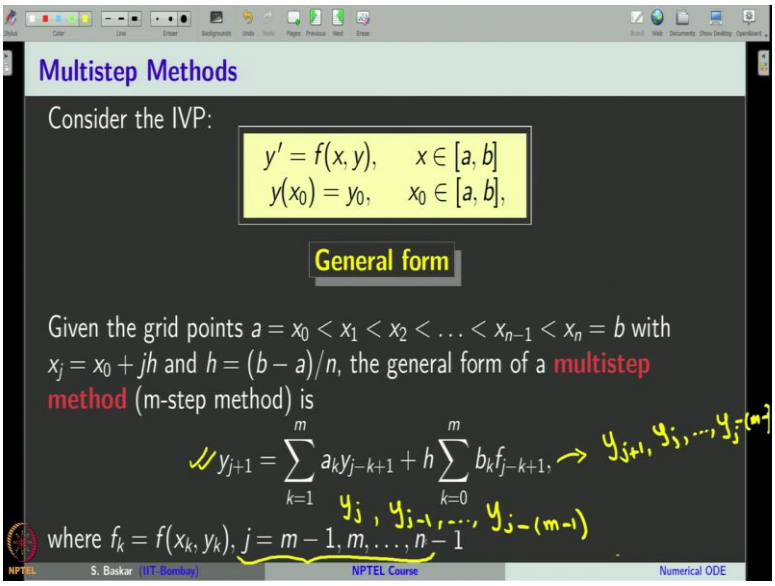
Numerical Analysis
Prof. S. Baskar
Department of Mathematics
Indian Institute of Technology - Bombay

Lecture - 59
Numerical ODEs Multistep Methods

Hi, we are learning numerical methods for initial value problem of first order ODE. We have learned Euler method, Runge-Kutta methods. We have also learned some modified Euler methods. In the last class, we have derived midpoint method and the trapezoidal method. Midpoint method is a 2-step method and trapezoidal method is an implicit method. In this lecture, we will generalize these ideas and develop multi-step methods involving explicit and implicit methods.

(Refer Slide Time: 01:00)



Recall that we are interested in approximating solution of the initial value problem $y' = f(x, y)$, where the equation is posed on a closed and bounded interval $[a, b]$ and we are also given an initial condition $y(x_0) = y_0$, where x_0 is some point in the interval $[a, b]$. Generally, we take $x_0 = a$, just for the sake of simplicity. The first step towards developing a numerical method, is to generate a partition for the interval $[a, b]$.

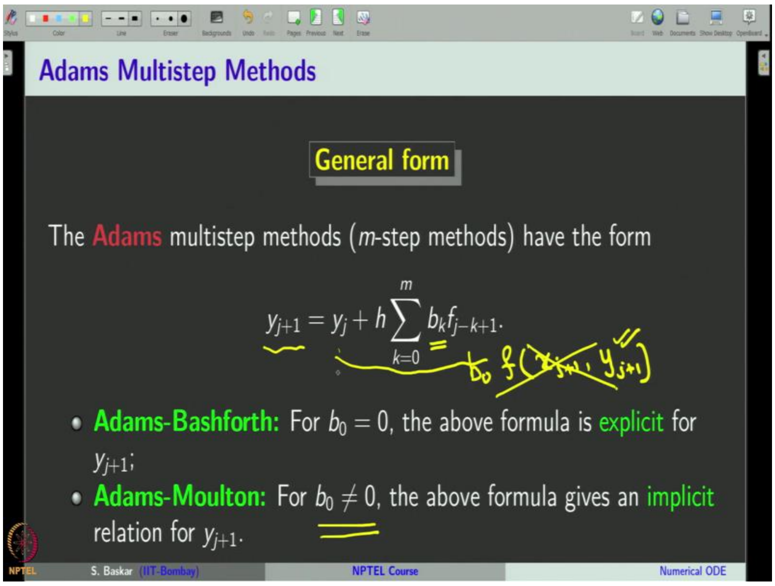
Let us take it to be equally spaced partition, with the step size as h given by $\frac{b-a}{n}$. Thereby we have $n + 1$ node points which is also called grid points and they are given by $x_j = x_0 + jh$. The general form of the multi-step method that we are interested in, is given by this expression. You can see that here y_{j+1}which is the approximate value of y at the point x_{j+1} is given by the first term involving the linear combination of y_j's.

And the second term involves the linear combination of the function value at $(x_j, y_{j)}$ is where the function f is coming from our initial value problem. If you recall, the Euler forward formula is given by $y_{j+1} = y_j + hf(x_j, y_j)$. You can clearly see that this method is also a particular case of this general multi-step method where a_1= 1 and all a_k's are equal to 0 for $k = 2,3, \cdots, m$.

