Computational Techniques.

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Module No. # 07

Lecture No. # 09

Ordinary Differential Equations

(Initial Value Problems)

Hello and welcome to this last lecture - lecture 9 of module 7. What we have been doing so far, is consider several methods for solving initial value problems, of our ordinary differential equations. We started off with Runge-Kutta family of methods, talked about the stability analysis, the error analysis for this method, saw that the essentially the implicit methods are much more stable than the explicit methods; implicit methods are in fact globally stable methods. And then, we talked about in the previous a couple of lectures, some of the advanced techniques for adaptive step sizing and improving the accuracy of the overall numerical solution. And finally, what we discussed in perhaps the last 10 or 15 minutes of the previous lecture was another set of, another family of methods called the multi-step methods.

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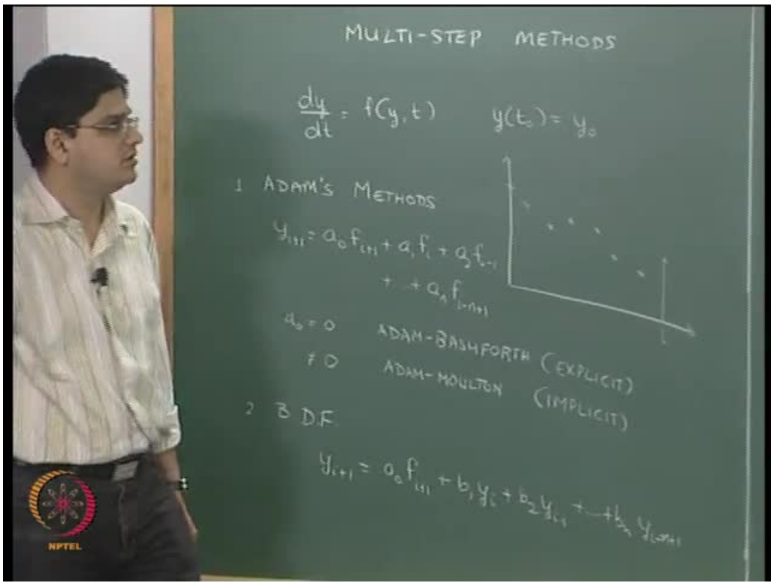

So, that is what we are going to discuss in this particular lecture. So, the difference between the Runge-Kutta family of methods and the multi-step methods is this: the multi-step methods, we are going to use the past information, whereas in the Runge-Kutta methods, we discarded all the past information and used the information only at y i and t i. However, in order to reach y i from y 0, we have collected information y 0, y 1, y 2, up to y i and that information can presumably be used in order to, one - improve the accuracy of this method and second perhaps to improve the stability of this methods.

So, what we are trying to solve is the equation of the type, dy by dt equal to f (y, t) starting with y at t 0 equal to y 0. And using the chosen method, we have somehow reached at time t i. And at time t i, we have data at various past values and this is the time, t i. And we can use the data, at this various past values, in various different ways. And the two main family of methods, that use this particular data is the Adam's family of methods and BDF or Backward Difference Formula based methods.

The Adam's family of methods, they do not use the y i per say, but they use the function f (y i, t i). So, what you try to do, is try fit a polynomial to the function of the past values of f i's, so that means f i, f i minus 1, f i minus 2 up to f i minus n, you fit a polynomial and then you use that particular polynomial instead of f (y,t). That is what we do in Adam's family of methods; as a result of this, the value in Adam's family of methods is going to be obtained as, y i plus 1 equal to a 0 f i plus 1 plus a 1 f i plus a 2 f i minus 1 and so on up to a n f i minus n plus 1. So, this is how we are going to use the Adam's methods in order to compute the y i plus 1. What we need to do, is find out the coefficients a 0, a 1, a 2 up to a n. Now, again in the Adam's family of methods are of two types: a 0 equal to 0 is Adam-Bashforth methods and a 0 not equal to 0 is Adam-Moulton's method; Adam-Moulton's is implicit, Adam-Bashforth is explicit. So, these are Adam's method.

The second set of methods are what is known as Backward Difference Formula - BDF methods and over there we write, y i plus 1 equal to a 0 f i plus 1 plus b 1 y i plus b 2 y i minus 1 and so on, up to b n by i minus n plus 1; this is going to be our Backward Difference Formula. Now, let us look at how to derive this Backward Difference Formula. It is fairly straight forward; what we have is, dy by dt equal to f (y,t); we express dy by dt using an appropriate backward numerical differentiation and that is how we derive the Backward Difference Formula.

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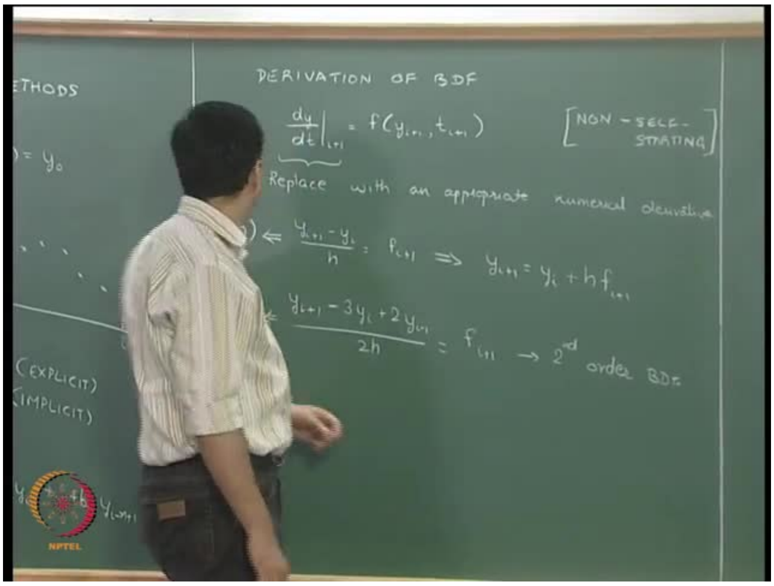

So, dy by dt computed at i plus 1 is going to be f of y i plus 1,t i plus 1; y i plus 1, keep in mind is not yet know. What we can do is, what we can do now is replace with an appropriate numerical derivative. So, the first order Backward Difference Formula, as you might expect, is essentially going to be the implicit scheme or implicit Euler's method. So, if we were to replace this with a first order Backward Difference Formula, it is going to be, y i plus 1 minus y i divided by h is going to be equal to f i plus 1, which will essentially give us y i plus 1 equal to y i plus h times f of i plus 1. This is nothing but our implicit Euler's method. So, this is the first Backward Difference Formula of order 1. Now, if you want to derive the Backward Difference Formula of order 2, we have to replace dy by dt with the numerical derivative of the second order.

What that means, is it is going to be equal to, y i plus 1 minus 3 y i plus 2 y i minus 1 divided by 2 equal to f of i plus 1 divided by 2 h equal to f of i plus 1; and we just rearrange this appropriately in order to get our result for y i plus 1. And this will give us the second order BDF. Recall, that this particular derivative was order h accurate, as a result, the error in first order Backward Difference Formula is of the order of h. This particular method was order h squared accurate, as a result the accuracy of the second order Backward Difference Formula is order of h square. We can have third order, fourth order, fifth order Backward Difference Formula so on and so forth. And we will be able to use an appropriate Backward Difference Formula with an appropriate amount of accuracy.

So, that is it about Backward Difference Formula; there is one more thing, that I will discuss and that is that the BDF methods like Adam-Moulton's method or any multi-step method are non-self-starting. What that means, I will come to that in in a few minutes. Let us go back go forward and discuss about how to get derivation for the Adam's methods. We will just derive for the Adam-Bashforth method, just one derivation for Adam-Bashforth method, would be enough. And I will just talk about Adam-Moulton's method and we will then talk about the range of techniques called Adam-Bashforth Moulton's methods of solving these equations.

