the value has gone below 1; so, perhaps our solution is going to be between… not perhaps definitely our solution is going to be between 6.2 and 6.25. So, let us try to actually get that solution also. So, 6.2, 6.21, 6.22, 6.23 and so our solution is somewhere between 6.2 6.22 and 6. 23.

And let us go and look at what Newton-cotes integration formulae had given us, as the volume that will give us 90 percent conversion and the Newton-cotes formulae - the one third rule results that we got was 6.2262, that was the volume of the reactor that gave as 90 percent conversion and the analytical solution gives us the value as 6.22 something.

We can we can just go a little bit further and we can get the actual result and we will be able to find that the values indeed that we obtained using integration over the same as the values that we will obtain using the true solution - the true analytical solution.

(Refer Slide Time: 35:40)



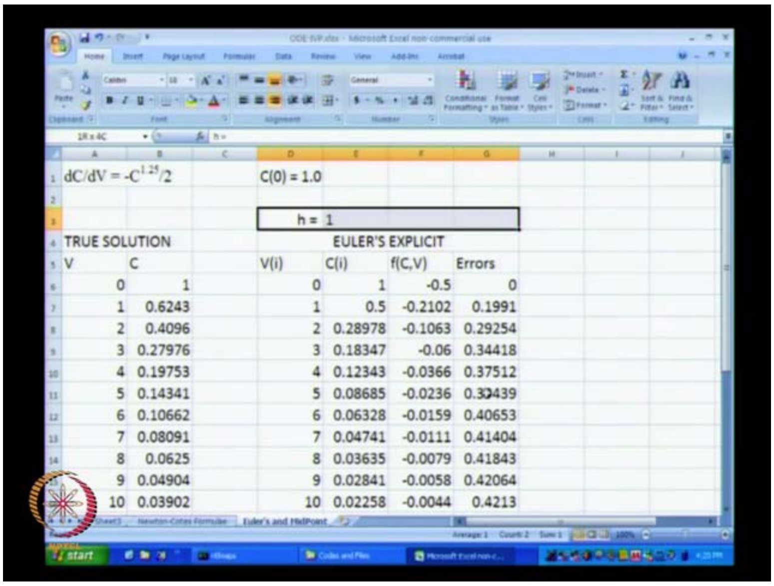
So, this we can use as one more check to check our integration that we did in our previous lecture. Now, let us use Euler's method - Euler's explicit method - with certain value of h. Let us let us choose the value of… I will just insert; so let us let us choose the value of h equal to 1 and see what the Euler's method gives us. And one of things that that happens with Euler's method is that Euler's method is not always Euler's explicit method is not always stable, what that means we will we will talk about soon.

So, C i I will I will write over here; so initial C i is going to be equal to 1; the V i, V i is nothing but the independent variable; the value of C i at V i equal to 0 was equal to 1. I will just move this over here; we will we usually put our independent variable in the first column. So, V i equal to 0; our C i is equal to 1. Let us compute our f of (c, v) and our function f is d c by d v equal to minus C to the power 1. 2 5 divide by 2. So, it is going to be equal to… I will increase the font size; so this is going to be equal to minus C to the power 1. 2 5 the whole thing divided by 2 that is going to be our value of f.

So, the value of f is going to be minus 0.5. Now, this guy is going to be equal to previous guy plus h and I will put dollar signs over here. And remember, the Euler's explicit method is y i plus 1 equal to y i plus f i that was the expression sorry y i plus h multiplied by f i.