Similarly, you can see that from this term $b_0 = 0, b_1 = 1$ and all b_k's are 0 for $k = 2, 3, \cdots, m$. So, that gives us the Euler forward formula. If you carefully observe you can see that the formula involves $y_j, y_{j-1}, \cdots, y_{j-(m-1)}$. And also, from here you can see that the formula involves the value of f at y_{j+1}, y_j and so on up to $y_{j-(m-1)}$. Thereby, you can apply this formula again only for j starting from m - 1 onwards, whereas for first m - 2 points, the value of the solution cannot be obtained from this method.

Whereas you have to use some lesser step methods, something like Euler method or Runge-Kutta method to find $y_1, y_2, \cdots, y_{m-2}$ then y_{m-2+1} onwards you can go with this method.

(Refer Slide Time: 05:03)



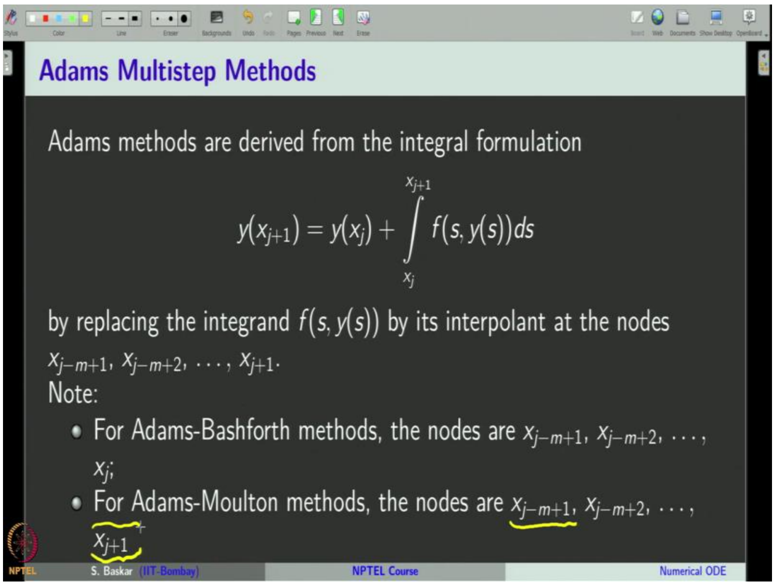
Recall that we have derived the midpoint method in the last class and it is given by $y_{j+1} = y_{j-1} + 2hf(x_j, y_j)$. You compare this with the general form of the multi-step method that we have given in the previous slide. You can see that we have to take $a_1 = 0, a_2 = 1$ and that will match the first term and similarly $b_0 = 0$ and $b_1 = 1$, to match with the second term of the general form.

And therefore, midpoint method is also a particular case of the general multi-step method. If you observe Euler method is a 1 step method whereas midpoint method is a 2-step method. The method that we have shown in this general form, is a m step method for some given positive integer m. We are interested, in particular, in a class of methods called Adams multi-step methods and these methods are written in the general form as this.

Where you can observe that this is also a particular case of the general form that we have stated in the last slide and this form of the method is of interest to us. Here you can observe that when you take $b_0 = 0$, recall that the first term b_0 appears with $f(x_{j+1}, y_{j+1})$. So, if $b_0 = 0$ then this term will not appear and you will have all the terms involved in this expression, are known to us already, from our previous calculation. In that way, we obtained an explicit relation for y_{j+1}.

Such methods are called Adams Bashforth method and they are basically explicit methods whereas if $b_0 \neq 0$ then the right hand side involves the function value evaluated at y_{j+1}. In that way, we have an implicit relation just like what we got in the trapezoidal rule. And therefore, these methods are implicit methods and they are also called as Adams Moultonl method.

(Refer Slide Time: 07:58)



Let us see how to derive this Adams methods. Again, we will have to use the integral form of the given initial value problem and here you have to note that to derive Adams methods, you have to take the limit in the integral as x_j to x_{j+1}. So, don't choose anything else you just have to take x_j to x_{j+1} and thereby the integral equation is taken only in this form for deriving the Adams method.

