Computational Techniques

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Module No. # 06

Lecture No. # 05

Differentiation and Integration

Hello and welcome to lecture five of module 6. This is going to be the last lecture in this module. We are going to look at couple of methods for numerical integration and finally summarize what we have done in numerical differentiation and integration, in this particular module.

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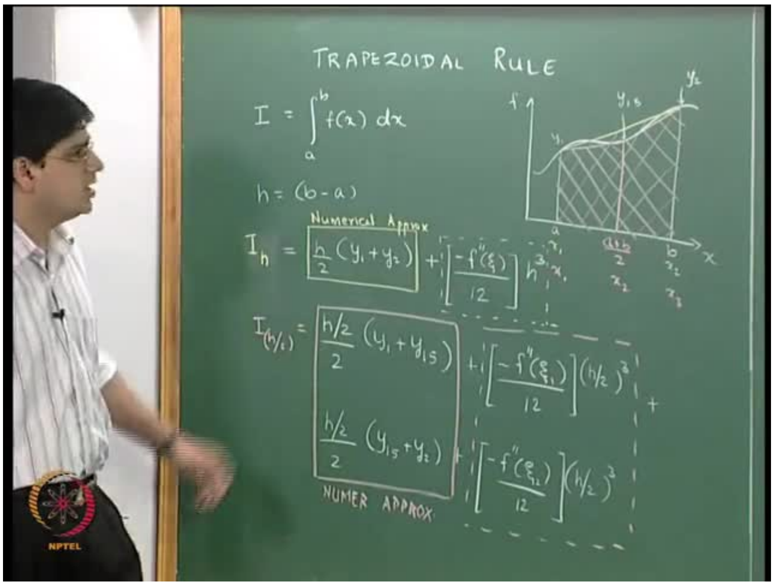

Once when we apply the trapezoidal rule, let say we want to find integral I, which is going to be integral from a to b, f of x d x, and the area under the curve between a and b is what we want to find out. So, what we can do is we can write our x 1 equal to a, and x 2 equal to b, and connect them with a straight line and that becomes the trapezoidal rule.

So, our h in this particular case, is just going to be equal to b minus a. With h equal to b minus a, we will apply the trapezoidal rule and the result that we will get is I is going to be equal to basically h divided by 2 of y 1 plus y 2, where y 1 is f of x 1 and y 2 is f of x 2. So, I equal to h by 2 plus this (Refer Slide Time: 01:49) plus negative f double dash of zeta, divided by 12 and multiplied by h cube.

This was our value of integral I, when we computed the integral I, as the area under the straight line joining these two points. So, the area under the yellow curve was I, and I will just use a yellow chalk over here to represent the area under the yellow curve and call this as I of h, to represent the fact that we have taken h equal to x 1 minus x 2; the entire region we have taken that as equal to h.

Now, let us consider another case where we have use the area, the calculated area as area under two different curves; first going from a plus b by 2 and then going from a plus b by 2 to b. So, we will consider a midpoint of this and that midpoint is going to be a plus b divided by 2. So, in the red case, we will have x 1, x 2 and x 3. In this case, our area will be area under the red curve, which I will represent with the red hatch lines, and in that case, I will write I of h by 2 equal to h divided by 2 or b by a divided by 4 is going to be our results. So, h by 2 is, because we have taken half the h and we will call this as y 1 plus y 1.5. Let us call that and let us call that as y 1. This particular guy, we will call it as y 1.5 and this as y 2.

So, the first integral that is going from y 1 to y 1.5, is going to be h divided by 2, whole divided by 2, because this is our new step size multiplied by y 1 plus y 1.5, plus negative f double dash and let us call this as zeta 1 divided by 12, multiplied by step size to the power 3. In this case, the step size is h by 2, so we will have h by 2 to the power 3, so that is. Now, what I have written over here is the integral under the first interval. I will write down the integral under the second interval also, and that is going to be just h by 2 divided by 2 multiplied by y 1.5 plus y 2 plus negative f double dash of zeta 2, divided by 12, h by 2 to the power 3.

So this is what we have as the two I's. Over here, is the numerical approximation (Refer Slide Time: 05:41) (no audio between: 05:41-05:51) using h equal to b minus a. The red box is the numerical approximation; using h equal to b minus a divided by 2 and this is the overall error term. This is the error also the error term.

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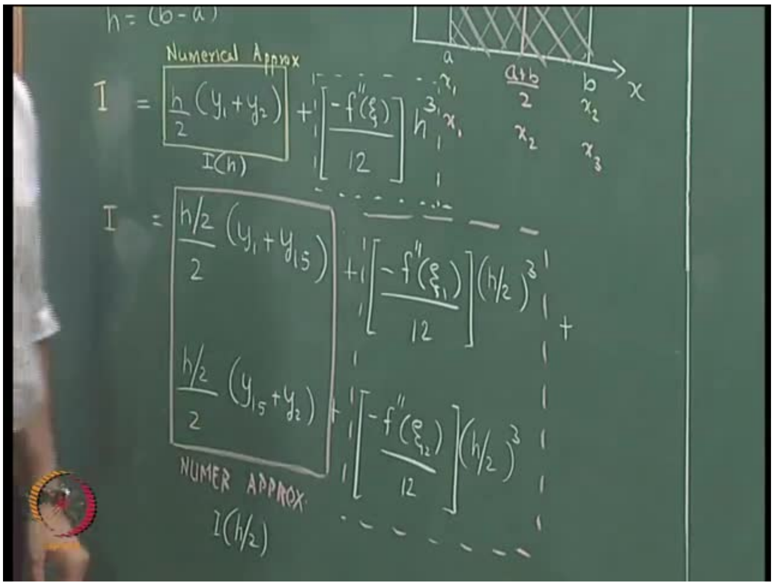

The new value of integral is the numerical value plus the error, so I will just drop this subscript from over here and we know that this particular guy and this particular guy are going to be exactly the same. This we will write as I in bracket h and this is basically I in bracket h by 2, not the previous notation.

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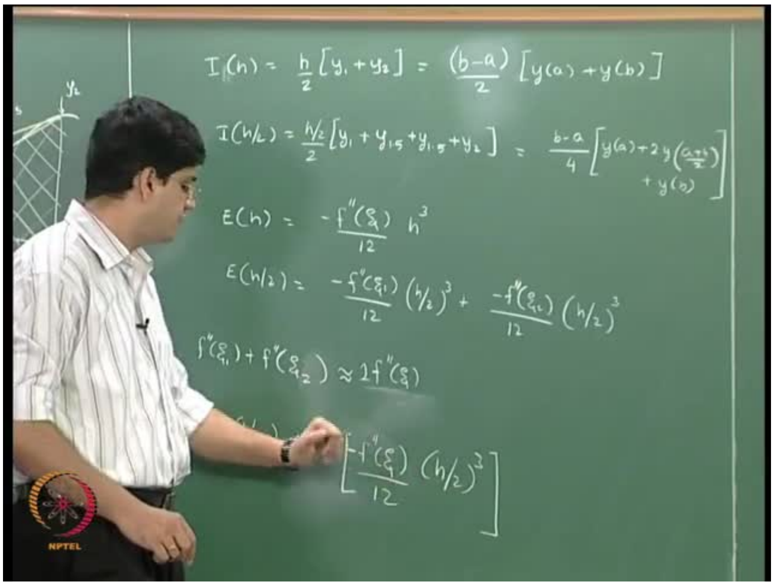

So, the numerical approximation is I of h and I of h by 2. I will just write down what those values are; I in bracket h is going to be equal to h by 2 of y 1 plus y 2 is equal to b minus a divided by 2 multiplied by y of a plus y of b. So, that is going to be our I h and I h by 2 is going to be equal to h by 2, divided by 2, multiplied by y 1 plus y 1.5 plus y 1.5 plus y 2, which is equal to b minus a, divided by 4, y of a plus 2, y of a plus b by 2, plus y of b. That is going to be our, I of h and I of h by 2. The dotted boxes that we have over here we will call them as errors E h and E h by 2.

