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Module No. # 07

Lecture No. # 04

Ordinary Differential Equations (Initial Value Problems)

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Hello and welcome to lecture 4 of module 7. In this module, we were considering numerical methods for solving ordinary differential equations initial value problem. In the previous lectures, we have covered several numerical methods for solving ODE problems; specifically we started off with Euler's method - the Euler's explicit and implicit method. And in the previous lecture, we did error analysis of for this Euler's for Euler's explicit method and we found that the Euler's explicit method had a local truncation error of the order of x squared, that means, that the error varied with square of the step size that we choose in order to solve the ODE problem using Euler's method.

Then we considered Runge-kutta family of methods and it is not just a single method, but it is a family of methods and we called it nth order Runge-kutta method. And the second order Runge-kutta method had an accuracy of order of h cubed; r k - 4 had accuracy of the order h to the power 5; we had derived the error analysis for r k - 2

method, we did not derive it for r k 4 method, we only stated the results for the r k - 4 method.

And then, we also stated that r k - 5, the best r k - 5 that we could get that also has an error of the order h to the power 5. As a result of this, when we actually go from a fourth order of an r k - 4 method to an r k 5 method, we do not get an improvement in the local truncation error and that is the reason why the r k - 4 method is perhaps one of the most popular methods for solving the ODE initial value problems of what we said was non non-stiff nature.

So that is what we considered and then, we looked at solving a particular problem for a plug flow reactor. and So, the physical problem means that there is a tube of a certain length 1 and we have the way of certain length 1 and volume v, and we have species a flowing through the tube and we said that the flow rate was some va[lue]- some value f, and there is the rate rate of rate that of reaction that is taking place. There is a reaction taking place, A going to B with rate of reaction equal to k times C A to the power 1.25 and we solved this particular problem analytically algebraically and we got the solution.

And then in the previous lecture of this module, we looked at Euler's explicit method. and to solve the problem And the overall problem that we get problem definition that we get is d C by d V, where C is concentration of species a at any location in the plug flow reactor and V is the volume of plug flow reactor. Starting from this end of the reactor was equal to minus k by f times c to the power 1.2 5 and this was the problem that we were trying to solve for value of k equal to 1 and value of f equal to 2. As a result, we we obtained the the ODE that we we had to solve in the form 1 by 2 C to the power 1.25 as the right hand side for this ODE.

Starting with the concentration C at volume V equal to 0 as 1; so, whenever we have ODE, we also require the initial conditions. In this case, since there is a single variable and it is a first order ODE, we require one initial condition. And given this initial condition, we solve this problem using the Euler's method. And we solve this problem for three different values of h for h equal to 1; h equal to 0.5 and h equal to 0.2 5.

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So, what I will do now is, I will go back to Microsoft excel, we will take off from this particular location and then compare what what the results of Euler's method are with results of the r k - 2 method. And the r k - 2 method that we will choose for today is the midpoint method, and for the midpoint method what we obtained was k 1 equal to f of (y i , t i) and k 2 equal to f of y i plus h k 1 by 2, t i plus h by 2, and the slope S that we said was just equal to k 2, which resulted in y i plus 1 equal to y i plus h times k 2, where k 2 was nothing but our S.

So, this is the midpoint method. We will also use the midpoint method in order to solve this problem and finally, we will use the r k - 4 methods as well. So, most of this lecture will essentially cover the solving the same ODE problem with first with r k - 2 method and then with the r k - 4 method. And in r k - 4 method, we had k 1 as same f of (y i, t i); k 2 we computed at f of (y i plus h k 1 by 2, t i plus h by 2); k 3 we computed at f of (y i plus h k 2 by 2, t i plus h by 2) and k 4 was computed at f at (y i plus h k 3, t i plus h). And then, S was just the weighted average 1 by 6 multiplied by k 1 plus 2 k 2 plus 2 k 3 plus k 4, and our y i plus 1 was, y i plus h times S.

So, all these derivations we have done in lecture 3 of this particular module; solving the the Euler's method using excel also we have covered in the previous module. In this particular module, we were going to cover the midpoint method and then, we are going to cover the r k - 4 method.

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So, let us now, go on to Microsoft excel, to try to solve the problem that we are interested in. So, let us now use our Microsoft excel to solve the problem using the higher order our more accurate methods and what I have in front of me is just the method that we had used in the previous module previous lecture sorry of this module. And the we are trying to solve d C by d V equal to minus C to the power 1. 2 5 divided by 2 starting with C 0 equal to 1. 0 and we had solved it for h equal to 1 for h equal to 0.5, and for h equal to 0.25.

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So, this is what we had done in in the previous lecture of of this module and this these were the error values that we that we obtained. So, I will so this is what we had obtained and for h equal to 1, this is how the error changes.

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As we had seen that the error starts with 0, because at volume equal to 0, we exactly know what the starting condition is. And as we move away from that particular volume and as the volume increases, we see that the relative error increases. (Refer Slide Time: 08:58) In this particular example, it increases monotonically, but there is no reason why

this particular error needs to increase monotonically always. The other thing that we also observe is that the error more or less falls linearly. So, when we go from h equal to 1 to h equal to half, there is this much big jump in the error - this much big decrease in the error; when we go from h equal to half to h equal to one-fourth, the decrease in the error is half of what the original drop in the error was. And we can look at this when we see the results for volume V equal to 5, there is a 40 percent error for h equal to 1; for h equal to 0. 5 we get the error almost at 19 percent; and for h equal to 0.5, we get error at 9.5 percent.