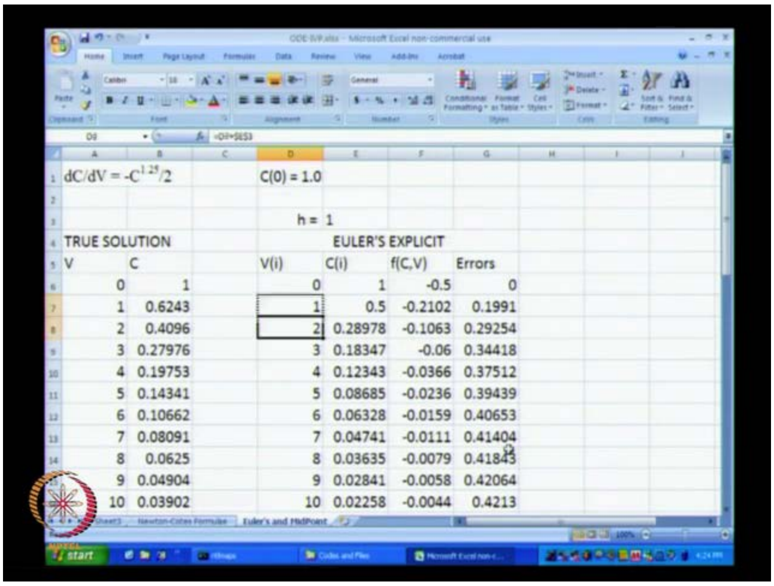
So, y i plus 1 equal to y i plus h multiplied by f i. Now, we will go and put dollar signs in front of h so that when we drag and drop this, we do not have to go and change our our h and now we will just drag drag it down up to 10 and then drag this f value below.

(Refer Slide Time: 39:53)



And we will just go ahead and check what we see with this. So, f 2 is going to be in sorry c 2 is going to be nothing but c 1 plus h multiplied by f 1 that is what we get over here. Now, we will check the value of f of (C i, V i), of course f of (C i, V i) again we get as negative C i to the power 1.2 5 divided by 2; so this is what we get. Now, if we if we compare the Euler's explicit method, the errors that we get with the true solution - we see that there are some amount of errors between the true solution and the Euler's explicit method and so we will just plot the errors over here. So, errors are going to be equal to the absolute value of the difference between C i true minus C i that is obtained from the numerical solution divided by the C i true. So that is the error; error of course, write in the beginning the error is 0 and as we proceed further, the error is…

(Refer Slide Time: 40:51)



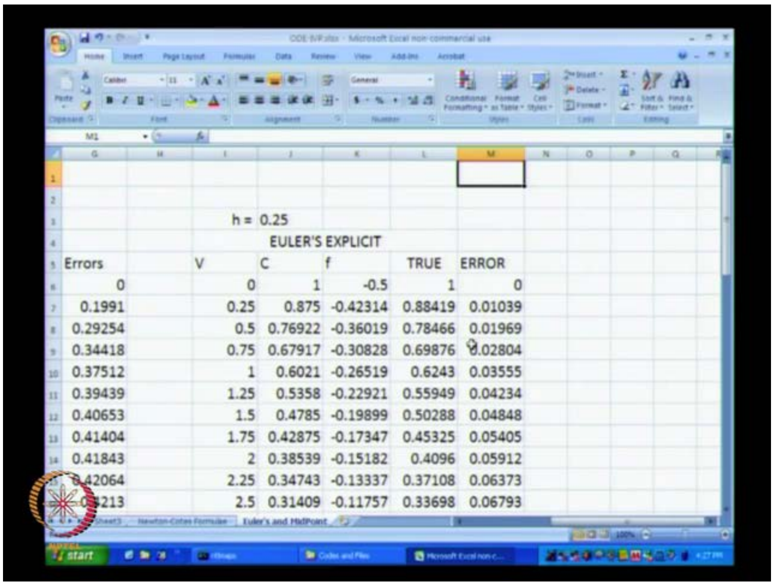
So, this is relative error and the relative error is actually as high as… So, its starts with 20 percent goes to approximately 30 percent and eventually we get error as high as 40 percent using the Euler's explicit method, if we choose h equal to 1. So, this is what we get with Euler's explicit method for h equal to 1. Now, we will again use Euler's explicit method for with h equal to 0. 5.