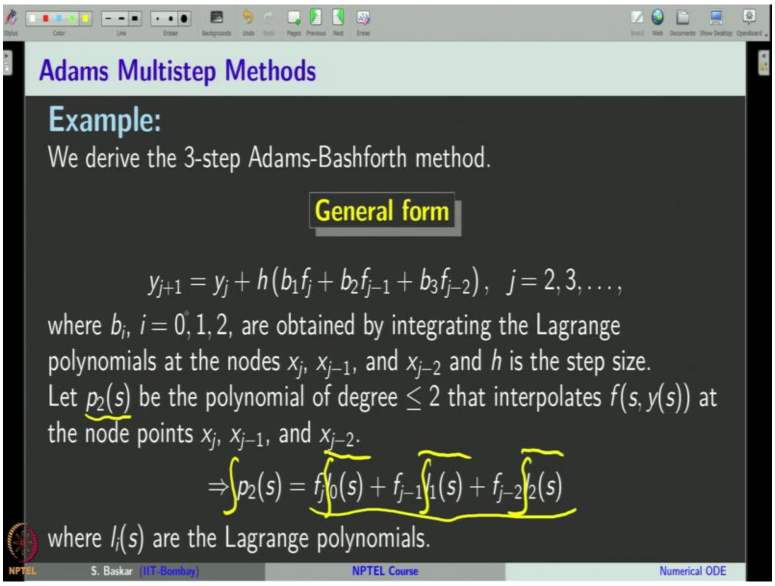
And now how to derive the Adams method? You can see that we need to precisely get the values of b_k. That is the only work involved in deriving Adams method of any particular number of steps. So, what you have to do is, first decide the value of *m* and then you replace the integrand $f(s, y(s))$. Remember, the integrand is basically a function of 2 variables but since we know *y* in terms of *x*, you can view *f* as function of *x* only.

And thereby, you can construct an interpolating polynomial for the function *f* as a function of *x* at the grid points x_{j-m+1} to x_{j+1}. So, once you are given these nodes and the function values, for that you of course need to know the function values, then you can construct an interpolating polynomial and then say it is denoted by $p(x)$ then replace this integral by $\int_{x_j}^{x_{j+1}} p(x)dx$ or $p(s)ds$.

So, that is the basic idea of deriving Adams methods. For Adams Bashforth method remember we should not take x_{j+1}, why? Because in Adams Bashforth method, which is an explicit method, in the previous slide we have seen that explicit methods come with $b_0 = 0$ and therefore you do not need to include x_{j+1} as a node in your interpolation for Adams Bashforth method. And thereby, the nodes for Adams Bashforth method are taken as x_{j-m+1} to x_j only. You do not need to include x_{j+1} because this is an explicit method.

On the other hand for Adams Moulton methods, we need to have the node points starting from x_{j-m+1} to x_{j+1}. So, x_{j+1} is included in the nodes because Adams Moulton methods are basically implicit methods.

(Refer Slide Time: 11:24)



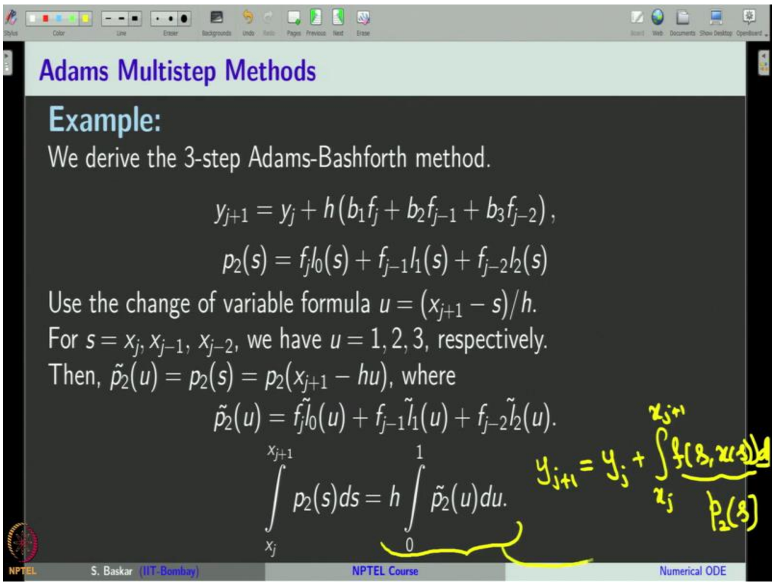
Let us try to illustrate the construction of Adams Bashforth method with 3 steps, means we are taking $m = 3$. Let us see, how to derive the method in the case of $m = 3$. We basically have to obtain the values for the coefficients b in the general expression. So, when you take $m = 3$, Adams method in the Bashforth form will be given like this. Note that you do not have $b_0 f_{j+1}$ term here. We do not have this, we only have the explicit relation.

So, thereby when you go for Adams Bashforth method, you have to take $b_0 = 0$ in the general Adams expression. And now, we have to find this b_i's where i is equal to 1, 2 and 3. We do not need to find 0, but we have to find b_1, b_2 and b_3. b_0 is already taken as 0. So, how to obtain this? Well, that is not very difficult. What you do is, you get the interpolating polynomial $p_2(x)$ with grid points or node points as x_{j-2}, x_{j-1} and x_j.

And from there, you take the integration of this polynomial to get the values of b_i's. Remember, these are given precisely as $f_j l_0(x) + f_{j-1} l_1(x) + f_{j-2} l_2(x)$, therefore when you integrate you just have to integrate the Lagrange polynomials that is why we can see that these b_i's are obtained as the integral of the Lagrange polynomials. As I told, we have to approximate the integrand by the quadratic polynomial interpolating the function f at the node points x_j, x_{j-1} and x_{j-2}.