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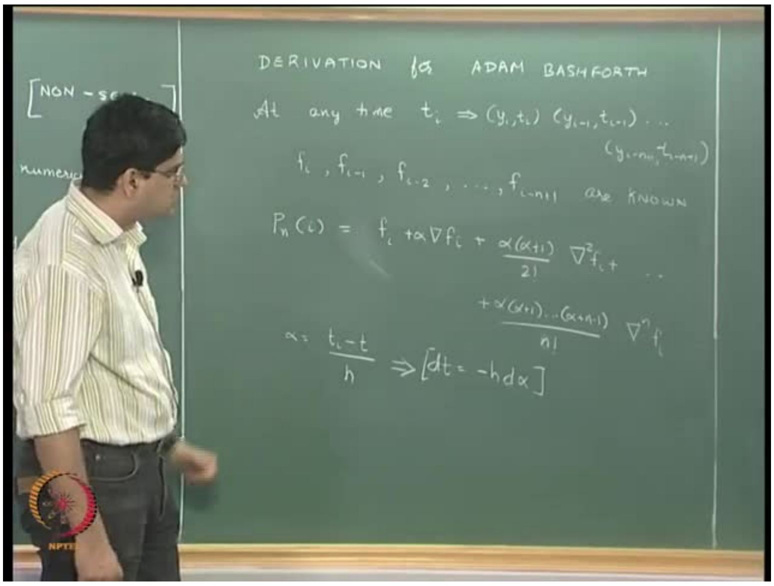

So, derivation for Adam-Bashforth - at any time t I, what we assume is that the data is available for us for the past n times; that means at any time t i, what is available to us is (y i ,t i) (y i minus 1 , t i minus 1) and so on up to (y i minus n ,n t i minus n plus 1). So, n past data points current and past data points; we assume or available to us, if y i t i y i minus 1 t i minus 1 and so on are actually available to us, we can compute f i f i minus 1 so on and so forth.

So, based on this, what we will say is essentially f i, f i minus 1, f i minus 2, and so on up to f i minus n plus 1 are known. So, what we do is we will fit a polynomial to this n past values, what type of polynomial will fit, will go back to, what we discussed in module 5 and we will fit essentially a Newton's backward difference polynomial.

So, a Newton's backward difference nth order, Newton's backward difference polynomial p n; we had written this as equal f P n computed at location i, is going to be equal to f i plus backward difference f i, multiplied by alpha plus alpha plus 1 divided by 2 factorial delta square f i plus So on up to alpha alpha plus 1 alpha plus n minus 1 divided by n factorial delta to the power n f i.

And this is essentially the type of similar type of derivation, if you recall, we had done, when we were trying to derive the Newton's cotes integration formulae also. So, it is the same idea in the Newton's cotes integration formulae, because all the functions where known to us; we could just use the forward difference formulation or we could over there also we could use the Backward Difference Formulation. In this case, the values at y i plus 1, i plus 2, i plus 3, and so on are not known to us; as a result we have to use a Newton's Backward Difference Formula and using this particular Newton's Backward Difference Formula.

Now, we have an estimate of what the slope is going to be, alpha at any time is t i minus t divided by h. So, at i alpha is going to be equal to 0 at i plus 1 alpha is going to be equal to minus ;1 given the data we will now have fitted, let us assume that we have now fitted a polynomial to the past n points.

So, if i plot f versus t, I have this particular polynomial up to the location i, keep in mind here, i am plotting f and not y; what we will assume is we will extrapolate this particular value of polynomial, for this region between i and i plus 1.

So, y i plus 1 is going to be nothing but integral from t i to t i plus 1 P n i dt. So, we have essentially this or rather it is y i plus 1 minus y i is going to be this particular integral. So, we have this particular polynomial that we have just derive, we go from t i to t i plus 1, we integrate that with respect to d t. Now, based on this particular equation dt is going to be equal to minus h times d alpha, and note that we are integrating from t i to t i plus 1 t i represents 0 t i plus 1 equal to minus 1.

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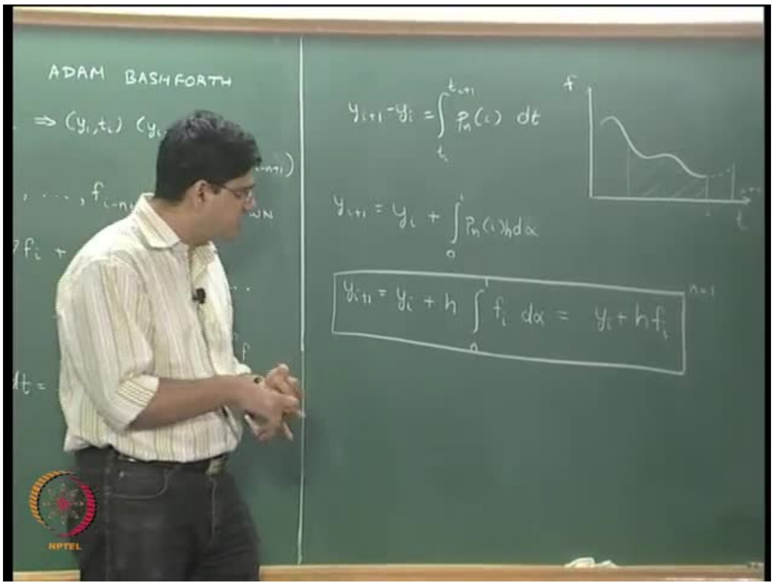

So, the limits of integration are going to be from 0 to minus 1 and we can substitute alpha equal to minus alpha and redo it the and solve this particular derivation and will be able to get y i plus 1 is going to be equal to y i plus integral from 0 to 1 P n of i dt, no matter what value of n we choose the limits of integration are going to remain from 0 to 1 this should not be t it should be actually alpha.

So, now, let us look at the first order Adam-Bashforth method. First order Adam-Bashforth method is going to lead us to nothing but the Euler's explicit method. So, first order Adam-Bashforth method, basically is going to be that we will be left only with f i and if that means we are only going to use 1 previous point f i.

So, if we were, we were, to in put this over here, what we are going to get is y i plus 1 equal to y i plus h multiplied by it; this should be h d alpha, when we replace dt is going to be h d alpha and that is where this h comes from 0 to 1 is going to be f i multiplied by d alpha, which is going to lead us to y i plus h times f i. So, this is going to be our first order Adam-Bashforth method. So, n equal to 1 Adam- Bashforth method is nothing but the Euler's method, the beauty about all these derivations, that where you have seen so far is the first order Runge-Kutta method reduces to nothing but the explicit Euler's method, the BDF formula we of first order reduces to implicit Euler's method, Adam-Bashforth method reduces to for n equal to 1 reduces to nothing but the explicit Euler's method; likewise the Adam-Moulton's method, which we would not do the derivation for in this lecture is going to reduce to nothing but the implicit Euler's method.

And the second order Adam-Bashforth method, if we go on to this particular type of a formula. Second order Adam-Bashforth method, is going to use f i and f i minus when reduces f i and f i minus 1 in this particular polynomial that we have we will be left with these 2 terms.