E h we are going to write this as minus f double dash of zeta divided by 12, multiplied by h cube. E of h divided by 2, we can write that as minus f double dash of zeta 1, divided by 12 h by 2 cubed, plus minus f double dash of zeta 2, divided by 12 multiplied by h by 2 cubed. At this point, what we will do is we will write f double dash of zeta 1, plus f double dash of zeta 2. That value we will write that as approximately equal to f double dash of zeta divided by 2. (No audio between: 09:19-09:32) This is more accurate way of saying rather than saying f double dash of… sorry, this not (Refer Slide Time: 09:47) divided by two, it is equal to two f double dash of zeta, sorry that is the mistake.

F double dash of zeta 1 is approximately equal to f double dash of zeta and f double dash of zeta 2 approximately to equal f double dash of zeta; rather than saying then in this way, a more appropriate way of saying is f double dash of zeta is approximately the average of f double dash of zeta 1 and f double dash of zeta 2. That is essentially, what we are saying at this particular stage.

So, what we actually have is that f double dash of zeta can replace essentially this particular value (Refer Slide Time: 10:27) when we add them up. So, what I will do is I will right that as E of h by 2 is going to be equal to 1 by 12 multiplied by h cubed. So, what we are actually going to do at this stage is this particular values that we have over here we will just write them that as equal to f double dash of zetas and we will have a two factor of two, because these are the two values over here.

Again, there are approximations involved in that. So, this is not an exact way of writing these things down. So, we will have this written as 2 or approximately equal to 2 multiplied by f double dash of zeta, divided by 12 of h by 2 cubed. So, h by 2 cubed divided by 12 comes out of the bracket and we will have minus of f double dash of zeta 1 plus f double dash of zeta 2, which we are writing as two times f double dash of zeta. I forget the minus sign over there. So, this is going to be our error in the computing the numerical derivative using h, h by 2 using the trapezoidal rule.

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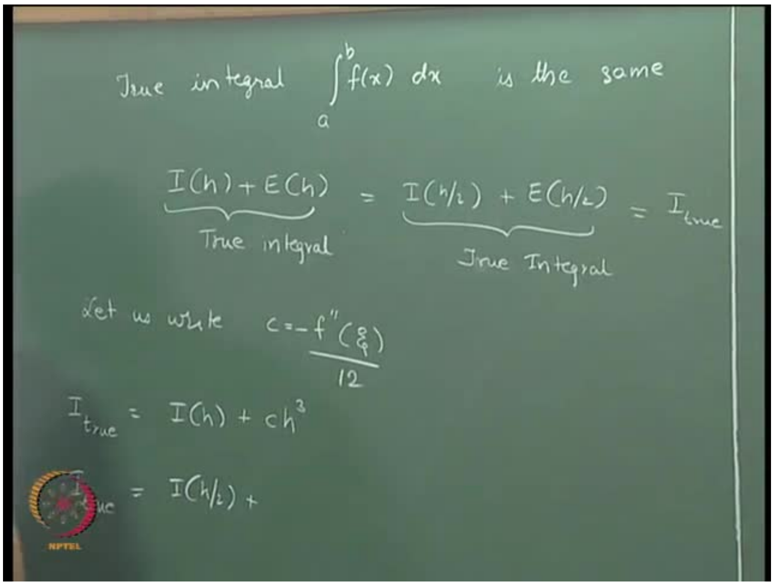

So, that is essentially what we are going to get at this stage, so we will write now the true integral (no audio between: 12:08-12: 25). So, the true integral a to b f of x d x is the same. As a result what we can say is I h plus E h is the true integral, and is going to be equal to I h by 2 plus E h by 2, (no audio between: 12:52-13: 06)which we will write that equal to some I true. Let us also write this particular constant as f double dash zeta divided by 12 as sum constant c. So, let us write (no audio between: 13:25-13:34) or let us write negative f double dash of zeta divided by 12.

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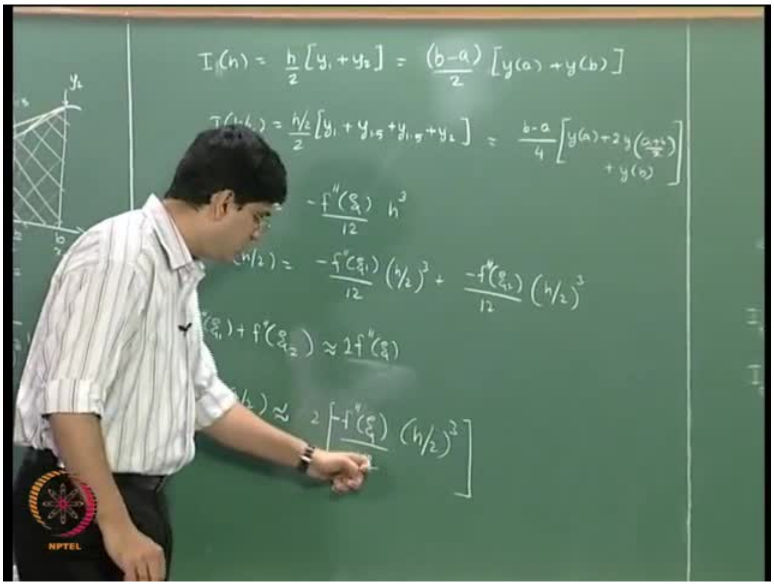

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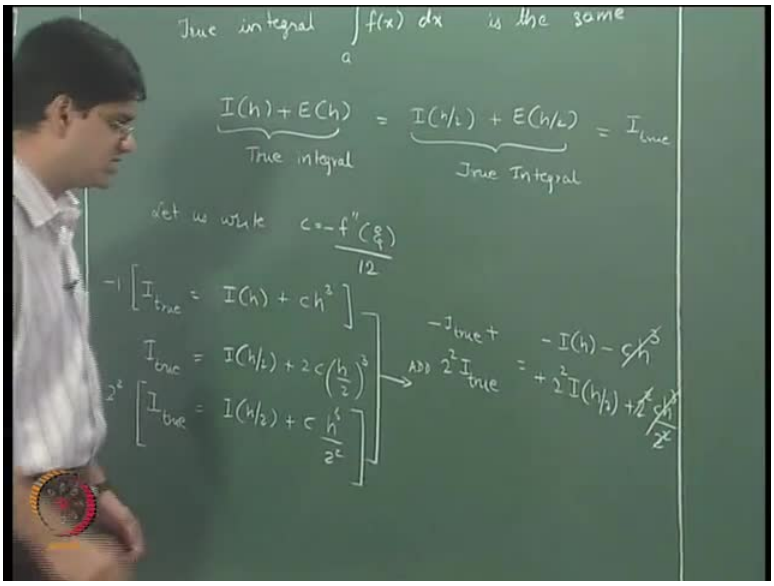

As a result, we will write or we can write I true as equal to I h plus c times h cubed. we can also write I true as equal to I h by 2 plus and if you go to this particular expression, (Refer Slide Time: 14:06) it is 2 multiplied by c multiplied by h by 2 cubed; 2 c h by 2 cubed, which is going to be equal to I of h by 2 plus c divided by h cubed divided by 2 squared. So, now what we will do is multiply this equation by 2 squared and multiply this equation by minus 1 and then add the two. So, we will get minus I true plus 2 to the power 2, I true will be equal to minus I h plus c h cubed, plus 2 to the power 2 I h by 2, plus 2 to the power 2 multiplied by c h cubed by 2 squared.