And in the Lagrange form $p_2(s)$ is given like this, where l_i's are the Lagrange polynomials. And now you can see that if you take the integral, you have to perform these 3 integrals in order to get b_1, b_2 and b_3.

(Refer Slide Time: 14:28)

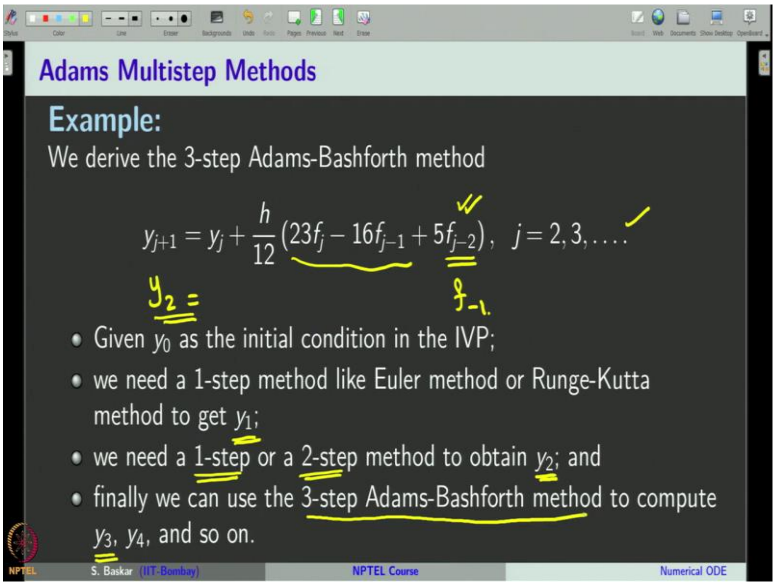


So, in order to simplify our calculation, we will use a change of variable formula whereby we will change the variable s to u given by this expression. With this, you can see that the nodes $x_j, x_{j-1}$and x_{j-2} are transformed to 1, 2 and 3 and thereby integrating the Lagrange polynomials becomes little easier, if you use this change of variable formula. That is why we are going for this. With respect to the variable u, the quadratic interpolating polynomial is denoted by $\tilde{p}_2$ and that is precisely equal to $p_2(s)$, which we want to actually use in our calculation.

But just for the sake of easy evaluation of the integrals, we are going for $\tilde{p}_2$ with the variable u. Let us see, how $\tilde{p}_2$ looks like, $\tilde{p}_2$ is precisely $f_j\tilde{l}_0(u) + f_{j-1}\tilde{l}_1(u) + f_{j-2}\tilde{l}_2(u)$, where $\tilde{l}$ are the Lagrange polynomials with respect to the variable u. And now you can also see that $\int_{x_j}^{x_{j+1}} p_2(s)ds$ is precisely $h\int_0^1 \tilde{p}_2(u)du$. If you recall, we want to replace the integral in our integral equation $y_{j+1} = y_j + \int_{x_j}^{x_{j+1}} f\big((s), x(s)\big)ds$.

So, here we want to replace f by $p_2(s)$ but for the sake of simplicity, we are now going to replace this integral here and thereby get an approximate value for our solution.

(Refer Slide Time: 16:42)



Let us go to do that. So, we want to replace our original integral by this. Let us see how this integral looks like. It is nothing but $h(f_j \int_0^1 \tilde{l}_0(u)du + f_{j-1} \int_0^1 \tilde{l}_1(u)du + f_{j-2} \int_0^1 \tilde{l}_2(u)du)$. So, let us evaluate these 3 integrals and see how they look like. Let us take the first integral $\int_0^1 \tilde{l}_0(u)du$.

Now you see, the Lagrange polynomial is given like this. It is more easy for us to integrate it because the grid points are now the integers and that can be easily evaluated and obtained as $\frac{23}{12}$. It is not very difficult, you can directly get it. Similarly, $\int_0^1 \tilde{l}_1(u)du$ is given by $\frac{-4}{3}$. Recall, this is b_1 this is b_2 and similarly $\int_0^1 \tilde{l}_2(u)du$ is given by $\frac{5}{12}$ and that is b_3.

So, we got b_1, b_2 and b_3. We can substitute these values to get the Adams Bashforth method which is a 3 step method. For that, we just have to replace the integral in our original integral equation by this quadrature formula. Now let us do that and that gives us $b_1 = \frac{23}{12}$, $b_2 = -\frac{4}{3}$ and $b_3 = \frac{5}{12}$, which gives us finally the 3 step Adams Bashforth method as this expression.