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So, we see that the error is approximately decreasing linearly as we are halfing the h value. Now, what I will do is, I will try to solve this particular problem using the midpoint method. So, first what I will I will just do is, I will just copy this particular worksheet at the end and I will just rename it as midpoint method and I will just delete all this and we will just go for now midpoint method.

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And first, we will use this midpoint method; we will use midpoint method with h equal to 1, then we will use midpoint method with h equal to half and will show how the error behavior changes.

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So, I will just delete all the results that we had obtained. I will just move this particular error graph over here; so what I am to plotting over here. what is what What I have over here is the volume of the reactor, and the volume of the reactor, we start off with volume V equal to 0. The initial value for this particular problem is the concentration starts at 1 and so, we have the concentration C i plotted over here. We do not need f anymore; we need k 1, we need k 2 and we need our slope value S; those are the things that we are going to require for solving this method using the midpoint method. Keep in mind, the midpoint method is a second order r k r k method, which means we need k 1 and k 2; for a 4th order r k method, we will k 1, k 2, k 3 and k 4.

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So, our k 1 was nothing but f k 1 was f computed at y i; I am not writing t i right now, because our expression over here in this particular problem, if we compare this this expression with d y by d t our concentration C is the variable y and our concentration V is the independent variable t. k 2 was going to be function f computed at y i plus delta divided by 2 that is the midpoint between t i and t i plus 1. So that is y i plus h multiplied by k 1 divided by 2 that is where that is the location at which we compute our f for getting our value k 2.

So, k 2 is going to be negative 1 by 2 multiplied by C i plus h into k 1 by 2 right. So, this is the overall expression that we are to get. Now, I will replace this C i with the location of the cell over here. So, I will just go go over here and click; so the location of the cell is c 6; our h value is the step size. So, I will choose the step size over here and as and if you recall what we use to do earlier was put the dollar signs, so that when we drag and drop this in Microsoft excel, this does not change and k 1 we are going to replace with this quantity.

So, this becomes our f computed at y i plus h times k i k 1 divided by 2; this is y i, that means the value in this particular cell plus h; this is the value in this cell multiplied by k 1, which is the value in this cell divided by 2 and the whole thing has to be raise to power of 1. 25 and that is our expression. So, we will just review that expression it is half or

rather its minus half multiplied by C i plus h times k 1 divided by 2 the whole thing to the power 1.25, this is the exponent 1.25, that we have over here.



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Now, the S value for our midpoint method is equal to 0 multiplied by k 1 plus 1 multiplied by k 2. So, our S value is nothing but k 2. Now, we have everything that we need in order to compute our C 1, I will delete these 2 guys over here and our C i plus 1 was nothing but C i plus 1 is nothing but C i plus h multiplied by S and now what I will do is, I will replace C i h and S with appropriate values.

So, C i is this particular value; our h step size is the value in this cell and our slope is the value in this cell. And as we have been doing all the time, I will put the dollar signs over here to represent that as we drag and drop this particular quantity, this h should not change. So, I will again drag this; down over here; drag my k 2 down and drag my S down; the true value that we have I will just drag this all throughout. And now what we need to do, as this is what we have been doing throughout the various modules in this particular lecture, we can highlight this entire row and drag it until the value of V reaches 5.

So, I am we will just go ahead and check whether for an n any arbitrary point, whether the our equations or correct or not. We will press f 2 and this is what we see; C i plus 1 is C i plus h multiplied by S i computed at time i. So, everything depends on the values that

are previously known at time i; everything at i plus 1 depends on values previously known at time i and therefore, this is an explicit method. We will check our value of k 1; k 1 should be minus C i to the power 1.25 divided by 2. So, it is minus C i to the power 1.2 5 divided by 2; this is exactly what we get; and k 2 is again minus half multiplied by C i plus h by 2 multiplied by k 1 whole to the power raise to the power 1.25.

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So, is minus half multiplied by this is C i plus h multiplied by k 1 divided by 2; this divided by 2 is because we are computing it at the midpoint and the entire thing to raise to the power 1.25. So, everything that we have over here is... Now, we are assured that this is correct and we can now look at the errors and the errors or this these are the errors that we get. So, the error initially, of course is 0, because there is no error; the value of concentration- initial concentration is known perfectly and then, the overall error starts increasing gradually. And at for volume V equal to 5, we have 10 percent error in computing the numerical value using the midpoint method. If you recall what we had in Euler's method, we had I believe 40 percent error. right yes.

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So, we had 39.4 percent error. When we use the Euler's method and when we are using the midpoint method, we have 10 percent error. What I have done is, I have also created another worksheet, where I have just written down all these errors; these are the errors that I have obtained for the Euler's method and I have just written them down. This is the error for midpoint method; we have just calculated 10. 3 2 percent, which I have just put it put over here. I have also pre-calculated errors of r 4 and error of midpoint method for different h values.

We will get to that particular slide in a few minutes. What I am going to do is, I am going to show you, how easy it is to go from this stage to calculating for doing the calculations from midpoint method for different h for h equal to 0. 5.

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So, I will just delete all these guys that I had developed before. So, these where the results using midpoint method; we highlight this entire row and we just drag it below until the value of V reaches 5.