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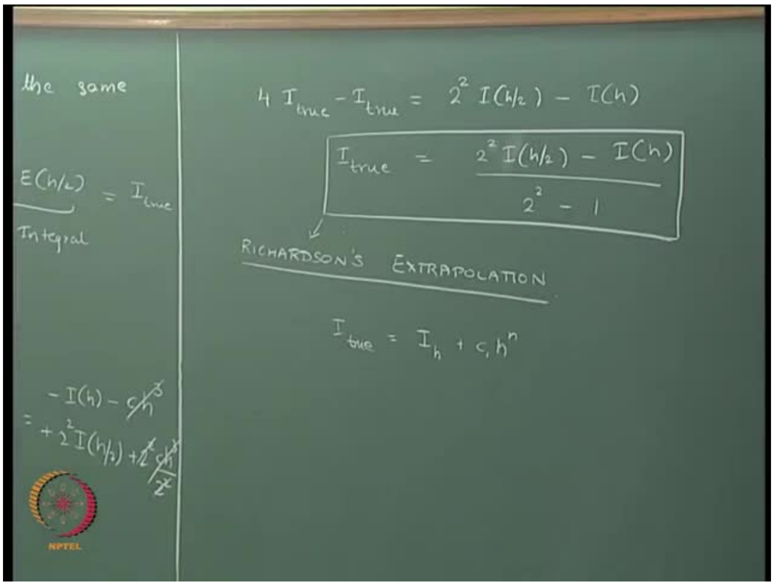

So, this and this also gets cancelled, so we will have from this expression we can have 4 times I true minus I true equal to 2 squared I h by 2 minus I h, which is going to be our expression. Dividing throughout, we will get I true is two to the power of 2, I h by 2 minus I of h, divided by 2 to the power 2 minus 1.

This particular method of getting an improved value of I true is called Richardson's extrapolation. So, the idea behind Richardson's extrapolation is this any true integral I can be written as I numerical using the value of h plus some constant multiplied by the leading error term. So, let us write that as constant c 1 multiplied by the leading error h to the power n. Keep in mind that this we are able to write, because of this we are able to write because of the mean value theorem.

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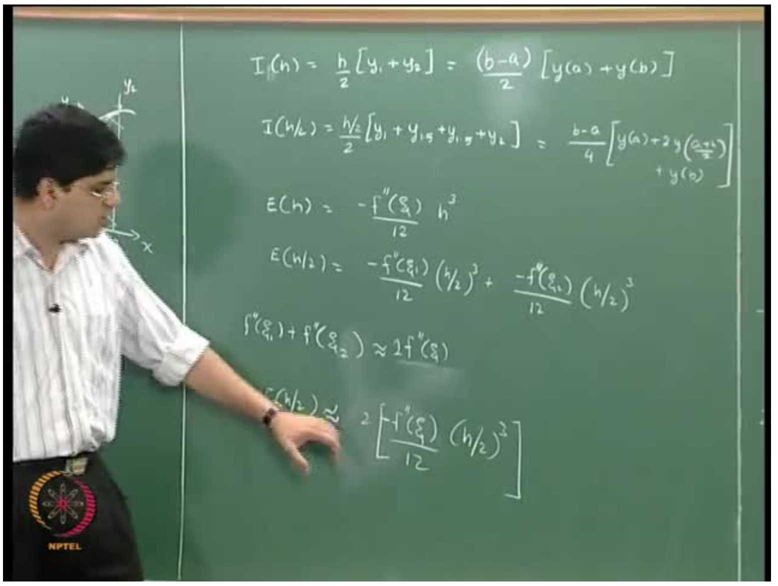

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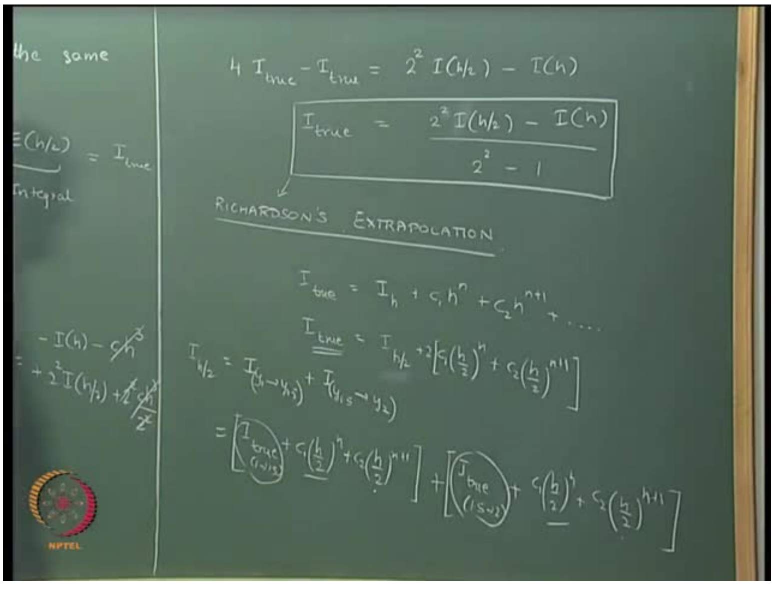

If we go back and look at the expression that we have over here like E of h by 2 is not exactly equal to 2 times f double dash of zeta, but it is approximately equal to 2 times h double dash of zeta. So, instead of that if we were to write the entire series of rather than truncating it using the mean value theorem, if we write the entire series, we will get this as c 1 h to the power n plus c 2 h to the power n plus 1 plus so on. So, this is what we will get using I h.

If we were to use two implementations of the same method, we will have this as I using h by 2 plus c 1 using h by 2 to the power n plus c 2, using h by 2 to the power n plus 1. This particular guy will actually have c 1 h by 2 to the power n, because of the first implementation, c 1 h by 2 to the power n because of the second implementation. So, that actually we will get multiplied by 2. in other words, what we are saying is that we have I h by 2 is actually going to be written as I going from y 1 to y 1.5 plus I y 1.5 to y 2.

And this guy is going to be I true plus c 1 h by 2 to the power n plus c 2 h by 2 to the power n plus 1. This is I true from 1 to 1.5, plus I true from 1.5 to 2, plus c 1 h by 2 to the power n, plus c 2 h by 2 to the power n plus 1. So, this plus this, is going to be equal to I true. This term plus this term will get added and we will get factor of 2. This term and this term will get added and we will again get a factor of 2. That is essentially how that the factor of 2 comes into picture over there.