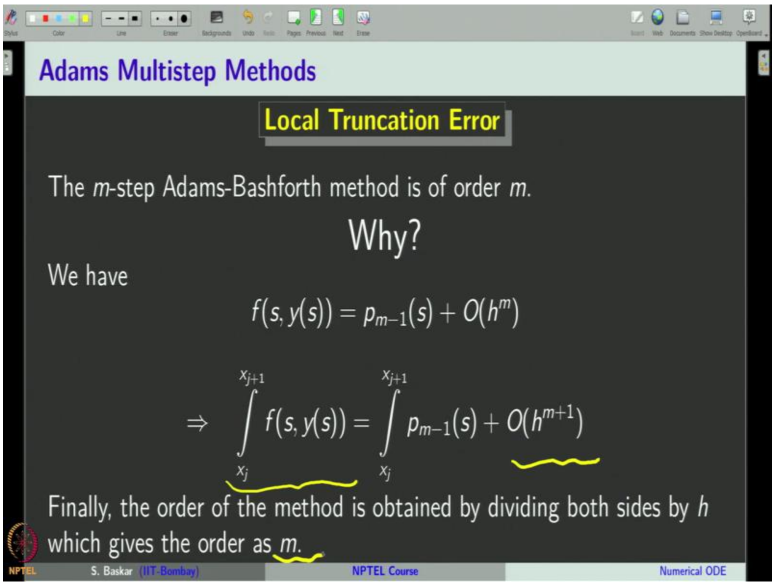
So, it is not very difficult for us to derive this method. Similarly, you can also get the Adams Bashforth method with step 2, 3, 4, and so on. Let us have some observations. Here, you can see that y_0 is of course given from our initial condition. once we have this, can we get y_1 from the 3 step Adam Bashforth method? Just observe that in order to get y_1, you need to take $j = 0$ in this expression.

That gives us $y_1 = y_0 + \frac{h}{12}\big(23f(x_0, y_0)\big)$, that is what is denoted by f_0 here. Up to here, it is ok, no problem. Let us see the next step. The next step is $\frac{h}{12}16f(x_{-1}, y_{-1})$. What is x_{-1}? x_{-1} is nothing but $x_0 - h$. Again, you can see that $x_0 - h$ is not in our domain of interest. Because we have only the interval $[a, b]$ on which we have defined our initial value problem. We always take $x_0 = a$ and therefore $x_0 - h$ is lying outside the domain of interest.

Therefore, we do not know whether y_{-1} exists or not. Even if it exists, we have no interest to calculate it. Therefore, we cannot apply the 3 step Adams Bashforth method for computing y_1 because we do not know these terms. Similarly, you can also cannot get y_2 because to get y_2, you can see that you have to put $j = 1$ and that makes this term to be f_{-1}. Up to this, it is ok but this term is outside our domain of interest.

Therefore, even y_2 cannot be obtained from this method. So, what we have to do is, we have to use some other one step method like Euler method or Runge-Kutta method to get y_1. And when you go to y_2, you may use a 1 step method or 2 step method to get y_2 and then y_3 onwards you can use the 3 step Adams Bashforth method. So, that is the idea of implementing the 3 step Adams Bashforth method.

(Refer Slide Time: 21:58)



Now coming to the local truncation error, we can see that the m step Adams Bashforth method is of order m. If you recall, we have seen that the forward Euler method is of order 1 whereas we have also derived Runge-Kutta method of order 2 and order 4. You can see that Adams

Bashforth method with *m* step is of order *m*. Why it is so? Well, it is not very difficult for you to see.

What we are doing in the derivation of the Adams Bashford method, we are replacing this function which is appearing as the integrand in the integral equation. We are replacing this by the interpolating polynomial and thereby we are committing an error, which from the interpolating polynomial theory, we call it as the mathematical error. We can also call it as a local truncation error here. And if you recall from theory of polynomial interpolations, that the mathematical error involved in the interpolating polynomial is given by this expression.

Here you can see that *s* belongs to the interval $[t_j, t_{j+1}]$. Therefore, this is something like *h*, may be less than *h* and this is something like some constant times *h* and similarly, everything in this product will be some constant times *h*. And therefore, this product will be some constant times *h* to the power of how many terms are there. Here there are *m* terms therefore this contributes to h^m.