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So, all we had to do was change the value of h over here to 0. 5 and we can just check the values of C i. So, c i is C i plus 1 is nothing but C i plus h multiplied by S; k 1 should be minus C to the power 1. 2 5 divided by 2. So that is minus C to the power 1. 2 5 divided by 2; our k - 2 should be minus half multiplied b y C plus h by 2 multiplied by k 1 the whole thing to the power 1. 25.

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8			MID-	POINT							
1	V(i)	TRUE	C(i)	k1	k2	S	Error				
8	0	1	1	-0.5	-0.4231	-0.4231	0				
7	0.5	0.78466	0.78843	-0.3715	-0.3176	-0.3176	0.0048				
	1	0.6243	0.62963	-0.2804	-0.242	-0.242	0.00854				
	1.5	0.50288	0.50865	-0.2148	=-1/2[* (0	9 + B\$3*0	09/2)^1.25				
10	2	0.4096	0.41524	-0.1667	-0.146	-0.146	0.01376				
11.	2.5	0.33698	0.34222	-0.1309	-0.1154	-0.1154	0.01556				
12	3	0.27976	0.28451	-0.1039	-0.0922	-0.0922	0.01697				
13	3.5	0.23419	0.23842	-0.0833	-0.0743	-0.0743	0.01807				
54	4	0.19753	0.20127	-0.0674	-0.0604	-0.0604	0.01892				
10	4.5	0.16777	0.17106	-0.055	-0.0495	-0.0495	0.01957				
8	6 5	0.14341	0.14629	-0.0452	-0.0409	-0.0409	0.02006				
l'	the second	Meduant	IN-4 Evers-	2 Had Print I	Hethod Dear	Comparison	1.00			-	
Tine .	-	_						- 1	303	8	
1	start	e 💼 🙂 👘	COLUMN ST	1 E					5 1 8 × 8	# 13.0.7 #	

So, I will click f 2 and we will able to see the formula. So, C is equal to minus half multiplied by this C i plus h multiplied by k 1 divided by 2; this whole thing raise to the power 1. 25.

So, now, what now what we are going to do is just the compare the errors of the two methods of sorry compare the errors of the midpoint method using h equal to 1 and h equal to 0. 5. So, with h equal to 0. 5 at volume 5, the error is 2 percent; the error was about 10 percent when we started with h equal to 1.

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Cores .	A CENTRAL	COUNCY EXCEL IN	e connerce o					 -	-	
	LOUIN .	0125 0						 	_	
1.4	dC/dV = -	-C**/2		C(0) = 1.0						_
2										
2	h =	1								
4			MID-F	POINT						-
	V(i)	TRUE	C(i)	k1	k2	s	Error			
	0	1	1	-0.5	-0.349	-0.349	0			
7	1	0.6243	0.65102	-0.2924	-0.2128	-0.2128	0.04281			
	2	0.4096	0.43826	-0.1783	-0.1342	-0.1342	0.06997			
	3	0.27976	0.30408	-0.1129	-0.0873	-0.0873	0.08693			
10	4	0.19753	0.21674	-0.0739	-0.0585	-0.0585	0.09725			
11	5	0.14341	0.15821	-0.0499	-0.0403	-0.0403	0.1032			
	-									
13										
14										
35										-
20										-
1.0										
29										
20										
21										
22										_
-	~									-
5.8	1									-
*	50									
100	1									

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So, now, that we have solved this problem using the midpoint method, what I am going to do is, we will just compare the midpoint method with the previous Euler's method. What we will do is, we will just see we are starting from the same initial volume and the same initial concentration and we are plotted both the con[centration]- how the con[centration]- numerical values of the concentration are changing as well as the true values of concentrations are changing. And here, I have noted down the error between the true and the computed value, the C i; these are the relative errors not the absolute errors. And what I am going to do now is, for volume V equal to 5, I will see what the error we are getting from the midpoint method is, and I will copy this error into a different worksheet and in this worksheet, I have already I have the errors from the Euler's method that I have put over here and on this place, I will just to paste special and I just want to copy the value, I do not want to copy the formula and the value of the error using the midpoint method for h equal to 1 was 10. 3 percent; so that is what I have put over here.

(Refer Slide Time: 22:09)

				0	1	1	6	1.987	1	4	- 1
1	dC/dV = -	-C ^{1.25} /2		C(0) = 1.0	i.						
2											
8	h =	0.5									
			MID-	POINT							
5	V(i)	TRUE	C(i)	k1	k2	S	Error				
	0	1	1	-0.5	-0.4231	-0.4231	0				
7	0.5	0.78466	0.78843	-0.3715	-0.3176	-0.3176	0.0048				
1	1	0.6243	0.62963	-0.2804	-0.242	-0.242	0.00854				
2	1.5	0.50288	0.50865	-0.2148	-0.1868	-0.1868	0.01147				
30	2	0.4096	0.41524	-0.1667	-0.146	-0.146	0.01376				
11	2.5	0.33698	0.34222	-0.1309	-0.1154	-0.1154	0.01556				
12	3	0.27976	0.28451	-0.1039	-0.0922	-0.0922	0.01697				
u	3.5	0.23419	0.23842	-0.0833	-0.0743	-0.0743	0.01807				
34	4	0.19753	0.20127	-0.0674	-0.0604	-0.0604	0.01892				
8	4.5	0.16777	0.17106	-0.055	-0.0495	-0.0495	0.01957				
24	5	0.14341	0.14629	-0.0452	-0.0409	-0.0409	0.02006				
17	5.5	0.12332	0.12583	-0.0375	-0.034	-0.034	0.02041	1			
14	6	0.10662	0.10883	-0.0313	-0.0285	-0.0285	0.02066				
19	-							8			-
R	1										
Ż	R										-

Now, if we if I want to run this particular problem for a different value of h, for h equal to 0.5 that is also pretty simple. I just need to change this to 0. 5 and everything is taken care of over here; I will just take this last line and just drag it down, until I reach volume V equal to 5. I can delete rest of the stuff and the error that I get for h equal to 0. 5 is excuse me the error that i get for h equal to 0. 5 is 2 percent error; again this 2 percent

error I will just copy it and past it in the new worksheet that I have called as comparison; so this is comparison between errors from various methods.