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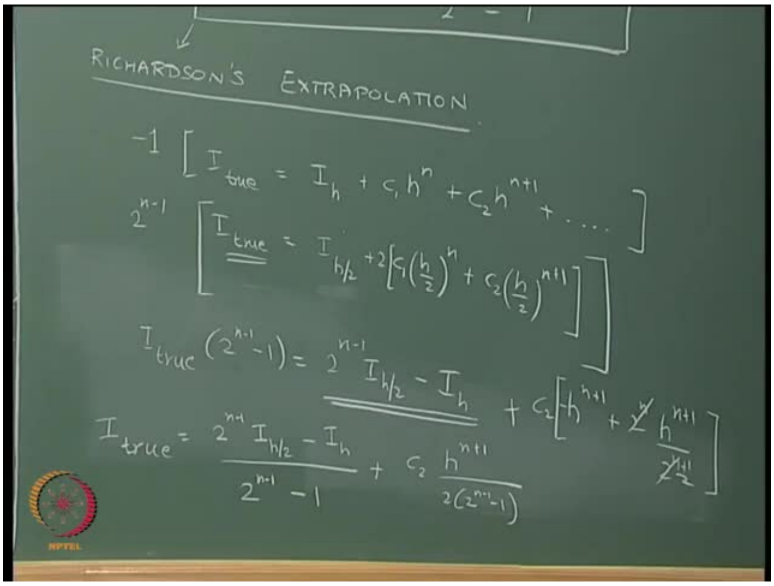

So, now what we can do is we can multiply this particular expression by 2 to the power n minus 1, and this expression we can multiply this by minus 1, and then when we add up we will get I true multiplied by 2 to the power n minus 1 minus 1, is going to be equal to 2 to the power n minus 1 I h by 2 minus I h. This is going to be the numerical integral plus this term and this term is going to get cancelled, when we multiply this guy by 2 to the power n minus 1, because 2 to the power n minus 1 multiplied by 2 is going to be 2 to the power n, 2 to the power n and 2 to the power n is going to get cancelled.

Plus we will get c 2 h to the power n plus 1 and a negative sign over there, plus 2 to the power n multiplied by h to the power n plus 1, divided by 2 to the power n plus 1. So, this and this will get cancelled and we will have this, the denominator as 2. As a result of this when we divide by 2 to the power n minus 1 minus 1, what we will get as the I true using Richardson's extrapolation. We will get this as I true as 2 to the power n minus 1, I of h by 2 minus I of h, divided by 2 to the power n minus 1 minus 1 plus c 2 multiplied by h to the power n plus 1 divided by 2. We will have this two factor that comes in and then this is 2 to the power n minus 1 minus 1. So, we will have 2 multiplied by 2 to the power n minus 1 minus 1. This is going to be the Richardson's extrapolations.

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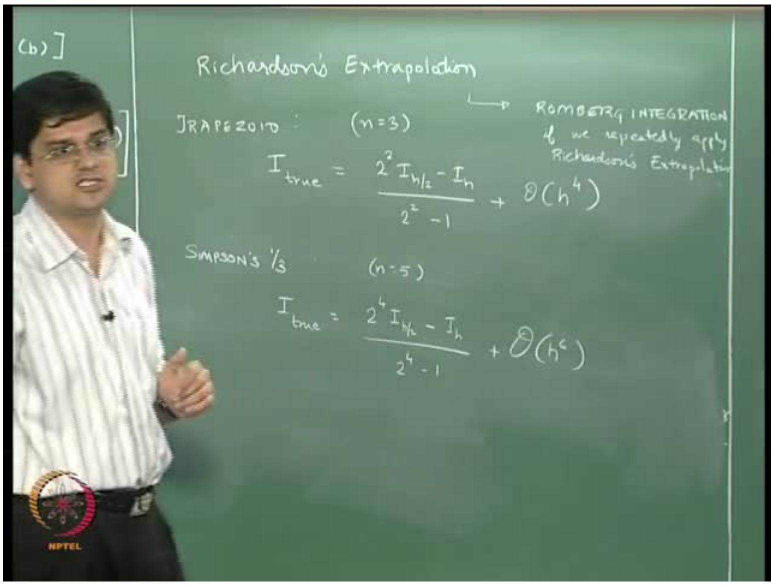

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So, for trapezoidal method, n was equal to 3. When we substitute that in this particular expression, what we are going to get is I true, which is going to be 2 to the power 3 minus 2 and that is 2 to the power 2 minus I of h, divided by 2, to the power 2 minus 1 plus error of the order of n plus 1; n was three, as a result the error is of the order of h to the power 4. Simpson's one-third, in this case, n was equal to 5, so I true is going to be equal to 2 to the power 4 I of h by 2 minus I of h, divided by 2 to the power 4 minus 1 plus order of h to the power 6.

Why h to the power 6? Because, the Simpsons' one-third rule is h to the power 5 accurate and we increase they order of accuracy by 1, while when we implement the Richardson's extrapolation. Likewise, we can have Simpson's three -eight rule so on and so forth. If we iteratively apply Richardson's extrapolation, then we come to a special method of integration called Romberg integration (no audio between: 25:54-26: 12). Beyond stating that, I would not go into the details of Romberg integration. You can look up any standard text book for numerical method and you will be able to see what Romberg integration means.

So, what do we do in Richardson's extrapolation is we obtain an integral under a curve using one single interval for the trapezoidal rule or two intervals for the Simpson's one-third rules or three interval for the Simpson's three -eight rule. So, that gives us the value of h. In the three cases, h is going to be b minus a, b minus a by 2 and b minus a by 3, respectively. Then we go on and use half that particular h values. So, in case of trapezoidal rule, we will redo the simulations or we do redo the calculations using 2 intervals. In the case of one-third rules, we redo the calculations using 4 intervals, and in the three -eight rule we redo the calculations using 6 intervals.

So, we will get I h by 2 as the result that we get using in this particular case in 2 intervals. In this particular case, 4 intervals, and that particular value multiplied by 4 minus the previous integral value that we have computed using just one single interval, is the numerator divided by 3 is the denominator. The new integral value that we are going to get is one order more accurate than our either of our older integral values. So, that is the idea behind the Richardson's extrapolation and that is summarizes our Richardson's extrapolation.

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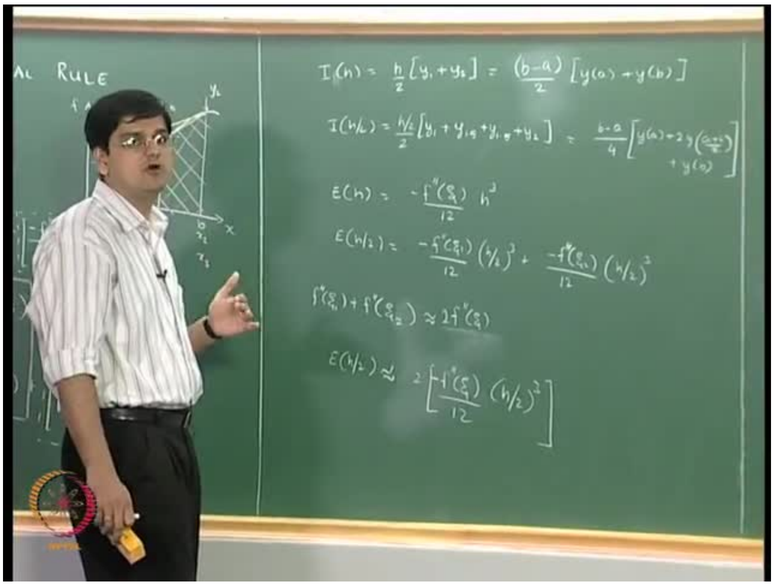

What I will do is very quickly is show one more way of deriving the trapezoidal rule and then talk very quickly about a new another method called Gauss Quadrature method.