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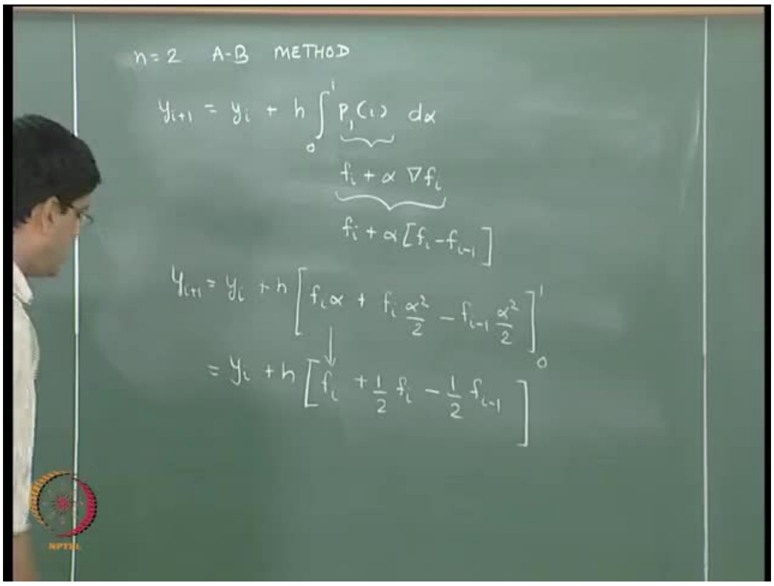

So, for the second order Bashforth method, the derivation is going to be y i plus 1 equal to y i plus h times integral from 0 to 1 p 1 i d alpha based on the notations that we have been using consistently since module 6 p 1 i is nothing but f i plus alpha times delta f i, which is nothing but f i plus alpha times f i minus f i minus 1.

So, we substitute this over here and integrate, we will get y i plus 1 equal to y i plus h multiplied by f i alpha plus f i multiplied by alpha square by 2 minus f i multiplied by alpha square by 2 going from 0 to 1.

So, this will reduce to f i multiplied by 1 minus 0, which is going to be f i. This is going to be nothing but f i multiplied f i multiplied by half minus 0 that is going to be plus half f i and this is going to be f i multiplied by 1 by 2 minus 0 that is going to be f i minus 1 that is going to be f my i minus 1 multiplied by half and that is the negative sign over here.

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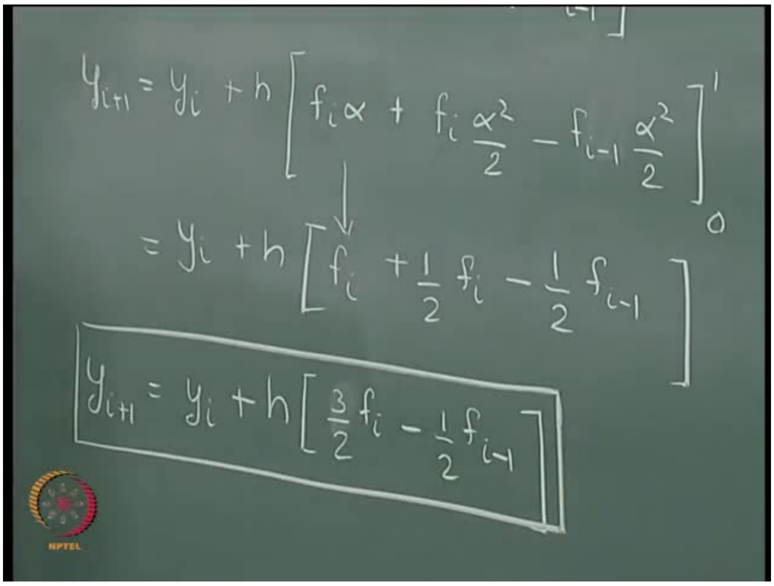

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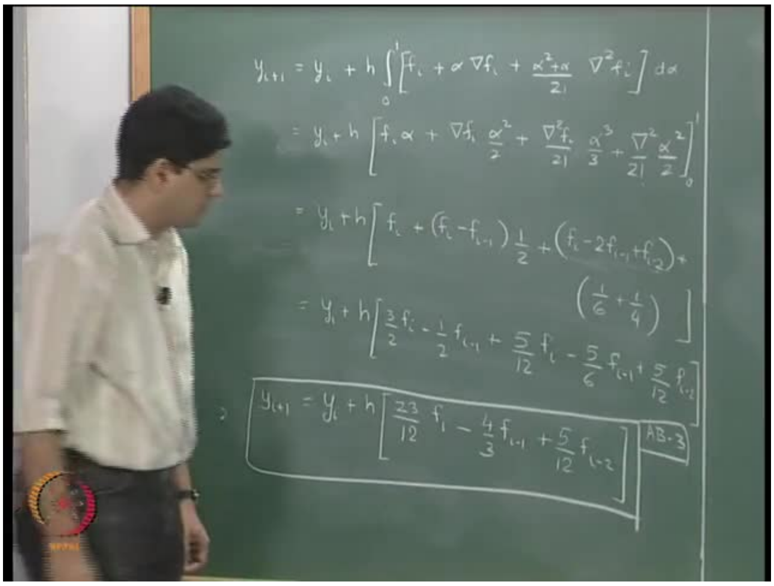

So, it is half f i minus 1 multiplied by h plus y i and finally, our result is going to be y i plus 1 equal to y i plus h times 3 by 2 f i minus 1 by 2 f i minus 1 this is Adam-Bashforth method of order 2. And in deriving third order of Adam-Bashforth method, we are going to say y i plus 1 equal to y i plus h times again integral from 0 to 1 p 2 of i multiplied by d alpha.

Now p 2 is going to be f i plus alpha times del f i plus alpha alpha plus 1 del square f i. So, this is going to be f i plus alpha del f i plus alpha square plus alpha by 2 del square f i d alpha, which is going to be equal to y i plus h f i alpha. So, now we are just integrating this, there is no alpha over; so, it is going to be f i alpha plus del f i alpha square by 2 plus del square f i by 2 factorial multiplied by integral of alpha square d alpha that is going to be alpha cube by 3 plus del square by 2 factorial alpha square by 2 alpha going from 0 to 1.

And that we will be able to write as, y i plus h since alpha goes from 0 to 1, the difference is just going to be equal to this is going to be 1,(Refer slide time 22:22) this will be replace by 1, this will be replace by 1 and this also will be replace by 1.

So, we will have f i multiplied by 1 plus del f i del f i is nothing but f i minus f i minus 1 f i minus f i minus 1 multiplied by half plus del square f i del square f i, if we recall, it is f i minus 2 times f i minus 1 plus f i minus 2.

So, this entire term is going to be multiplied by 1 by 6 plus 1 by 4. So, that is going to be y i plus h times 3 by 2 f i minus 1 by 2 f i minus 1 plus; this term is going to be 4 plus 6 10 by 24 10 by 24 is 5 by 12 plus 5 by 12 f i minus 2 multiplied by 5 by 12 that is 5 by 6 f i minus 1 plus 5 by 12 f i minus 2.

And this finally, will lead us to y i plus h multiplied by 3 by 2 plus 5 by 12. So, that is 6 18 by 12 so 18 plus 5 is 23 23 by 12 f i minus half plus 5 by 6 that is going to be 3 by 6 plus 5 by 6 that is going to be 8 by 6. So that will be 4 by 3 f i minus 1 plus 5 by 12 f i minus 2 and this is going to be our, Adam-Bashforth third order method. So, this is the results for Adam-Bashforth third order method, for a forth order method in addition to this we will have alpha alpha plus 1 alpha 2 divided by 3 factorial multiplied by del square f i over here will do that integration, will do the substitution and will get a forth order, fifth order,sixth order and higher order Adam-Bashforth method.