And then, again I want to calculate this value at 0. 2 5; I just change the value of h since the value of h is change to 0. 25, the final volume- value of the volume is 2.5, because we have just computed it ten times. So, I will just drag it ten more times for ten more roles and I should be able to get volume V equal to 5. And now, the error has decreased from 2 percent to about 0. 4 percent, 0.4 5 percent to be more precise, and I will paste this error again over here.

So, the error in midpoint method has gone down from 10 percent to 2 percent from 2 percent to 0. 5 percent approximately, so it is almost the error is decreasing almost one fifth and again the error has decreased by almost one fourth or one fifth when we go for when we half the h value. And what I will do is, I will half the h value further and go to 0 .12 5, and for 0. 1 2 5, again this I will have to drag it for twenty more columns and when I drag it for twenty more columns and twenty more rows sorry I will delete these guys and now the error is 0.1 percent. So, error is approximately decreasing by one fourth when the step size is decreasing by one half. So, it looks like what happens is the error is decreasing by 1 by 2 to the power 2 every time I am halfing the step size.



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So, on this log-log so what I have done over here is for the Euler's method I have plotted h, the step size in the y axis- x axis sorry and the error using Euler's method on the y axis and I have made them both lo[g]- log-log plot, and on the log-log plot, the error h versus error becomes a straight line for Euler's method. Actually the slope of the straight line is going to be equal to 1 for the Euler's method what I will do is, I will also plot the midpoint method.

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So, the way to plot an additional data set of data on this plot is right click and choose select data, add the data, the series name is going to be midpoint method; the x values are going to be the step sizes and the y values the original y values I will just delete them and then, again click on this and I will choose the values in the midpoint column and it is done.

So, now, what we have is this particular line represents the Euler's method and this particular line represents the midpoint method. So, what we see is that the errors in

Euler's method are greater than the errors in midpoint method. The slope of the Euler's method is lower than the slope of the midpoint method. The slope of Euler's method is actually slope equal to 1, it does not seem like 1 from this particular graph simply because the step size goes from 0.1 to 1, whereas the error goes from 0.00 to1 and that is the reason why it does not look as if the slope is 1 and this slope is 2, but actually the slope of this line is approximately 1; the slope of this line is approximately 2.

So, this was the results using Euler's method and using the midpoint method. What I will do next is we will try to use the Runge-kutta method in order to solve this problem.

	A		2	0			0	 1	1	
1	dC/dV =	C1.25/2		C(0) = 1.0						
2										
8	h =	0.125								
			MID-	POINT						
5	V(i)	TRUE	C(i)	k1	k2	S	Error			
8	0	1	1	-0.5	-0.4805	-0.4805	0			
7	0.125	0.93987	0.93993	-0.4627	-0.445	-0.445	6.9E-05			
8	0.25	0.88419	0.8843	-0.4288	-0.4126	-0.4126	0.00013			
	0.375	0.83257	0.83273	-0.3977	-0.383	-0.383	0.00019			
30	0.5	0.78466	0.78486	-0.3694	-0.3558	-0.3558	0.00025			
11	0.625	0.74016	0.74038	-0.3434	-0.331	-0.331	0.0003			
17	0.75	0.69876	0.69901	-0.3196	-0.3082	-0.3082	0.00036			
11	0.875	0.66022	0.66048	Move or Co.	77	2	0.0004			
34	1	0.6243	0.62457	Safook	(della)		.00045			
13	1.125	0.59078	0.59107	COR DIF Labo			.00049			
20	1.25	0.55949	0.55979	CONTRACTOR OF	921.		.00053			
17	1.375	0.53024	0.53054	Newton-Cole	s fundae		.00057			
28	1.5	0.50288	0.50318	Reprint Bal-4	-4		0.0006			
2	1.625	0.47726	0.47756	Page-Proper Page	field		.00063			
-	1.75	0.45325	0.45356	C) Quale a c		1.000	.00067			
2	875	0.43074	0.43104		_ a		0.0007			
1	A. Barr	0 1000	A 1000	Hid Point)	A * E OO	0 1500	0.00073		-	×.
T.	start	0 00 20	-		Person Caroline	nc 💽 🗤		 	18.0.0 .	

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So, in order to use Runge-kutta method what I will do is, I will just copy this midpoint method to a new sheet; I will so i have what I have done, I will just show you again what I have done is right clicked on this tab, click on move and copy; I click on create a copy, that means, this particular midpoint method work sheet is going to be copied and I will choose to copy before the work sheet call comparison.

And now, this midpoint method has now been copied as midpoint method 2; I will rename this as r k - 4 method. And again for r k - 4, we are trying to use the same same type of scheme to compute d c by to compute C at various time given d C by d V equal to minus C to the power 1. 2 5 by 2, and C 0 is 1. 0. And we want to compute with h equal to 1, I will just go down over here and excuse me and delete all these guys.