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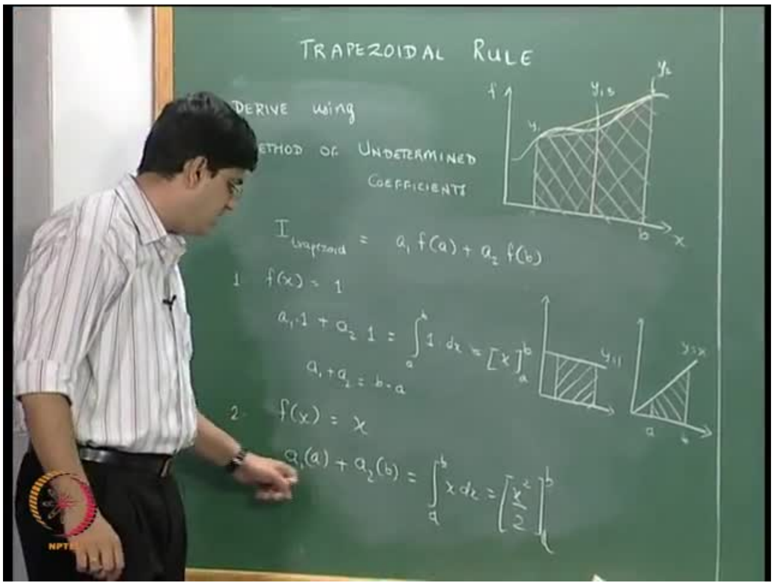

So, we will derive using method of undetermined coefficients. (No audio between: 28:22-28: 35) In this particular case, in the method of undetermined coefficients, we will write, I trapezoidal is going to be equal to a 1 multiplied by f of a, plus a 2, multiplied by f of b. This is how we are going to write a 1 and a2. Sorry! This is how we will write our I trapezoid. What we know with the trapezoidal rule is this if our curve was a flat line, and we wanted to find area under this particular curve, so in other words, if our curve was a constant function, we know that the value that the trapezoidal rule gives us is going to be the exact value under that curve. Second case, we also know is that if this was aligned with unit slope. Let us say y equal to x, and in this particular case with the curve is y equal to 1, and if we were to find area under this curve between a to b.

This area obtain through the trapezoidal method is also going to be exact. That is the property that we are going to use in order to use the method of undetermined coefficients. So, the first case is, if f of x is going to be equal to 1, then the trapezoidal rule is exact. In that case, I trapezoid is a multiplied by f of a, f of a is a 1 multiplied by f of a, f of a is nothing but 1. So, a 1 multiplied by 1 plus a 2, multiplied by f of b, we substitute x equal to b in this case again f of x equals 1. So, this is what we will get, is going to be equal to integral from a to b f of x d x. That is one multiplied by d x. Now, this is going to be nothing but, x going from a to b, which is nothing but, b minus a.

So, a 1 plus a 2 is going to be equal to b minus a, is our first equation. I will just write this in a more descriptive from. Our second equation is that for f of x equal to x also, the trapezoidal rule gives us the exact result. So, we again substitute f of a in this particular case is going to be equal to a, f of b in this case is going to be equal to b. So, the I trapezoid is going to be a 1 multiplied by a, plus a 2 multiplied by b. that is going to be equal to integral from a to b, f of x d x; f of x is x, so we will have x d x, which is equal to x square divided by 2, going from a to b. So, writing those equations down, writing both those equations down over here what we get is this.

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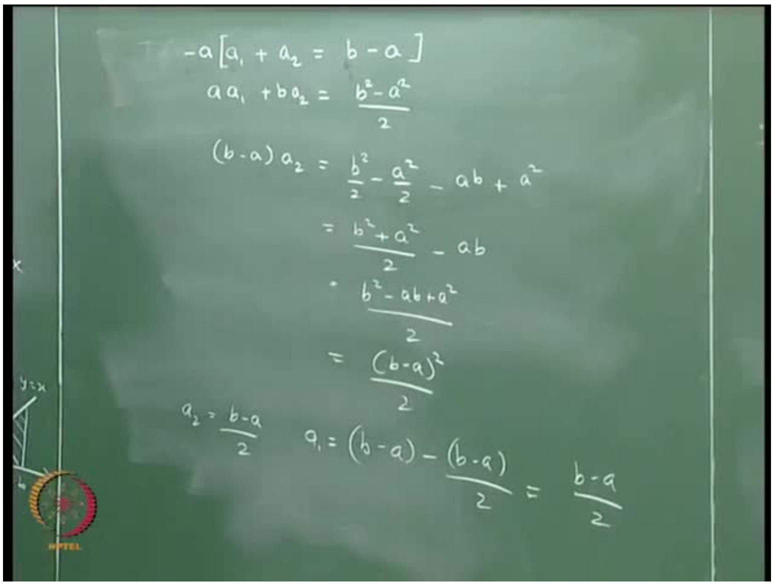

So, our first equation is a 1 plus a 2 equal to b minus a, this is our first equation. Our second equation is a multiplied by a 1 plus b multiplied by a 2, is b squared minus a squared divided by 2. So, what we will do is we will multiply this equation by minus a, and add these equations up, so we will get b minus a, multiplied by a 2, is going to be equal to b squared by 2 minus a squared by 2. This is what we get by writing here, minus a b plus a squared.

So, this is going to be b squared plus a squared, divided by 2, minus a b, which is equal to b squared minus a b, plus a squared divided by 2, which is b minus a, the whole squared divided by 2. That is going to be equal to a 2 multiplied by b minus a. So, a 2 is going to be equal to b minus a, divided by 2. So, a 1 is going to be equal to, a 1 is going to be equal to b minus a, minus b minus a by 2, which is equal to b minus a divided by 2.

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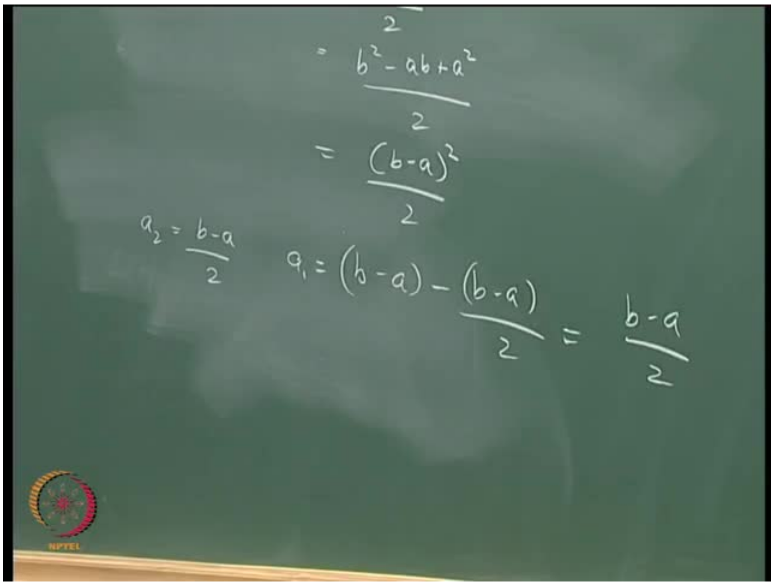