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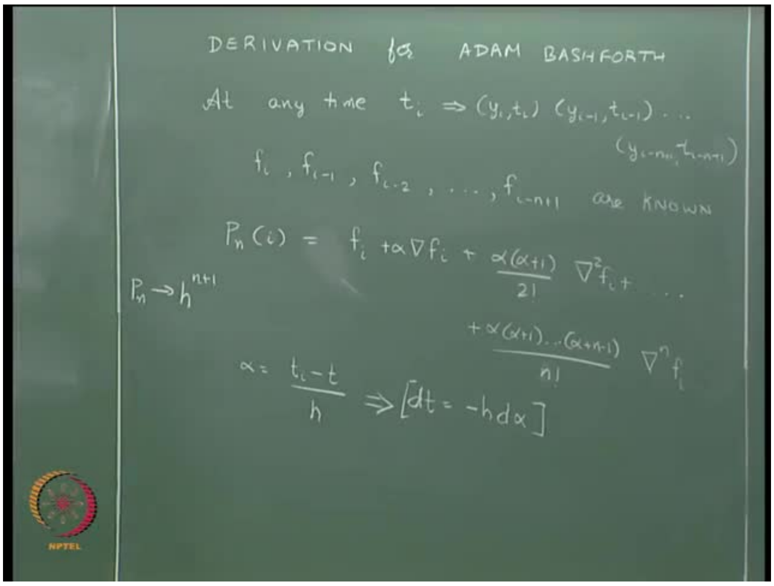

Now, what is the accuracy of nth order Adam-Bashforth method, if we go back and see what the errors are going to be for this? So, let us go back and look at the polynomial expression for an nth order polynomial expression for P n, the error is of the order of h to the power n plus 1.

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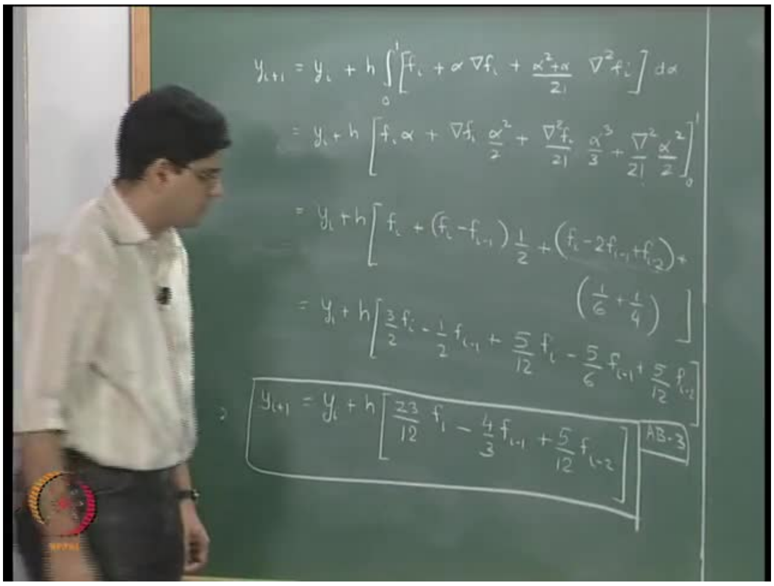

So, now, if we substitute that over here, an nth order Adam-Bashforth method uses P n minus 1. So, an nth order Adam-Bashforth method, because it uses P n minus 1 the order of accuracy of the polynomial used in nth order Adam-Bashforth method is h to the power n.

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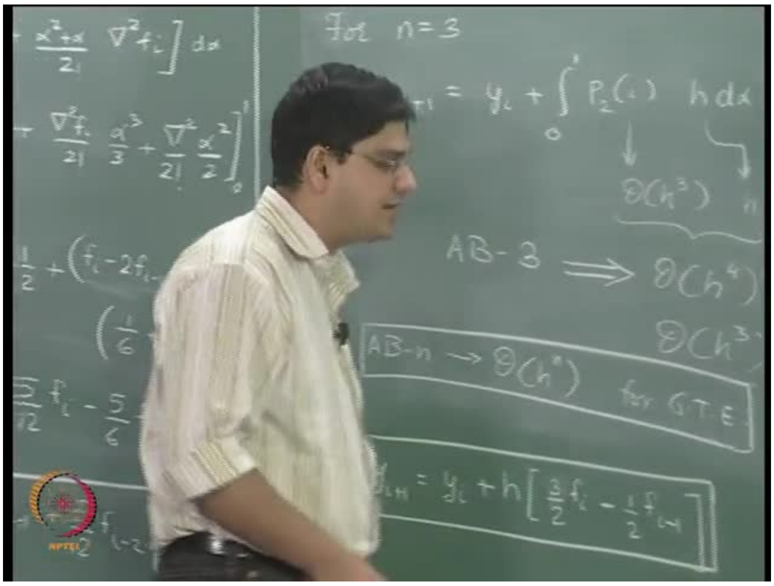

And now, there is this h term that comes in over there, which makes the nth order Adam-Bashforth method the local truncation error of that is going to be h to the power n plus 1, I will write down, what I have said over here, for n equal to 3 for n equal to 3 y i plus 1 equal to y i plus integral from 0 to 1 p 2 h d alpha.

Now, for p 2 the accuracy is of the order of h cubed. This is what we had derived when we talked about the backward difference Newton's backward difference interpolating polynomials in module 6 and then, there is this h term that comes over here.

So, h multiplied by a number that is order of h cube accurate becomes order of h to the power 4 accurate. As a result, Adam-Bashforth method of order 3 has a local truncation error of h to the power 4 and the global truncation error is going to be of the order of h to the power 3. And that will work for any nth order Adam-Bashforth method, as the order of the Adam-Bashforth method increases, the accuracy also tends to increase.

So, AB n accuracy of or the global truncation error is going to be of the order h to the power n for global truncation error. So, that is the result for Adam-Bashforth method what we do in Adam-Moulton's method is the same thing but will have to get the polynomials, which involve f i plus 1, also because what we are trying to do in the Adam-Moulton's method is we also have the f i plus 1 term.

So, in the first order Adam-Moulton's method, we have f i plus 1 and f i. Second order Adam-Moulton's method f i plus 1, f i, f i minus 1, so on and so forth. We fit an appropriate size polynomial and then proceeds in exactly the same manner, as we did for the Adam-Bashforth's method. I would not go over the derivation of the Adam-Moulton's method, but now i will talk about some practical issues in implementation of Adam-Bashforth method or in general for any of the multi-step method.

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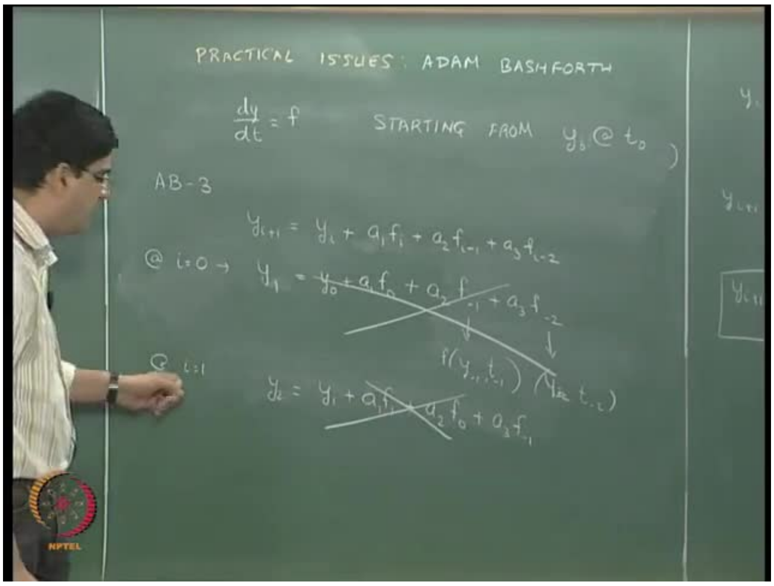

So, we start off with dy by dt equal to f starting from y 0 at t 0. Now, when we start let us consider the Adam-Bashforth third order method. So, y i plus 1 for Adam-Bashforth third order method is going to be y i plus a 1 f i plus a 2 f i minus 1 plus a 3 f i minus 2; where if we go back to this particular derivation a 0 a 1 is 23 by 12 a 2 is minus 4 by 3 and a 3 is 5 by 12.

So, these are the values of coefficients that we can use in this particular Adam-Bashforth formula. So, this is the overall Adam-Bashforth formula at i equal to 0. The formula is going to be y i plus 1 equal to y i plus a 1 or y 1 equal to y 0 plus a 1 f 0 plus a 2 f minus 1 plus a 3 f minus 2 f minus 1 is f computed at y i y minus 1, t minus 1 and this is at y minus 2 and t minus 2.