So, what we will do is, h we will redo this for h equal to 0. 5 and this is going to be this guy and I will put the dollar signs over there; our f is again correct. Now, let us get our C i plus 1 that we have C i plus 1 over here is going to be nothing but equal to C i plus h multiplied by f i.

And we will go back and put dollar signs in front of h so that we get this. We just drag and drop this over here and we will do this over here as well, drop this over there and we will just copy this down, and 0. 5 so that we are able to computed for the same set of values. And these are the errors that we get with h equal to 0. 5. Now, if we compare if we compare the errors that we are getting for the Euler's method using h equal to 1, I will just copy this and put them over here.

So, at at at the volume equal to 1, the error using the h equal to 0.5 in Euler's explicit method is all most 80 percent, whereas it was almost 20 percent using h equal to 1 for for this guy; the error is again again half of what we obtained using h equal to 1 so on and so forth. So, this is what we see for h equal to 4; again, the error is 38 percent, whereas error using h equal to 0.5 at volume equal to 4 is approximately 80 percent; so error is approximately half using h equal to half compared to h equal to 1.

(Refer Slide Time: 44:31



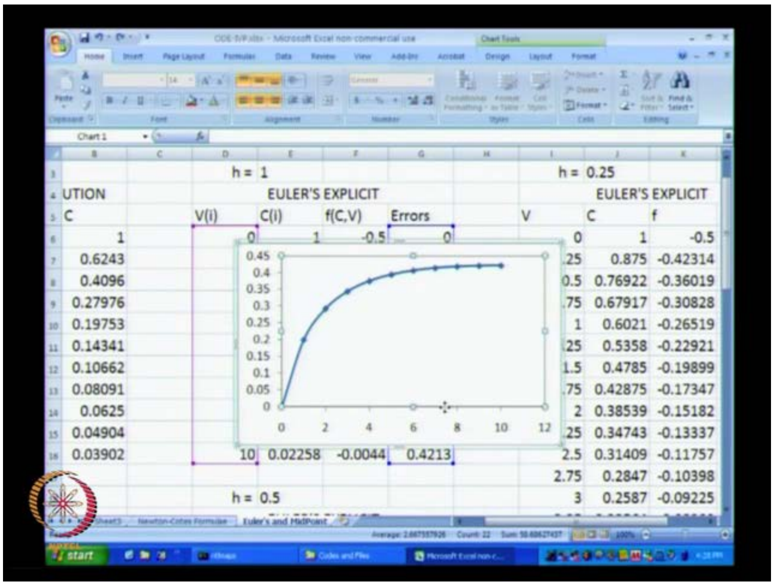
And what we will do is, we will just carry out until 10 and we will do the same thing over here as well. And these are the errors that we get. And the Euler’s explicit method, we will repeat at once again for h equal to 0.25 and then, we will do the plots. And volume is 0; at volume of 0, we will get C equal to this; our f, we will write this as again will just we can just copy and paste it that is not going to be a problem; we will write h equal to 0.25. And next value of V is going to be V i plus 1 is going to be V i plus h and then, we will again put… as we have been doing always, we will put dollar signs over there.

So that when we drag and drop, we do not get any problems and then, we will go right up to volume of the reactor equal to 10. And the concentration C is going to be equal to… So, C i plus 1 equals c i plus h, and for h we will put dollars, because h is not changing multiplied by f I; so C i plus 1 equal to C i plus h multiplied by f i.