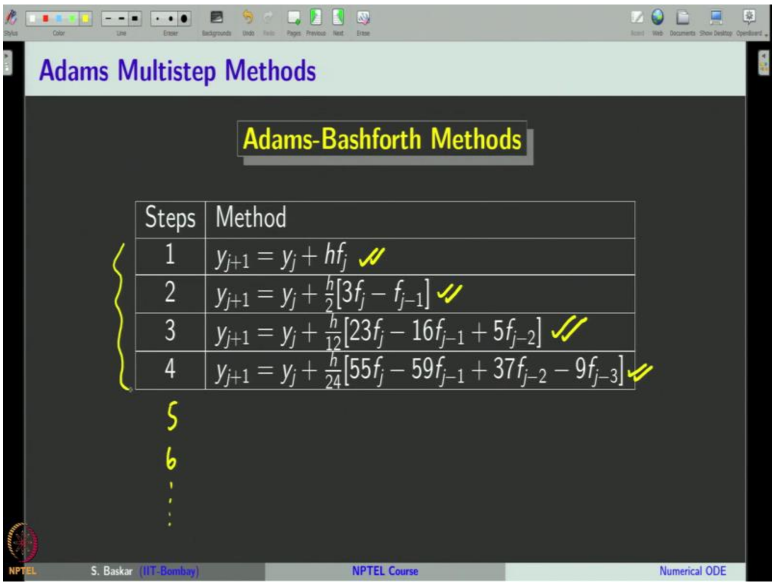
Thereby you can say that the function is approximated by the polynomial interpolating the function at some node points with the truncation error of order *m*. Then what we are doing, we are taking the integral of this function because in our integral equation this function is appearing with an integral over x_j to x_{j+1}. Remember $[x_j, x_{j+1}]$ is the interval with length *h*. We have this integral + the error that we are committing in this quadrature formula, is of order already you have h^m.

Now when you integrate that error, you are again accumulating one more *h* coming from the length of the integral, over which we have taken the integral. So, that contributes one more *h* here and thereby the integral will have the truncation error with order *m* + 1. Now if you recall, in Euler forward method we had the truncation error of order 2. But we have seen that the method is of order 1.

Similarly, when we derive the Runge-Kutta method of order 2, the truncation error was of order 3. So, this is because when we go to find the order, we are precisely taking the way we are approximating y'. When we go to approximate y', we have to divide by *h* on both sides of the approximation. That will generally reduce the order of the method by 1 when compared to the truncation error.

So, the same idea goes here also. You can see that the approximation that we have taken for the quadrature rule, is obtained with the error of order $m + 1$. Therefore, the truncation error is of order $m + 1$ and that implies that the method will be of order one less, that is m. So, in that way the Adams Bashforth method with m steps will be of order m. This is an important point, you have to keep this in mind.

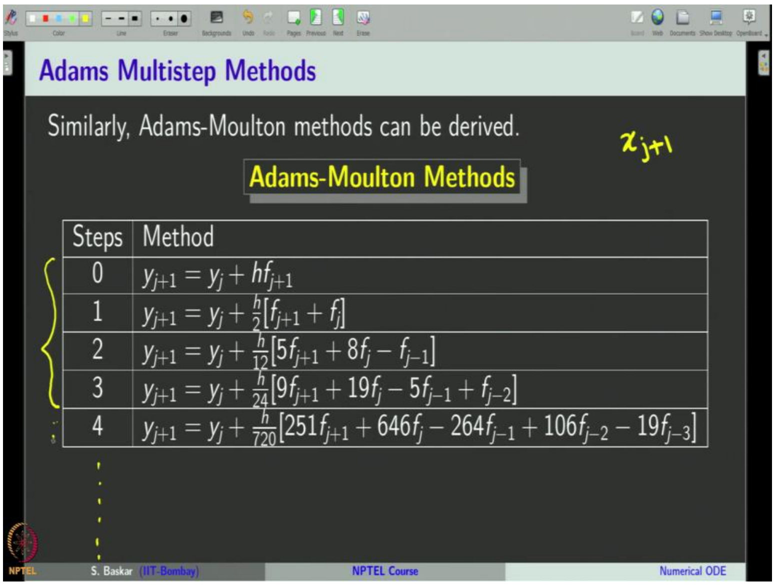
(Refer Slide Time: 26:42)



Now as I told you, we have derived the 3 step Adams Bashforth method. Similarly, you can also derive 4 step Adams Bashforth method, even 2 step, you can easily derive. One step is trivial but if you go on like this, five, six and so on, you can derive them. These expressions are there in the literature however these calculations are little difficult. We will not go to do any problem with Adams Bashforth method of order five six or so on.

Maximum, we will restrict ourselves to Adams Bashforth method with step 4 not more than that.