Keep in mind, that we know the value at y 0. we do not know the value at y minus 1; we do not know the value at y minus 2; so at i equal to 0 the Adam-Bashforth method cannot be used. Let see, what happens at i equal to 1 at i equal to 1 y 2 is going to be equal to y 1 plus a 1 f 1 plus a 2 f 0 plus a 3 f minus 1, again f minus 1 is not known to us, if a f minus 1 is not known to us we cannot use Adam-Bashforth method at i equal to 1 either.

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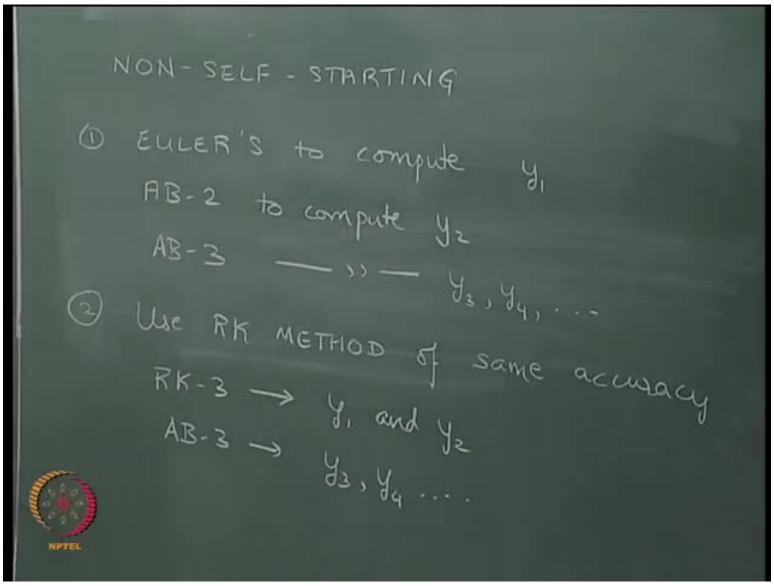

At i equal to 2, what happens y at i equal to 2 y 3 is going to be equal to y 2 plus a 1 f 2 plus a 2 f 1 plus a 3 f 0. Now, from starting from i equal to 2 we can actually use Adam-Bashforth third order method. So, Adam-Bashforth nth order methods can be used to compute y n onwards it cannot be used to the compute y 0 y 1 and so on up to y n minus 1 so this is what is known as these methods are non-self-starting.

So, when we are at y 0, we cannot use Adam-Bashforth method; when we are at y 1, we cannot use Adam-Bashforth method; when we are at y 2, we cannot use Adam-Bashforth method from y 3 onwards, we can start using the Adam-Bashforth third third order method.

So, what is the solution? They are various ways to do 1 is, you can use the Euler's method to compute y 1, you can use Adam-Bashforth second order method to compute y 2 and so on, you can use Adam-Bashforth third order method to compute y 3 and all the future wise.

So, this is 1 possibility. Now, the problem with this is the Euler's method is h square accurate, Adam-Bashforth second order method is h cubed accurate. So, we are losing on the accuracy; so, these are again the local truncation errors, we are losing on the accuracy by using the less accurate methods in order to start this particular system.

The second possibility is to use the self-starting methods, such as the Runge-Kutta method. And the RK method of the same accuracy, that we can use is essentially the RK 3 method, RK 3 method, will be used to compute y 1 and y 2 and Adam-Bashforth 3 method will be used to compute y 3, y 4 and so on. So, these are the two possibilities that we can use in that we can implement in order to use the Adam-Bashforth non-self-starting methods. So, this is 1 of the issues that the multi-step methods phases is not just the issue with Adam-Bashforth method it is issue with all the 3 methods Adam-Bashforth Adam-Moulton's and the Backward Difference Formula methods. And these are the ways to handle them, of this two ways - this is typically, the preferred way. It is preferred really because you can maintain, the same level of accuracy for very stiff problems and from for problems in which, the lambda values are very high. Under those conditions, what happens with the RK method essentially is that you need to use really small step sizes in order to get good solution from the RK method.

But other than that, this is essentially the procedure that is going to be use in order to start to use in all self-starting methods.

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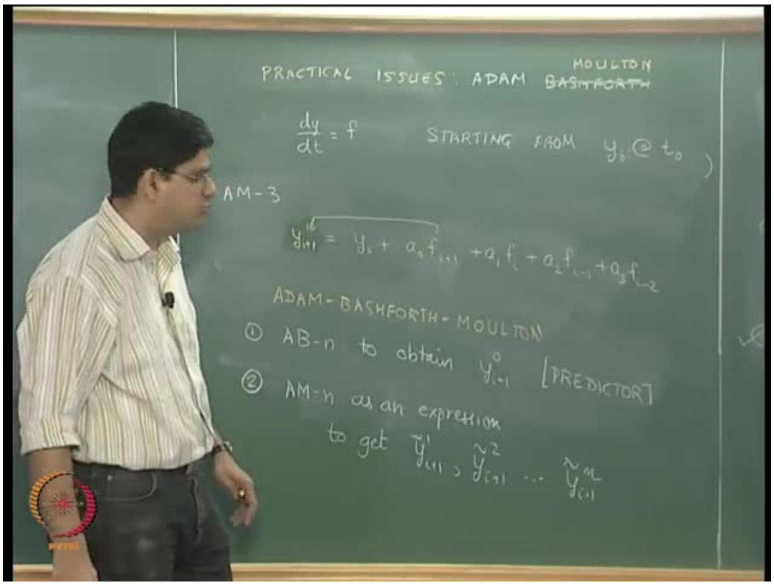

Now, when it comes to implementing the Adam-Moulton's method, we have we will have the same practical issues as the Adam-Bashforth method, there is 1 more challenge to it and that is these equations are written the AB AM 4 is going to be written implicitly, or AM 3 will be written in the form of y i plus 1 is going to be equal to y i plus a 1 a 0 f i plus 1 plus a 1 f i plus a 2 f i minus 1 plus a 3 f i minus 2.

So, now, this y i plus this f i plus 1 depends on y i plus 1 making this an implicit scheme. So, we have this non-linear equation, which we need to solve in order at each time interval, in order to get the Adam-Moulton's method. And finally, we come to the last technique and that is known as Adam-Bashforth Moulton method. And the relationship between Adam-Moulton and Adam-Bashforth method is the same as the relationship between the predictor corrector Heun's method and the implicit Crank-Nicholson method that is in implicit Crank-Nicholson method, we need to solve this equation repeatedly, until the convergence is reached. on the other hand in the predictor corrector method. What we do is we use a predictor equation and this particular equation is use as an expression that ends up the corrector equation.

So, what we do is in Adam-Bashforth Moulton method is first use, AB n to obtain y i plus 1 0. So, the Adam-Bashforth method is used as a predictor and next you use AM n as an expression to get y i plus 1, 1 y i plus 1 to and so on up to y i plus 1 m

So, we repeat the corrector equation fixed n number of times in order to get and improved solution using the Adam-Moulton's method, so Adam-Bashforth Moulton's method is a predictor corrector method.