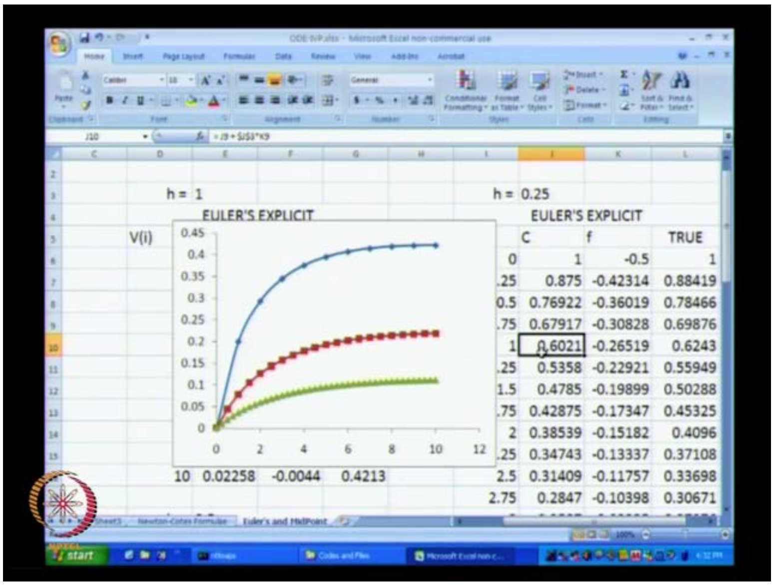
And then will just double click this and will double click this; so that our solution is now obtained. Now, we will plot the true solution is well and the true solution and this double click this and this will give us the true solution and then, I will compute the error as well.

Ok yes And we have computation at error over here and error is the absolute value of true solution minus the numerical solution divided by the true solution. And I will just double click this and we now have the error using h equal to 0. 2 5.

(Refer Slide Time: 48:17)



(Refer Slide Time: 48:50)



So, now, what I will do is create a plot of how the error changes with volume for the 3 different h values. So, I will choose this as our x axis; I will choose this error as the y axis; I will click on insert and then, we want scatter plot and this, we wanted connected by smooth lines. So, this is going to be our scatter plot; I will increase the font sizes now.

So, what we are plotting over here is how the error changes with with the volume for the P F R and then, I will add another set of data - the x values these are the x values; y values are going to be the errors over here.

So, the second series is Euler's method using h equal to 0.5 and we will add one more series with errors using 0.25. So, this blue line represents the error using the Euler's explicit method with h equal to 1; the red line indicates Euler's explicit method with h equal to 0.5; and green line indicates euler's Euler's explicit method with h equal to 0.25. One of things that you see is what is what is known as the propagation of errors; as we go further and further away from y 0, we see that there is that the overall truncation error increases. How the error changes from one point to another point is what is known as the local truncation error, and how the error changes over all throughout the overall ah solution is known as the global truncation error.

At each point we are trying to find out the at a difference between the true value of concentration and the numerical value of concentration. So, what we have plotted over here is not the local truncation error, but what we are actually plotted is the global truncation error. So, in case of Euler's method, although the local truncation error scales as h squared, the global truncation error scales as h. So, what we seen is, when we are going to half the ah the h value, the overall errors are also going to reduce by the same factor.

So, when we go from h equal to 1 to h equal to 0.5, the overall errors have half; when we go from h equal to 0.5 to h equal to. 2 5, again the errors have half. If we go from 0.25 to 0.1 to 5, again the errors are going to be half. Even further, keep in mind that when I say half, it is not exactly half it is approximately half. Because in the derivation using ah basically using our mean value theorem, we do get f of f at (t zeta , y zeta), where zeta is a point which lies arbitrary between t i and t i plus 1 and y i and y i plus; this particular point is not known a priory.

So, we cannot exactly say that the errors are going to reduce exactly by half, but approximately the errors are going to reduce by half and that is what we have consistently seen when we compare this blue line, which was for h equal to 1; with this red line for h equal to 0.5; with this green line for h equal to 0. 25.

So, this is now, where we come to end of this particular lecture of this module. So, what I am going to cover in the next lecture is, I will go over this results for Euler's explicit method once over again and show you how this over all error are changing when we change our h value for the Euler's explicit method. Then I will take on the midpoint method and solve using the midpoint method, also solve using the Heun's method. I will solve the same problem of O D E solving. Next, we will go on to the predictor corrector form of Heun's method.

Thanks and see you in lecture 4 of this module.