(Refer Slide Time: 27:28)



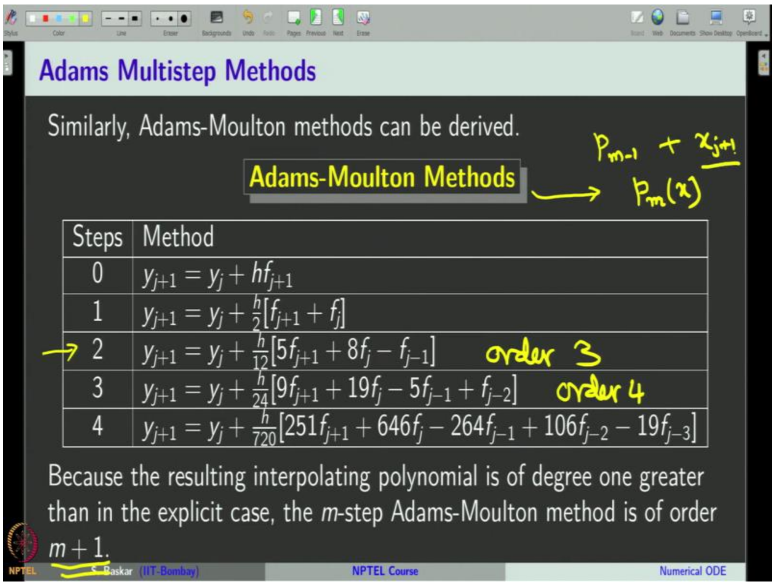
Once you got the idea of how to derive the Adams Bashforth method, you can also derive Adams Moulton methods similarly. The only difference is that you have to include one more grid point that is node point x_{j+1} and thereby you will be constructing a polynomial of degree one greater than the degree that you have with Adams Bashforth method. Otherwise, the derivation goes exactly the same as we have illustrated in the 3 step Adams Bashforth method.

You can easily derive the Adams Moulton method with step 1, 2, 3, 4 and so on. You can also go on, but we will only restrict ourselves to maximum 3 or at most 4. We will not go more than that. Of course, from the examination point of view we will not go more than 2 because it is very difficult for us to remember these formulas and even in the Adams Bashforth method we will not go more than step 3 in the examination.

And coming to the order of Adams Moulton methods, you can see that the order of the Adams Moulton method will be one more than what step you have taken. Say, for instance two-step Adams Bashforth method will be of order 3. Similarly, this will be of order 4, that is, the 3 step Adam Moulton method will be of order 4 and so on. Why it happens like that? Because, if you recall, in the Adams Bashforth method we approximated the integrand f by the interpolating polynomial of degree p_{m-1}.

Whereas, here you will be adding one more node $x_{j+1}$and thereby you are approximating the integrand by the interpolating polynomial of degree p_m. So, in that way the truncation error of the Adams Moulton method will be of order $m + 1$ and therefore the order of the method will be one less, that is, $m + 1$. That is how the Adams Moulton method, just because it is implicit you have to include one more node point into your polynomial construction and that will increase one order in the Adams Moulton method.

(Refer Slide Time: 30:16)



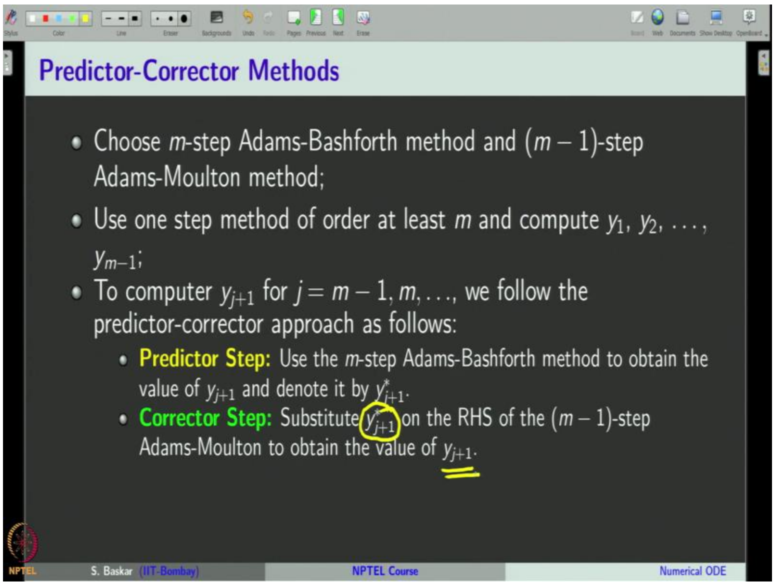
Now let us illustrate the predictor corrector method using the Adams Bashforth and Adam Moulton method. In this what you have to do is, first you have to fix the *m* value, which will tell what is the step that you are taking in Adam Bashforth method and then you have to go and choose one step less in the Adam Moulton method. Because if you take *m*-step method in the Adam Bashforth method thereby you get the order *m* in the explicit form. To match that with the Adams Moulton method, you have to take one less because Adams Moulton methods order is one greater than its step because of the implicit term.

So, that is the important point you have to keep in mind. So, use one step method of order at least *m* and compute $y_1, y_2, \cdots, y_{m-1}$. Remember, since we are fixing *m* step method, you cannot use Adams Bashforth and similarly Adams Moulton method for computing the values of *y* at first *m* - 1 grid points. Therefore, you have to go for some one step method. It is better to choose a method which is of order *m* something like Runge-Kutta method of higher order, you can take to compute these values.