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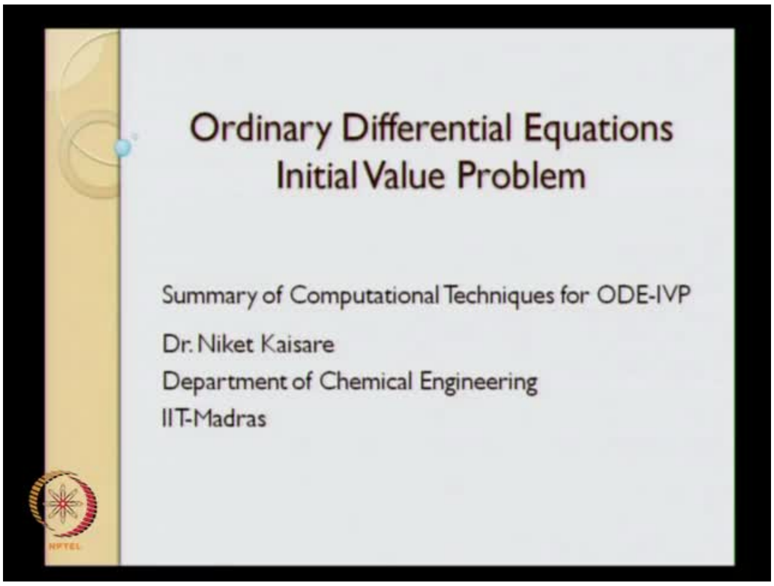

Where the Adam-Bashforth is used as a predictor, and Adam-Moulton is used as corrector. So that essentially finishes the what wanted to cover in module seven, what i will now do is spend a next 8 to 10 minutes recapping the every everything that we have manage to cover in this particular module.

Now, what i am going to do is spend the next few minutes, recapping what we have done in the last 9 lectures, in for the numerical methods for solving the ordinary differential equation initial value problem.

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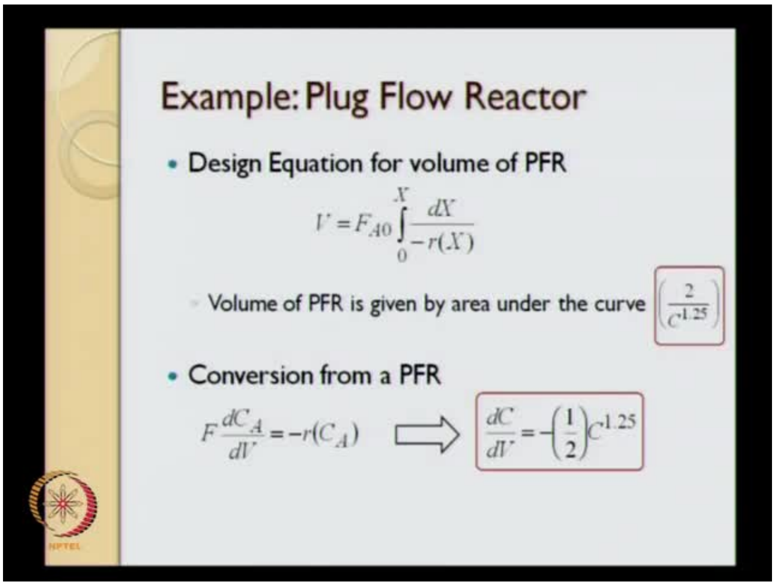

We started off with an example of the plug flow reactor, what we said is that for a state forward single reaction system, we have the design equation for the plug flow reactor, where the volume of the plug flow reactor is going to given by area under the curve for the specific example that we took the volume of the PFR was computed by area under the curve 2 divided by c to the power 1 point 2 5.

And this area gave us the total volume of the PFR required to reach a certain conversion x what we said was that this particular design equation is obtained from this particular ordinary differential equation. And then we recast the overall problem as a problem of solving the ordinary differential equation given the initial concentration C at volume v equal to 0.

And the entire lecture series, all the 9 lectures, in this particular module, what we have done is we have use this example in order to compare the various method contrasts the various methods and try to prove essentially some of the things that we were interested in knowing in this particular method.

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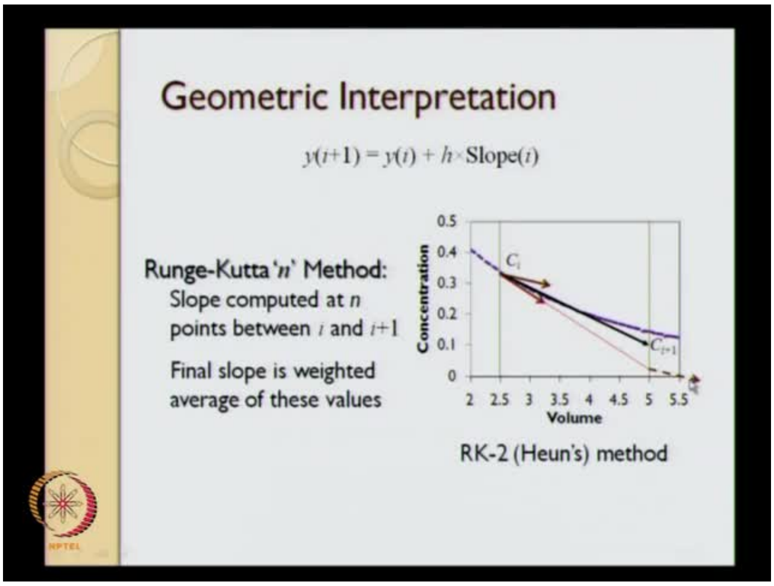

Now, let me just talk about the geometric interpretation, we have covered geometric interpretation multiple number of times, what we do in any kind of an o d e solving technique is y i plus 1 is given as y i plus h times certain slope. Now, this slope in Euler's explicit method is nothing but the slope computed at C i, V i in Euler's implicit method is nothing but the slope computed at C i plus 1, V i plus 1 in Runge-Kutta method; we use multiple points between t i and t i plus 1 in this particular case between v i and v i plus 1.

So, nth order Runge-Kutta method uses slope computed at n points between i and i plus 1 both this points may be inclusive and the final slope is nothing but the weighted average of these values. What am showing over here is RK 2 Heun's method. In Heun's method, what we do is this particular red arrow is the slope computed at C i, V i based on the slope computed as C i, V i, we project at this particular point.

Note that this is not c i plus 1, this is just the projection of C i at V i plus 1 using the slope at V i. So, this is the projection, we compute the slope over here. The slope is shown by this particular dotted line, the slope of this line and slope of this this particular arrow is the same and the average of these 2 slopes is the actual slope, shown by this black line; we use this slope in order to get C i plus 1 in the Heun's method.

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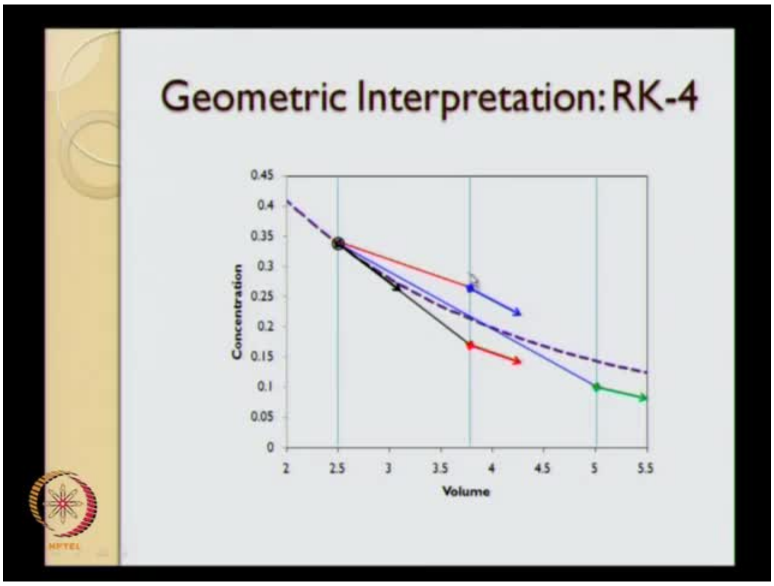