(Refer Slide Time: 28:04)

	a	8	¢	0	5		0	н	1	 -
2										- 0
3	h =	1								
2		-	MID-	POINT					-	
2	V(i)	TRUE	C(i)	k1	k2	k3	k4	S	Error	-
*	0	1	1	-0.5	-0.349			-0.349	0	-1
2	1	0.6243	0.65102	-0.2924	-0.2128			-0.2128	0.04281	
8	2	0.4096	0.43826	-0.1783	-0.1342			-0.1342	0.06997	
9	3	0.27976	0.30408	-0.1129	-0.0873			-0.0873	0.08693	
10	4	0.19753	0.21674	-0.0739	-0.0585			-0.0585	0.09725	
11	5	0.14341	0.15821	-0.0499	-0.0403			-0.0403	0.1032	
12										
23										
34	-									
25										
10										
17										
2	~									
S	2									
R										-1
22		at 864 8	sters-2- Md	Post Method	RK-4 Hethod	Comparison	100			

This error column i will and the slope columns, these two columns I will move it two positions to the right, one and two and the reason for that is I want to accommodate k 3 and k 4. k 3 and k 4

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21	A		6	0	1		6	14	1	1
1	dC/dV =	-C ^{1.25} /2		C(0) = 1.0	0					
2										
8	h =	1								
4			MID-	POINT						
5	V(i)	TRUE	C(i)	k1	k2	k3	k4	S	Error	
	0	1	1	-0.5	=-1/2 * (0	6 + \$B\$3	*D6/2)	-0.349	0	
7.	1	0.6243	0.65102		-0.349			#REF!	0.04281	
2	2	0.4096	(0	1	
	3	0.27976						0	1	
10	4	0.19753						0	1	
11	5	0.14341						0	1	
12								0		
11										
\$4	RK-4									
23	k1 = f(yi)									
16	k2 = f(yi +	h*k1/2)								
17	k3 = f(yi+	h*k2/2)								
18	k4 = f(yi+	h*k3)								
2	5 = 1/6	* (k1 + 2*)	k2+2*k3	+ k4)						
1	6									
0	2					-	-			
-			-	Contraction of the	NACE PRENOT			-		

And so that everything is visible to you, I will just select this and change the font size to 18, so that everything is clear. Now, for r k (()) -method our k 1 remains the same; k 1 is just going to be f of y i.

So, k 1 there is no problem; k 2 is going to be f of y i plus h multiplied by k 1 divided by 2; this is our k – 2. Keep in mind that in this particular example, we the function f is just the function of y, it is not a function of t that is why I am using a short hand notation. If it was also a function of t, then instead this would have been f of (y i, t i).

So, I am just not writing this t i to simplify the notations at this point of time, because our function f is just a function of y i. Now, our k 3 that we had is function f of y i plus h multiplied by k 2 divided by 2, this is our k 3; and k 4 was nothing but f of y i plus h multiplied by k 3; this was our k - 4.

Remember, geometrically what what we said this means is k 1 means slope computed at the initial point y i; k 2 means the slope computed at midpoint y i plus half; k 3 means slope computed at midpoint again y i plus half, but in this case, y is computed using k 2 instead of computing using k 1; and finally, k 4 is the slope computed at the end point y i plus 1, sorry rather t i plus 1.

So, these are the various projected slopes that we compute and our S, the actual slope is going to be one-sixth multiplied by k 1 plus 2 k 2 plus k 3 plus k 4; so I will write that down over here as well; S equal to 1 by 6 multiplied by k 1 plus 2 multiplied by k 2 plus 2 multiplied by k 3 plus k 4. So, this is our S.

Now that we have all these; we are now ready to do all the computations. I will delete all these guys from here; the true values I do not need to delete, because true values remain the same. So, k 1 is the same as we had in the r k - 2 method; k 1 is always going to be f of y i. So, f of y i is a negative of c to the power 1. 2 5 divided by 2. So, we have this; this is not a problem. k 2 is now going to be again the same as previous, because in midpoint method also, we are going to use the the formula computed at the midpoint.

So, again k 2 we do not have to change, but why what I will do is just for our own sake, we will just copy down or we will rewrite or rewrite this formula for k - 2; I will increase the font size to 18. So, now, k 2 is going to be equal to f of y i plus h multiplied by k 1 by 2. So, let me just write what h multiplied by k 1 by 2 is; I will write that in brackets. So, this is h multiplied by k 1 is this guy divided by 2; so that is the value of our argument of this function. So, y i plus h multiplied by k 1 by 2; so y i is this guy plus h multiplied by k 1 by 2.

So, in the brackets the term that we have is the argument of the function f, C 6 is y i, b 3 is our h when we are going to drag and drop, we do not want our h to keep changing, so I am going to put dollar signs in front of this and then, our d 6 is our k 1. So, our argument is C1 plus h multiplied by k 1 divided by 2; it is just the h multiplied by k 1, which gets divided by 2. Now, this is our argument that has to be substituted over here. So, what we have is negative 1 by 2 multiplied by the argument to the power 1. 2 5; so I will write that down over here minus 1 divided by 2 multiplied by the argument raise to the power 1. 2 5 and this is our k - 2. So, just for comparison that is the same k 2 that we had obtained earlier.