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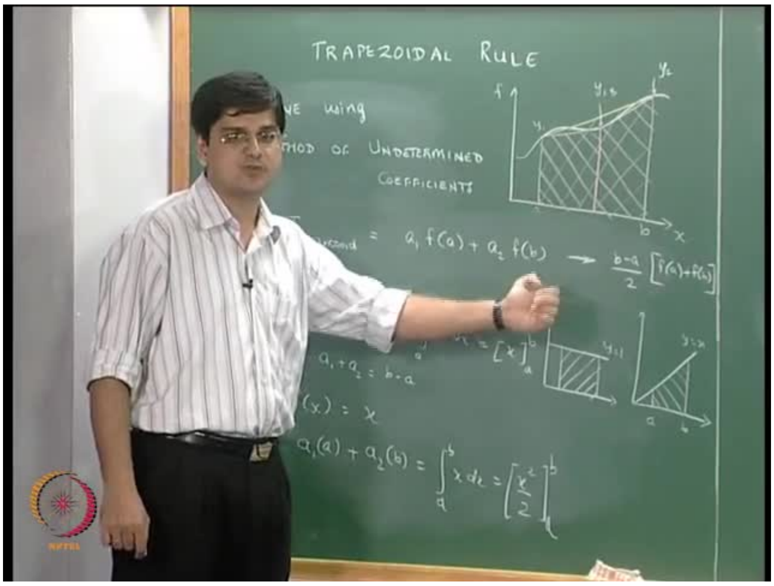

Substituting in this particular equation as a 1 equal to b minus a by 2, and a 2 equal to b minus a by 2, when we substitute this, we will get this as b minus a divided by 2 multiplied by f of a plus f of b, which is exactly what we had as the trapezoidal rule. That we have derived using three different method earlier, using the geometric method, using the algebraic method and using integral of the Newton's forward difference formula.

The new method that we introduced over here is method of undetermined coefficients where the trapezoidal rule is taken as a weighted average of the function computed at the two end points.

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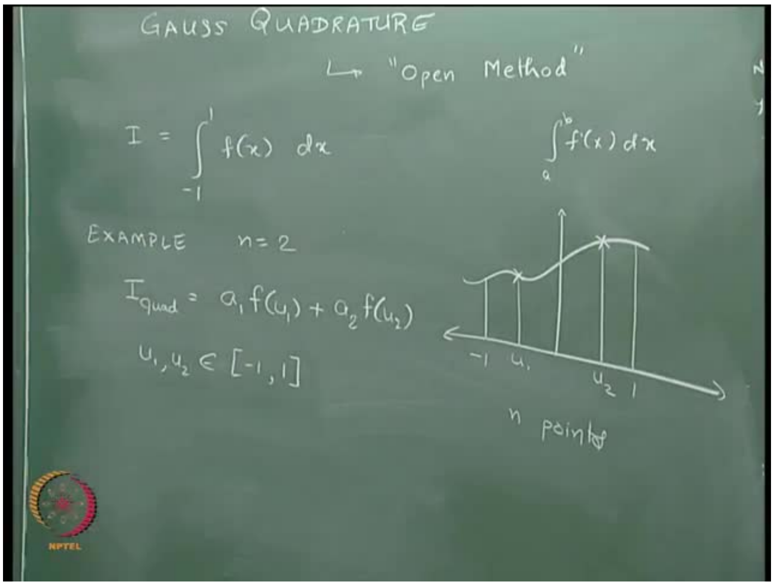

Gauss quadrature compare to the Newton cotes formulae, Gauss quadrature is an open method, and it is specifically used to calculate integral from minus 1 to 1 of f of x d x. It is specifically use to calculate this. Any integral, a to b of f of x d x, can suitably be converted through a linear change of variable x into the form minus 1 to 1. So, this is not a respective form. This is indeed a fairly general form of the expression.

So, the idea behind gauss quadrature, is this is given an arbitrary function f of x. You want to find integral from minus 1 to 1 f of x d x. What we do is we select n number of points, within this interval. We select n points within this interval such that these integral is a weighted average of the functions computed at those n points. Let us first consider the example as for n equal to 2. I, using the quadrature method, is going to be equal to some constant f 1 multiplied by f of x 1 or I will just write this as f of u 1, to separate out from x 1 plus f 2, multiplied by f of u 2, where u 1 and u 2 are the two values within the interval minus 1 to 1.

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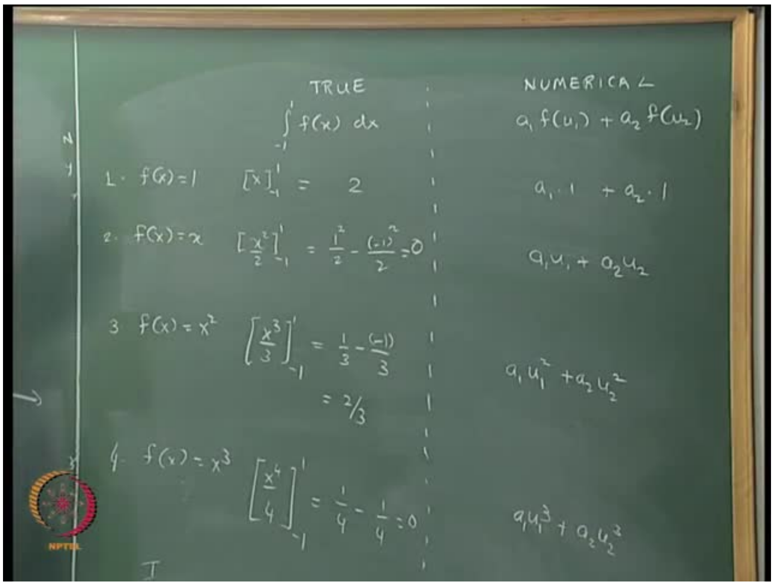

And our objective is to find a 1, u 1, a 2, u 2, and like we did in the trapezoidal rule what we are going to do in the Gauss quadrature method is the same idea, is for f of x equal to 1, f of x equal to x, f of x equal to x square and f of x equal to x cube, we will say that the gauss quadrature method should give us the perfect solution. So, here I will write the true integral and here I will write the numerical integral. This is going to be minus 1 to 1, f of x d x. This is going to be equal to a 1 f of u 1, plus a 2 f of u 2. In the first case, f of x is going to be equal to 1. So, integral from minus 1 to 1, 1 d x is x, from minus 1 to 1, which is equal to 2. It is 1 minus 1 equal to 2. When we substitute u 1 and u 2, in this particular case, we will get this as a 1 multiplied by 1 plus a 2 multiplied by 1.

So, that is going to be our first equation. The second equation is going to be for f of x equal to x, the integral from minus 1 to 1 f of x d x is x square by 2, going from minus 1 to 1, which is 1 squared by 2 minus of minus 1 squared by 2, which is equal to 0. In on to the right hand side, what we will get is a 1 multiplied by u 1 plus a 2 multiplied by u 2.

The third case is f of x equal to x squared, and this we will get it as x cube by 3 from minus 1 to 1, which is equal to 1 by 3 minus of minus 1 by 3, which is equal to 2 by 3. That is what we get on to the left hand side. And to the right hand side, we will get a 1 u 1 squared plus a 2 u 2 squared, f of u 1 is going to be u 1 squared, f of u 2 is going to be u 2 squared. So, a 1 u 1 squared plus a 2 u 2 squared. The fourth equation is going to be f of x equal to x cubed, and in that case, we will have x to the power 4, divided by 4, from minus 1 to 1, which is equal to 1 by 4 minus of 1 by 4 which is equal to 0 and this is a 1 u 1 cubed plus a 2 u 2 cubed.