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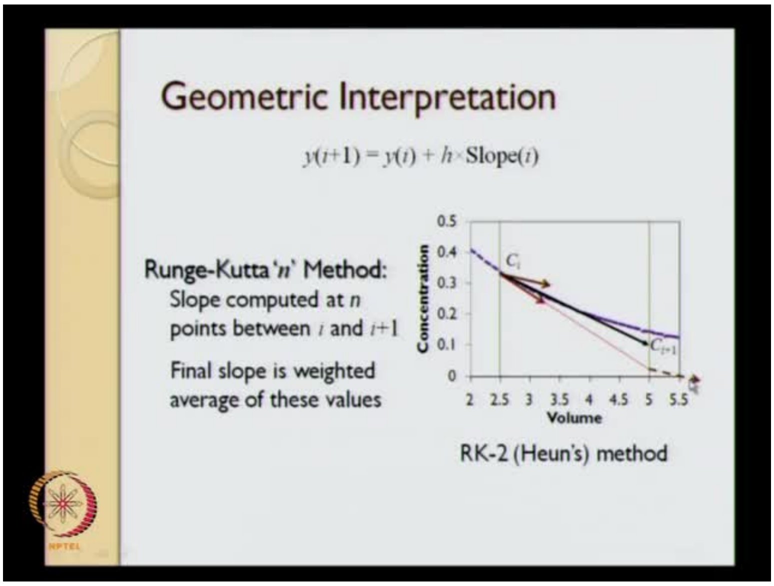

Then, we took up the geometric interpretation of the fourth order Runge-Kutta method. The classical fourth order Runge-Kutta method use slope at V i then, use slope at v i plus half then use slope at the improved value of V i plus half and then use the slope at V i plus 1. So, we had those 4 slopes. This black line, red line, blue line, and this green line and the final slope was nothing but the weighted average of all these 4 lines that was RK 4, Let us go back 1 more slide and just talk about the Heun's method. Again Heun's method computes the slope at V i computes the slope at projected value of C i plus 1 at V i plus 1 not the actual value of C i plus 1 and V i plus 1.

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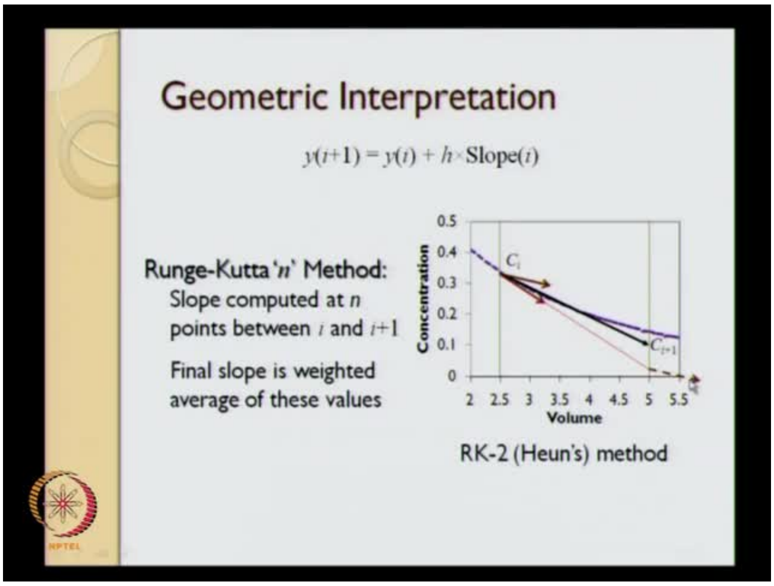

The predictor corrector method again does the similar things but in in an iterative way what we do is this red arrow is nothing but the predicted value C i plus 1. This predicted value of C i plus 1 is use to compute the new predicted value of C. The new corrected value of c i plus 1 first time this slope at C i plus 1 1 is come use to get the average again c i plus 1 to so on and so forth. We use this particular prediction and correction multiple number of times in order to finally get C i plus 1 and then we talked about crank-Nicholson method the idea of the Crank-Nicholson method is that this is the red line represents the slope at V i comma C i. This dotted line represents the slope at the final solution which is yet unknown because it is at the true solution at i plus 1, it is the slope at true solution at i plus 1 this is an implicit method why it is an implicit method because this true solution at i plus 1 is not known at time i.

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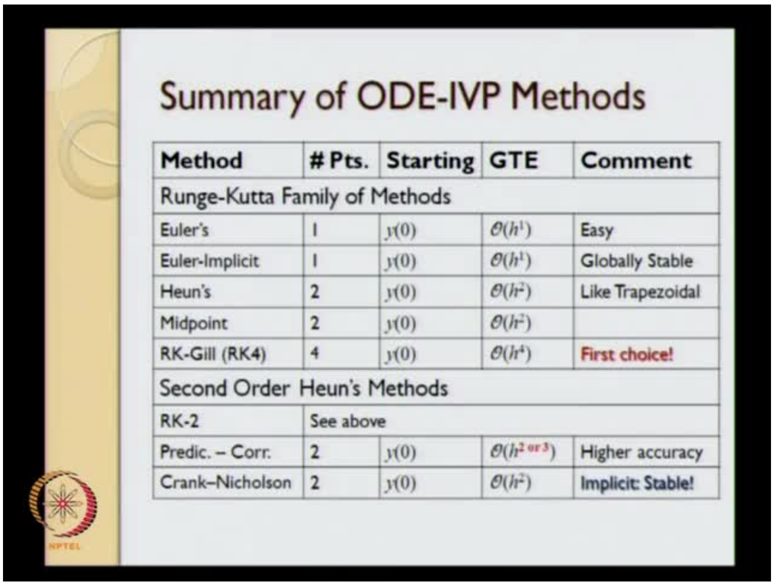

Summary of ODE-IVP Methods

Method	# Pts.	Starting	GTE	Comment
Runge-Kutta Family of Methods				
Euler's	1	$y(0)$	$\mathcal{O}(h^1)$	Easy
Euler-Implicit	1	$y(0)$	$\mathcal{O}(h^1)$	Globally Stable
Heun's	2	$y(0)$	$\mathcal{O}(h^2)$	Like Trapezoidal
Midpoint	2	$y(0)$	$\mathcal{O}(h^2)$	
RK-Gill (RK4)	4	$y(0)$	$\mathcal{O}(h^4)$	First choice!
Second Order Heun's Methods				
RK-2	See above			
Predic. – Corr.	2	$y(0)$	$\mathcal{O}(h^{2 \text{ or } 3})$	Higher accuracy
Crank–Nicholson	2	$y(0)$	$\mathcal{O}(h^2)$	Implicit: Stable!

So, we need to compute both C i i plus 1, as whereas c the slope at c i plus 1. Simultaneously that is the Crank-Nicholson method, so, this actual slope in the Crank Nicholson method is the weighted average of the slope computed at V i and the slope, actual slope computed at V i plus 1. Being an implicit method, it is a globally stable method.

So, this is all we covered in the Runge-Kutta family of methods. And lets us talk about the summary of all these methods, what i am showing over here is the method, the number of points between i and i plus 1 that is used whether, its self-starting or not the global truncation error and general commands. Euler's and Euler's implicit method both use only 1 point, Euler's method uses the point at i; Euler's implicit method uses the point at i plus 1. The global truncation error in both the cases is order of h to the power 1 accurate. Euler's method is very very easy to implement. Euler's implicit method is difficult to implement but it is globally stable. Heun's method is kind of like trapezoidal method, it is not exactly like trapezoidal (( )) it is kind of like trapezoidal method. The Heun's predictor corrector method is much more like a trapezoidal method. The corrector equation is indeed a trapezoidal method. Heun's method uses 2 points and therefore, it is an RK 2 method. Midpoint method, also uses is also an RK 2 method and RK gill method is an RK 4 method. And the global truncation error for second order Runge-Kutta method is h squared. And for the Runge-Kutta gills method is h to the power 4. In general command is, if you do not have any idea of what ODE solver to use, your first choice should be a fourth order Runge-Kutta explicit method.