So, now, we have k 1; now we have k 2 as well; k 3 has a similar formula, so I am just going to drag k 2 and drop it to the right hand side. However, there is a problem over here; so we will just do f 2 and see what that problem is. Now, for k 3 we have minus half multiplied by the argument to the power 1. 2 5; so minus half multiplied by this particular argument to the power 1.25, that argument is y i, which is this particular guy.

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So, it is actually y I plus h multiplied by k 2 divided by 2. So, now, our formula is correct its minus half multiplied by y i plus h multiplied by k 2 divided by 2 plus h multiplied by k 2 divided by 2 this whole thing to the power 1. 25. I will press enter and we will get the value of k 3. So, k 4 is going to be equal to negative half minus half multiplied by the argument the argument is y 1 sorry y i, which is this guy plus h multiplied by k 3; that is

the argument C i plus h k 3 is the argument; for h, we need to put dollar signs so that when we drag and drop, that thing does not change.

Now, this is our argument; the argument has to be raised to the power 1. 25 to the power 1. 25 is minus half multiplied by y i plus h k 3 to the power 1.25 that is our k - 4. And our S is going to be 1 by 6 multiplied by k 1 plus 2 multiplied by k 2 plus 2 multiplied by k 3 plus k 4 that is going to be our S. So, we now have k 1, k 2, k 3, k 4; now let us look at computed at time i. Now, let us look at C i plus1; C i plus 1 I will just write that down C i plus 1; C i plus 1 is nothing but C of i plus h multiplied by S.

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21			¢	0		1	0	191	1 1		
1	dC/dV = -	-C125/2		C(0) = 1.0							
2											
	h =	1									
		1	MID-	POINT				1			
5	V(i)	TRUE	C(i)	k1	k2	k3	k4	s	Error		
	0	1	1	-0.5	-0.349	-0.3934	-0.2676	-0.3754	0		
7	1	0.6243	0.62459	-0.2776	-0.2028	-0.2225	-0.1601	-0.2147	0.00047		
8	2	0.4096	0.40988	-0.164	-0.1241	-0.1336	-0.1002	-0.1299	0.00068		
	3	0.27976	0.27998	-0.1018	-0.0792	-0.0841	-0.0651	-0.0823	0.00077		
10	4	0.19753	0.19769	-0.0659	-0.0525	-0.0552	-0.0438	-0.0542	0.0008		
11	5	0.14341	0.14353	-0.0442	-0.0358	-0.0374	-0.0303	-0.0368	0.0008		
12									R.		
13											
14	RK-4										
13	k1 = f(yi)										
16	k2 = f(yi +	h*k1/2)									1
17.	k3 = f(yi+l)	h*k2/2)									
18	k4 = f(yi+i)	h*k3)									
-	5 = 1/6	' (k1 + 2*k	2+2*k3	+ k4)							4
1	$G(n_1) = C$	(i) + h*S									4
R.											4
1	No. Inclu	et BLA B	dera-2 1 MA	Point Method	RK-4 Hethod	Companyo	198				ani
ų	start	e 🛄 🦉 👘	Carlos -	8		NC- 🛃 🕅	nd formering -		1110-BB	「「日本の日本」」	

So, C of i plus 1 that we have over here is I will just rewrite this C of i plus 1 over here is equal to C of i plus h multiplied by S and for h, we will again put the dollar signs over here and that is our concentration computed at volume equal to 1. Then what we will do is, we will take this and we will just drag it to the next row. And now, we have concentrations and k 1, k 2, k 3, k 4 and S computed on the next row and we can just copy all of these and just drag them over here and we have the results.

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	ACIAV -	c125/2		(0) - 10		-	0	1		
1	ac/av =	-6 12		C(0) = 1.0	-					
ł	h									
-		*		OURTH-O		GE-KUTT	A METHO	0		
	V(i)	TRUE	C(i)	k1	k2	k3	k4	s	Error	
	0	1	1	-0.5	-0.349	-0.3934	-0.2676	-0.3754	0	
7	1	0.6243	0.62459	-0.2776	-0.2028	-0.2225	-0.1601	-0.2147	0.00047	
	2	0.4096	0.40988	-0.164	-0.1241	-0.1336	-0.1002	-0.1299	0.00068	
	3	0.27976	0.27998	-0.1018	-0.0792	-0.0841	-0.0651	-0.0823	0.00077	
10	4	0.19753	0.19769	-0.0659	-0.0525	-0.0552	-0.0438	-0.0542	0.0008	
11	5	0.14341	0.14353	-0.0442	-0.0358	-0.0374	-0.0303	-0.0368	0.0908	
12										
13										
54	RK-4									
15	k1 = f(yi)									
26	k2 = f(yi +	h*k1/2)								
17	k3 = f(yi+	h*k2/2)								
10	k4 = f(yi+i)	h*k3)								
13	5 = 1/6	* (k1 + 2*)	k2 + 2*k3 -	+ k4)						
-	C(1-1) = C	(i) + h*S								
2	S									
2	A	et . 864 . 8	Me's - 2 Md	Point Hathod	RK-4 Hathod	Greater	-			

So, now, what we see is and we need to change it from midpoint method, of course to Runge-kutta fourth order method, format cells, alignment merge cells, horizontal alignment will be centered, fourth order Runge-kutta method.