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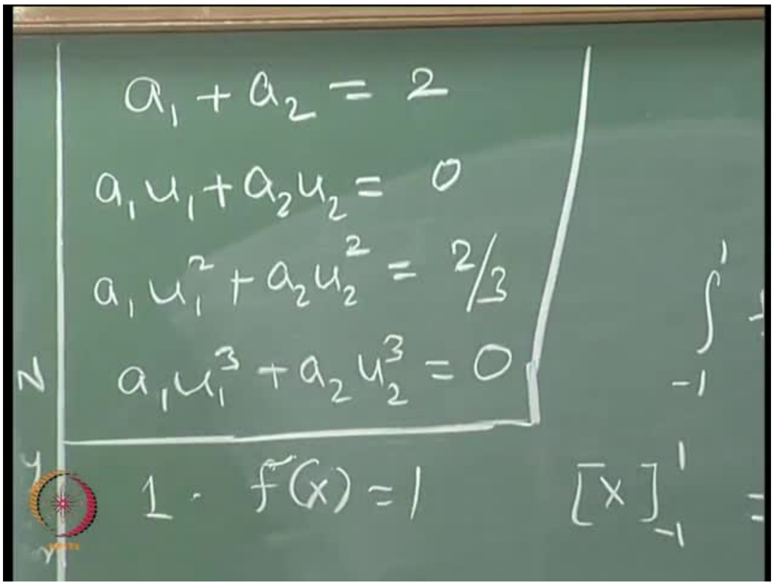

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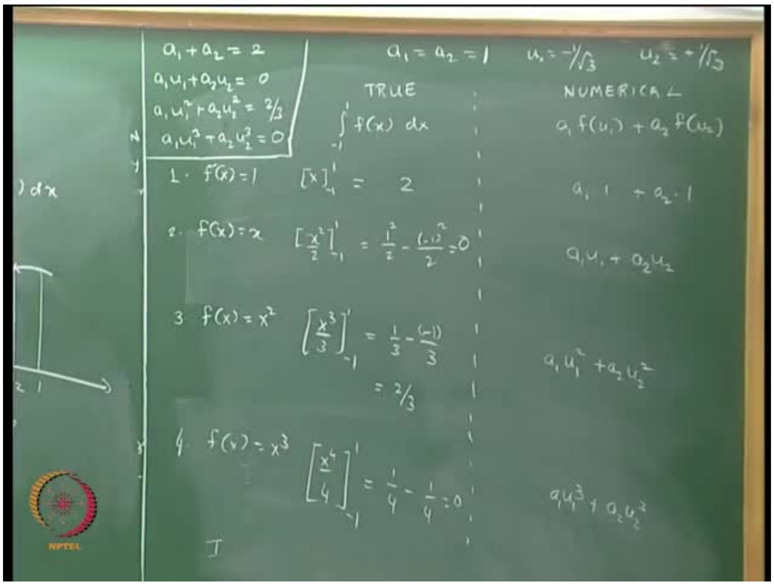

So, now we have the four equations; a 1 plus a 2 equal to 2, a 1 u 1 plus a 2 u 2 equal to 0, a 1 u 1 squared plus a 2 u 2 squared equal to 2 by 3 and a 1 u 1 cube plus a 2 u 2 cubed equal to 0. These are the four equations that we need to solve. When we solve this equation the value of a 1 and a 2, we get one; we will get a 1 equal to a 2 equal to 1 and u 1 we will get as minus 1 by root 3, and u 2 we will get as plus 1 by square root of 3.

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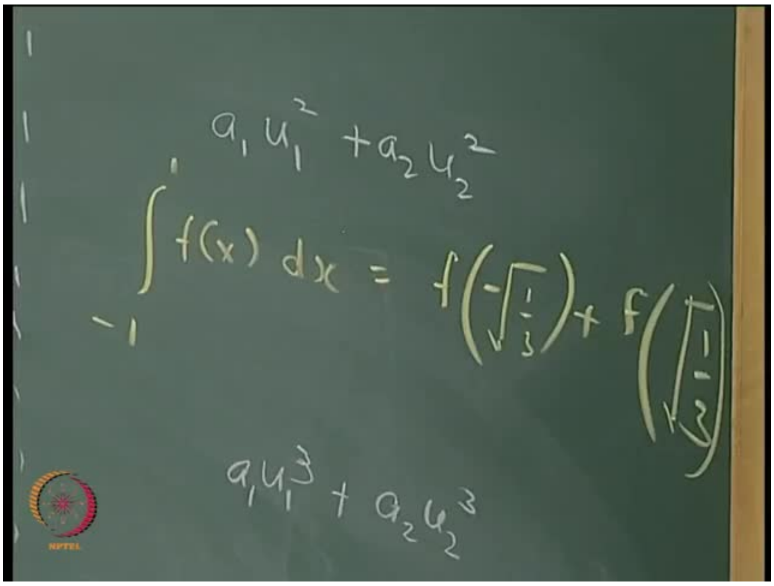

So, 1 plus 1 is 2, minus one-third plus one-third is 0, minus 1 by root 3 plus 1 by root 3 equal to 0, 1 by root 3 squared minus of 1 by root 3 squared is 1 by 3 plus 1 by 3, which is 2 by 3, and this is going to be minus of 1 by 3 root 3 plus 1 by 3 root 3, which is equal to 0. So, this is going to be satisfied. As a result, for the gauss quadrature method, the final result is going to be, integral from minus 1 to 1 f of x d x is going to be equal to f of square root of 1 by 3 plus f of square root of minus 1 by 3. This is going to be the gauss quadrature results.

So, that is essentially the numerical method that I wanted to cover for getting numerical integral of any function f of x. What we will do now in the next about 10 minutes are so is recap what we have done overall, for numerical differentiation and numerical integration, in this particular module. So, let us now recap the overall things that we have done for numerical differentiation and numerical integration.

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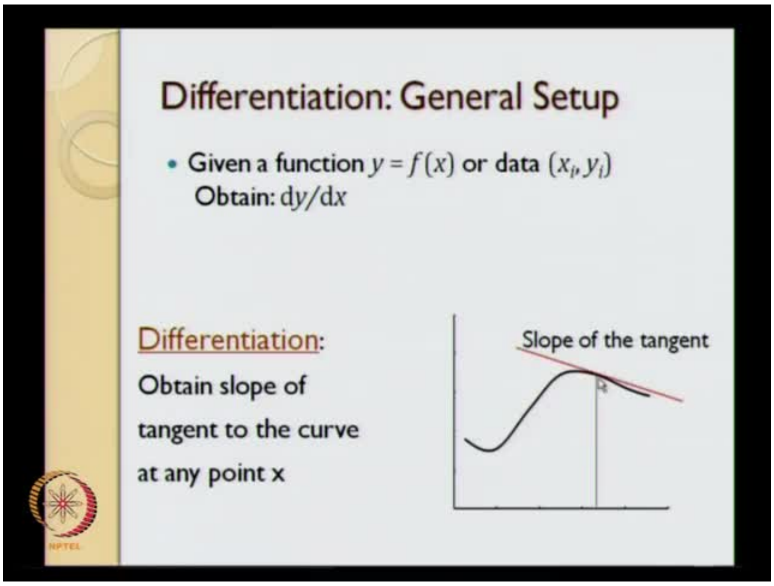

So, the general setup for differentiation was that given a function y equal to f of x, we wanted obtain d y by d x, which is essentially the slope of the tangent at the desired point.