If you know apriori that the system is very stiff, in that case, go ahead and use implicit methods. But if stiffness is not an issue, then you can go ahead and use the RK 4 method, aAs your first choice; lot of RK 4 methods are now available, if you go to NETLIB - N E T L I B that stands for Network Library NETLIB dot org - you will have a lot of o d e solver techniques that you will be able to download for Fortran, for Matlab essentially you can use ODE 45, which is a fourth order, fifth order Runge-Kutta Cash-Karp method.

Then, we talked about, just a few slides earlier we have talked about comparison of the second order methods. The RK 2 variant of Heun's method is what we have just discuss over here. The predictor corrector form of Heun's method, can be a order h square accurate or h cube accurate - i will come to that in a minute - and the Crank-Nicholson method is an implicit method and therefore, its stable and h squared accurate.

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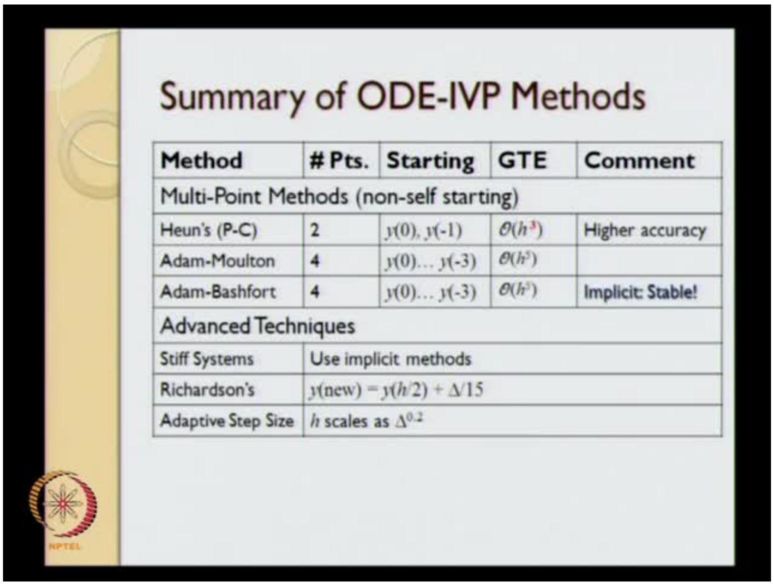

The two probably, the two most popular methods for solving o d e's are the RK 4 method, which is an explicit method and Crank-Nicholson method, which is an implicit method. these This in my experience, are perhaps the 2 most popular methods for solving ODE initial value problems. And then in essentially in today's lecture we covered what is known as the multi-point methods.

And an example of multi-point method is the Heun's predictor corrector; indeed Heun's predictor corrector method is an Adam-Bashforth Moulton method of second order. The Heun's predictor corrector method is a non-self-starting method, which has a global truncation error of h cubed. How it is different from multipoint from the original predictor corrector Heun's method is that; in the predictor corrector Heun's method we use essentially the Euler's method in order to compute the predictor equation.

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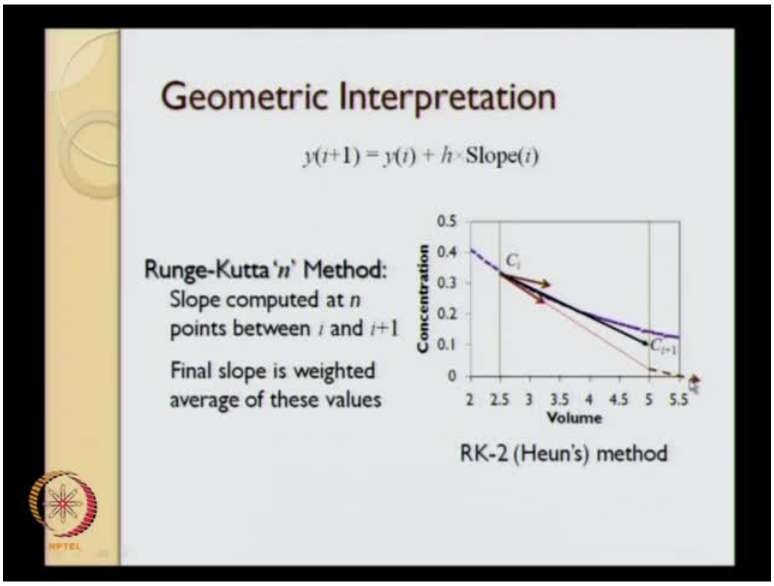

If we go back to this particular slide, what we do is at this particular point, we use Euler's method to project the point in the future. So, the first method is going to be h squared accurate that is the Euler's method.

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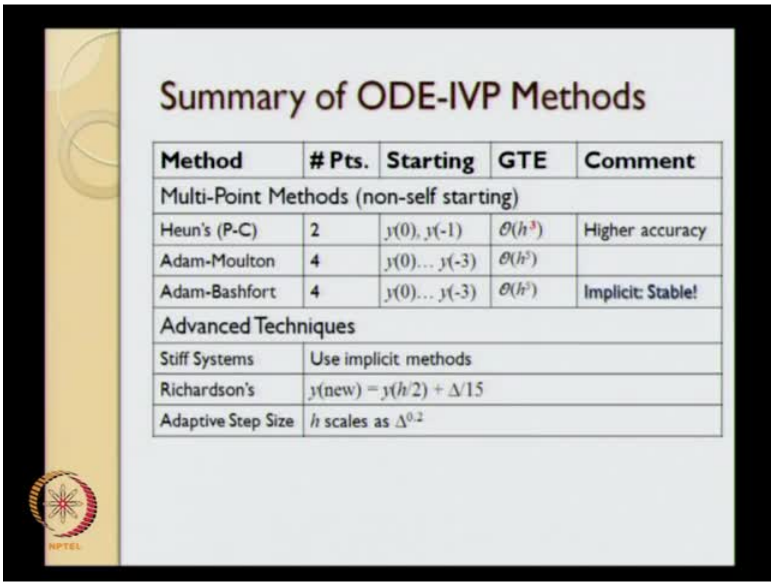

Instead we can replace the Euler's method by a trapezoidal like method and that will give us the multi-point predictor corrector Heun's method. And that is h cubed accurate the Adam-Moulton's method, which takes 4 points is h to the power 4 accurate, there is an error over here this should be h to the power 4. And the fourth order Adam-Bashforth method is an implicit method which is again h to the power 4 accurate.

We also talked about the backward difference methods. Backward difference methods are much more simpler to use than any of the other methods, that we have talked about any of the other implicit methods, that we have talked above except the implicit Euler's method. So, backward difference methods are also popular in what is known as differential algebraic equations? This is just something that i have information and if you do not understand the previous statement, you can ignore it. And then finally, what we have also done is covered the advanced techniques, we just talked about stiff systems.

If the ratio between the largest and the smallest eigen value in your system is greater than 10 to the power 5, do not even think about it just go and use implicit methods. The specific implicit method that i can suggest to you is either the Adam-Bashforth method or the Crank-Nicholson method, you have the choice to use one of the two in Matlab, we have ODE 15 s that solves a stiff system of equation.

The other thing we talked about is Richardson's method, in order to, improve the accuracy is the same idea, as we have covered in the numerical integration section of this particular course. And finally, the adaptive step sizing. And in adaptive step sizing for RK 4 method the step h step size h scales as delta to the power 0 point 2; likewise in fourth order Adam-Moulton's or Adam-Bashforth method h scales, as delta to the power 0 point. And you have the Adam-Bashforth Moulton's predictor corrector methods that ,that, can be used instead of the Adam-Moulton's implicit methods.

So, in summary, if you have to use an ODE solver, try to use the fourth order RK method with adaptive step sizing as your first choice, if that does not work try to use your Crank-Nicholson method. If you need a higher accuracy compare to what Crank-Nicholson method is going to provide you or you may either use the Adam-Moulton's method or backward difference fifth order or fourth order methods, in order to, get a higher set of accuracy. But with this, we end module 7, of our course and i will see you again in module 8, where we are going to discuss - ordinary differential equations boundary value problems.

Thanks.