So, now, we have the results for r k - 4 method using h equal to 1, and for h equal to 1 the error is 0. 0 8 percent, which is much lower than the errors that we had obtained earlier; I will copy this and paste it in our comparison section, paste special and we just want the values. Now, what I will do is I will just change the format of the numbers, rather than a general format, I will change it to the scientific format with two decimal places. So, we get 8 into 10 to the power minus 4 that is the error that we get you with h equal to 1.

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Now, I do not need all these; so I will just go ahead and delete them and now we want what we want do... I will just save the file right now yes. Now, what we want to do is recompute this for h equal to $0 \cdot 5$, and we want to see how the error decreases for h equal to $0 \cdot 5$. So, with that, now V has gone from h equal to zero v equal to 0 to v equal to 2. 5 when h is half. So, I will have to just select this last row and just drag it, until we reach 5.

So, now, when we half the overall h what happened is, the error decrease from 0.0 0 eight sorry . eight percent 0. 08 percent to 0.004 percent, which is approximately I would say eighteen times or twenty times decrea[ses]- reduction. So, if we take the coef[ficient]... divided this by this guy, we have essentially the error has decreased almost by a factor of 18.

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			c .	0	4			1.00	1	-	-
6.	0	1	1	-0.5	-0.4612	-0.4642	-0.4285	-0.4633	0		
7	0.25	0.88419	0.88419	-0.4287	-0.3965	-0.3989	-0.3691	-0.3981	4.5E-07		
	0.5	0.78466	0.78467	-0.3693	-0.3423	-0.3443	-0.3193	-0.3436	8.2E-07		
9	0.75	0.69876	0.69876	-0.3194	-0.2968	-0.2984	-0.2774	-0.2979	1.1E-06		
10	1	0.6243	0.6243	-0.2775	-0.2583	-0.2596	-0.2419	-0.2592	1.4E-06		
32	1.25	0.55949	0.55949	-0.2419	-0.2257	-0.2268	-0.2117	-0.2264	1.60E-06		
32	1.5	0.50288	0.50288	-0.2117	-0.1979	-0.1988	-0.1859	-0.1985	1.77E-06		
\$3	1.75	0.45325	0.45325	-0.186	-0.1741	-0.1749	-0.1638	-0.1746	1.92E-06		
34	2	0.4096	0.4096	-0.1638	-0.1537	-0.1543	-0.1448	-0.1541	2.03E-06		
35	2.25	0.37108	0.37108	-0.1448	-0.136	-0.1366	-0.1284	-0.1364	2.13E-06		
20	2.5	0.33698	0.33698	-0.1284	-0.1208	-0.1212	-0.1141	-0.1211	2.21E-06		
17	2.75	0.30671	0.30671	-0.1141	-0.1075	-0.1079	-0.1017	-0.1078	2.27E-06		
38	3	0.27976	0.27976	-0.1017	-0.096	-0.0963	-0.0909	-0.0962	2.32E-06		
13	3.25	0.25571	0.25571	-0.0909	-0.0859	-0.0862	-0.0814	-0.0861	2.36E-06		
20	3.5	0.23419	0.23419	-0.0815	-0.0771	-0.0773	-0.0731	-0.0772	2.39E-06		
23.	3.75	0.21489	0.21489	-0.0732	-0.0693	-0.0695	-0.0658	-0.0694	2.42E-06		
22	4	0.19753	0.19753	-0.0658	-0.0624	-0.0626	-0.0594	-0.0626	2.43E-06		
22	4.25	0.18189	0.18189	-0.0594	-0.0564	-0.0565	-0.0537	-0.0565	2.44E-06		
24	4.5	0.16777	0.16777	-0.0537	-0.051	-0.0511	-0.0486	-0.0511	2.45E-06		
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So, the error with h equal to 0 . 5 is approximately one eighteenth of the error with 0 . o[ne]- sorry with h equal to 1. Now, we repeat this with h equal to 0 . 2 5, again we will take the last row and just copy downwards and see check the error at volume equal to 5, and at volume v equal to 5 the error is 2 .44 into10 to the power minus 6. I will do this copy this and I will paste it over here, again paste special and value and again if we take the ratio of the two, the ratio of the two would be would lie somewhere around 15 to 20 that range **S** it does lie in that range, its 17. Actually what we had seen in the earlier class

is error for the local truncation error for the Runge-kutta method is h to the power 5 that was the local truncation error. This one shows the global truncation error, and global truncation error is are of the order of h to the power 4, which means every time we are going to half the h, we are going to increase the accuracy by approximately 16 fold. That is what we saw earlier; the accuracy was increased by approximately eighteen factor of 18; now the accuracy has increased approximately by a factor of 17 and half.

Let us now again repeat this r k method for h equal to 0. 1 2 5; I will just choose this particular row and this copy it below and this is the result that we get. So, now, the error has decreased to 1 .5 E minus seven. I will just paste special, I will just paste the values and again, I will try take the ratio; this divided by this and this ratio is now 16.7.

So, in all cases the ratio is indeed (()) around 16, that is, when we take the ratio of the accuracy of r k - 4 method using h eq[ual]- h and using h by 2. So, just recap what we get is, when we half the h in Euler's method, the accuracy also the error also half or the accuracy doubled; when we half the h in midpoint method, the accuracy changed by a factor of 4; and when we half the r k method, the h in the r k method, the accuracy changed by a factor of 16.

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These are all what are known as global truncation errors and I will I will add another plot over here, where the name of the plot is going to be r k - 4. The x axis values are going to

be the h values and the y axis value. You have to delete the value 1 over here, before we choose the row. So, here we have chosen this row sorry not the row the column and we have the result also over here.