Once you have these values then to compute y_{j+1} for j equal to *m* - 1 and so on, you will now go with the predictor corrector approach. If you recall in the last class, we have introduced the predictor corrector approach for the trapezoidal method. The same idea will go on here. What you do is, first find y_{j+1} using the Adams Bashforth method, there is no problem in doing this, because Adams Bashforth method is an explicit method. You have an explicit formula for y_{j+1}. Once you obtain the value of y_{j+1} from the Adams Bashforth method, you denote it by y_{j+1}^{*}.

And this is the predictor step, once you have the predicted value of y_{j+1}, you plug in that on the right hand side of the Adams Moulton method. Remember, Adams Moulton method is an implicit method therefore you have y_{j+1} term on the right hand side also. So, substitute this predicted value on the right hand side of the Adams Moulton method and get y_{j+1}. That is the corrector step in our predictor corrector method. So, this is the procedure you have to follow for the predictor corrector method.

(Refer Slide Time: 33:26)

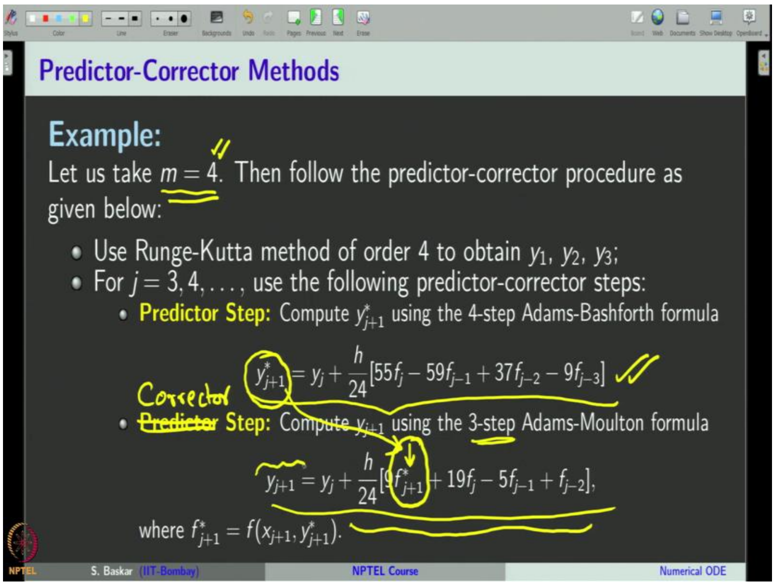


Let us just illustrate it with $m = 4$. Remember, to implement a predictor corrector method, you first have to decide what is m. Let us fix m as 4. Once you fix m you first go to the table given for Adams Bashforth. We have fixed it as 4, therefore you have to take this formula for the predictor step. That is what I am writing here, the predictor step will have this formula.

For the corrector step, you have to take the 3 steps Adams Moulton formula. In order to match the order, you have to take one step less, that is you have to take these 3 steps in Adams Moulton method and that is given by this formula. So, that will give you this formula, where the first term that is the implicit term is now obtained by plugging in the predicted value here and thereby the right hand side now becomes explicit.

So, you can get y_{j+1} without going for any non-linear iterative method. So, that is the idea of predictor and corrector method.

(Refer Slide Time: 34:58)



So, there is also another important class of methods called backward differentiation method. Remember backward differentiation method can also be obtained by approximating the function *f* by a corresponding interpolating polynomial. Only thing is, in the Adams method we will use the polynomial interpolation of *f* to approximate the integral. So, we will use the polynomial approximation to approximate the integral in the interval $[x_j, x_{j+1}]$. So, that is approximated by $\int_{x_j}^{x_{j+1}} p(s)ds$. So, that is for the Adams method.

Whereas in BDF method, we will approximate the unknown function *y* by the polynomial and then we will differentiate p' and use this as an approximation in our equation. So, that is the idea, we will go for the interpolating polynomial for the function $y(x)$ at these node points for some given *m* and then replace y' by p'_m and that gives us a general expression like this. Recall, what we had the general expression for *m* step methods, it is given like this, where the first term is given as it is whereas the second term is taken with $b_0 \neq 0$, whereas $b_1 = b_2 = \cdots = 0$.

So, that gives us BDF method whereas if you recall Adams method's general form is given like this. Where $a_1 \neq 0, a_2 = a_3 = \cdots = 0$, whereas *b*'s are kept as it is. So, similarly you can also get this $a_k's$ and b_0 by just replacing *y* by the corresponding interpolating polynomials but we will not give any weightage for BDF methods in our course. With this we will end this lecture, thank you for your attention.