As you can see r k - 4 method is significantly more accurate than than the Euler's method. The Euler's method using h equal to 0 .1 2 5 has an accuracy of about 4 percent, whereas r k - 4 method using h equal to 1 has an accuracy of 0. 08. Keep in mind that r k - 4 method uses four computations of the slope. So, the slope is computed at y i at the midpoint twice and at the end point, whereas Euler's method is just going to use the slope computed only once.

So, **f** for each implementation of Euler's method the function f of (y, t) is used once, whereas for each implementation of r k method, y of t is used 4 times. So, a fair comparison would be when Euler's method is used with h equal to 0 .1 2 5 versus r k - 4 method used for h equal to 1, and even that comparison shows a significant accuracy of the r k - 4 method over the Euler's method.

And this is the plot of the log-log plot of how error changes with this step size. And this particular line is going to have a slope of minus 4 this line has a slope of sorry a slope of 4; this line has a slope of 2 and this line has a slope of 1. Even though, it might not look this way, because of the range of this ordinate versus the range of the abscissa that we had over here.

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So, that is essentially what we have with respect to comparison for the various r k methods with the Euler's method. What I will do is, I will just recap what we have done so far in in the 4 lectures, in the previous three lectures in this particular module. The overview, we are going to consider Runge-kutta family of methods; we have considered Euler's method ;we have talked about implicit and explicit method; we have considered higher order Runge-kutta method; we have done error analysis, what is left to do is this stability analysis that will be do in the next lecture of this module.

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Now, let us give an overview of r k - 2 methods. We are going to use r k - 2 method as a weighted average of slope computed at two points between t i and t i plus 1, where k 1 is the slope computed at t i, and k 2 is the slope computed somewhere between t i and t i plus 1.

We use Taylor series expansion to get the derivation for r k - 4 method and these were the results that we got - some of the weights w 1 plus w 2 should be equal to 1; w 2 multiplied by p 2 should be equal to half and w 1 mul[tiplied]- w 2 multiplied by q 2 1 should be equal to half again.

In yesterdays sorry in in the previous lecture of this module, we had used the te[rm]term w 2 multiplied by p and w 2 multiplied by q, instead of that I have used the subscript 2 and subscript 2, 1 in a below p and q, and the reason for this I will be evident from when we go to extension to higher order r k methods.

And the standard way of writing these weights is in a tabular format of this type, we draw two lines, one vertical line and one horizontal line. To the left of the vertical line, we will write p 2 p 3 p 4 and so on for up to p n for r k n method and to below this horizontal line, we will write the weights w 1 w 2 and so on up to w n and the q values come over here.

So, for example, let us consider the midpoint method. In midpoint method, the value of p 2 was equal to the value of p 2 that we chose was half, because value of p 2 we chose was half, the value of q 2 was also half. And the weight that weights that we got were 1 for w 2; and for w 1 it was 0 and this is represented as half half for (Refer Time: 47:00) the p and q values, and 0 and 1 for the weight values. There is no q 2 term over q 2 2 term in second order r k method; the q 2 2 term would be y i plus q 2 2 1 multiplied by h k 1 plus q 2 2 multiplied by h k 2.

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But keep in mind, if we had q 2 2 multiplied by h k, we will not have an explicit method anymore, because k 2 itself will depend on k 2. So, this will become a semi implicit method, if we were to have this term as non- zero. And then, in Heun's method, for Heun's method what we said was p o[ne]- p 2 p we said was equal to 1; when p was equal to 1, q also we got equal to 1.

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So, p and q are both equal to 1; based on this our w 2 was equal to half, and w 1 was also equal to half. So, what we have is p and q were both 1 and 1, and w 1 and w 2 are both half and half, and there is no q 2 2 term and that is essentially the Heun's method. And finally, we also talked about the Ralston's method, and for Ralston's method our p 2 was equal to three fourths q 2 q q 2 1 was three fourths, and the weights were 1 by 3, and 2 by 3 that is about the r k - 2 method. We can then go on to discuss about a general r k n

method, and the general r k n method will be written as a weighted sum of slopes k 1, k 2, k 3 up to k m k n.

So, its h multiplied by w 1 k 1 plus w 2 k 2 and so on up to w n k n k 1 is of course, as before computed as f of (y i , t i) and k m is com[puted]- is a slope computed at some points within that particular rectangle that we had shown in the geometric interpretation.

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So, its computed at t i plus some quantity p m multiplied by h, and y i is h multiplied by again a weighted sum of k 1, k 2, k 3 up to k m minus 1 that is how the r k n method will look like. And for r k - 4 method, we will have k 1 and then, this expression for k – 2. k 2 will consider q 2 1 and p 2; k 3 will considered to q 3 1 q 3 2 and p 3; and k 4 will have q 4 1 q 4 2 q 4 3 and p 4.

So, the particular table in case of r k - 4 method will have p 2 p 3 p 4, q 2 1 q 3 1 q 4 1, q 3 2 q 4 2, q 4 3, under weights w 1 w 2 w 3 w 4. So, as long as this table is given to you and I tell you that this is going to be the r k - 4 method, we can then use these particular values in order to solve the ODE using r k - 4 method.

So that is where we will end this lecture of module 7. In the next lecture, we will start of again considering the r k – 4 method, we will again look at the geometric interpretation of r k - 4 once for one final time before proceeding on to the predictor corrector methods Thanks.