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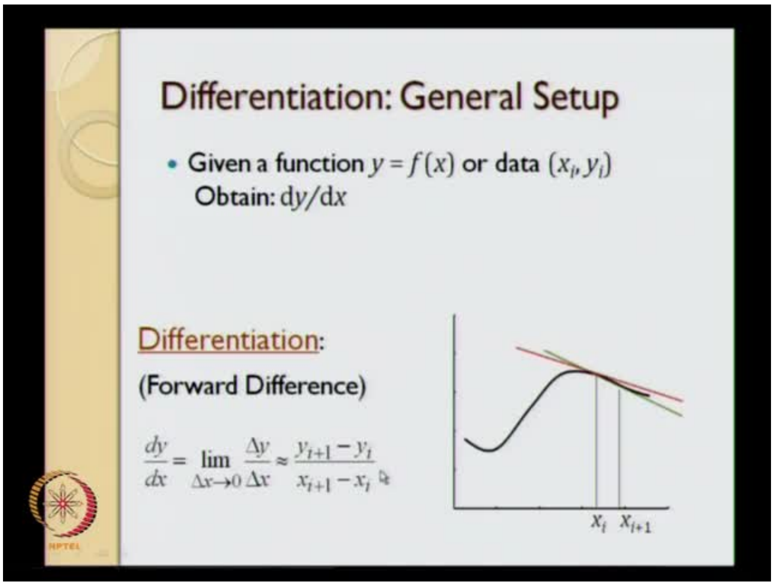

That is the geometric interpretation of differentiation. We then saw that we can use a forward difference formula in order to get the numerical differentiation, and the line over here shows the numerical differentiation using the forward difference formula, and the red line over here shows the tangent to that particular curve. And d y by d x, using forward difference was y i plus 1 minus y i minus 1 divided by delta x.

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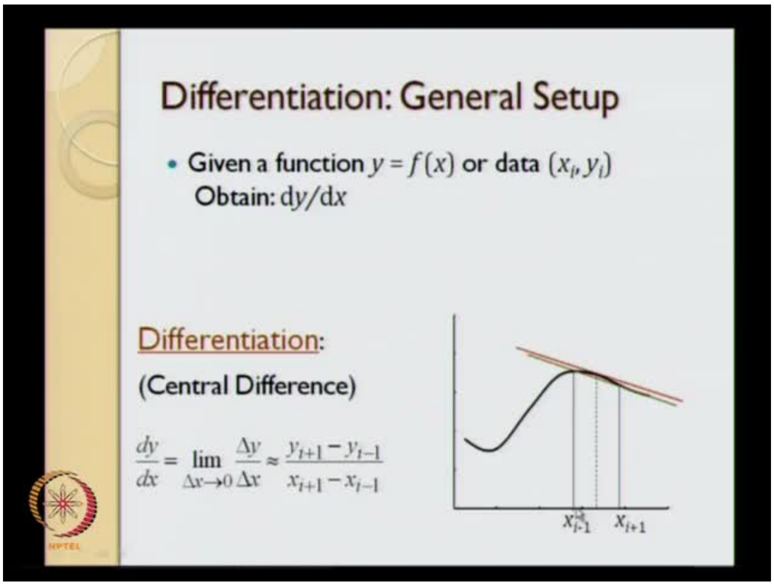

Then the other possibility is to use a central difference formula, so to find the slope at this particular point, we will do the numerical differentiation between x i plus 1 and x i minus 1, and based on the central difference formula we get is d y by d x equal to y i plus 1 minus y i minus 1 divided by 2 times delta x , where delta x is this particular difference between x i minus 1 and x i.

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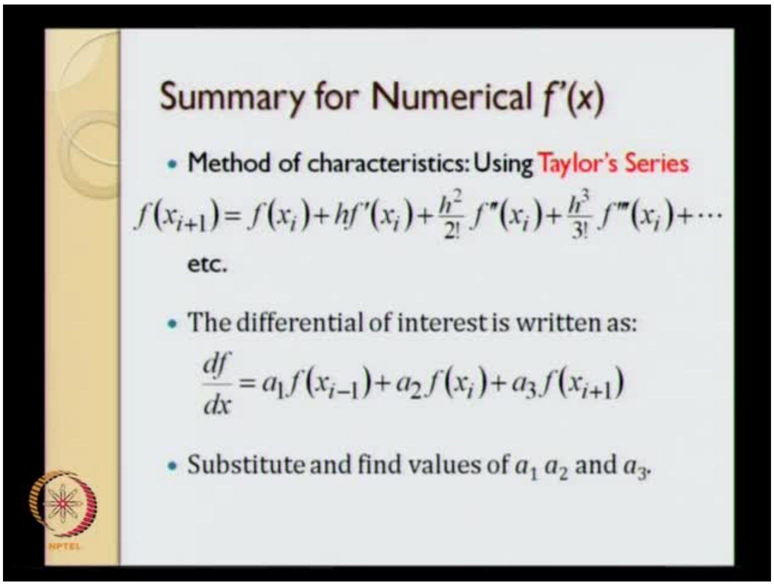

After that what we did was we use the Taylor's series expansion to find the numerical differentiation, for various different conditions. So, a summary of numerical f dash of x, we use method of characteristics where we write f of x plus 1 using the Taylor's series expansion, f of x minus 1 using the Taylor's series expansion, f of x plus 2 f of x minus 2 etcetera as needed, and differential of interest, we will write that as d f by d x as a weighted average of all these f of x. So, in case of the central difference formula where d f or d f by d x, we write this as a 1 f of x i minus 1 plus a 2 multiplied by f of x i plus a 3 multiplied by f of x i plus 1.

We substitute the Taylor's series in each of these, f of x i minus 1, f of x i plus 1. We do not have to substitute anything for f of x i, and then we equate the appropriate terms based on that we will get the values of a 1, a 2 and a 3. As well as, we will get the value of error of the leading term that we obtain.

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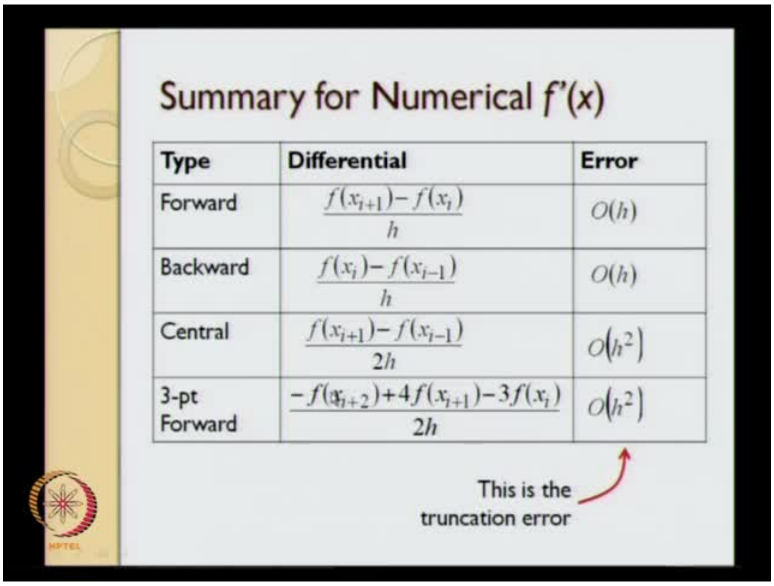

Based on this, we were able to derive all these formulae. This is the forward, the backward and the central difference formula. The forward and backward difference formula, the truncation error, is order of h and that is order of the difference delta x that we took. For the central difference formula, this is the actual formula that we derived which is accurate to h squared. We finally, derive three point forward difference formulas that mean it takes value of x i plus 2, i plus 1, and x i, to compute f dash of x i.

And that again we found was order of h square accurate and this was the overall expression for the numerical f dash of x.

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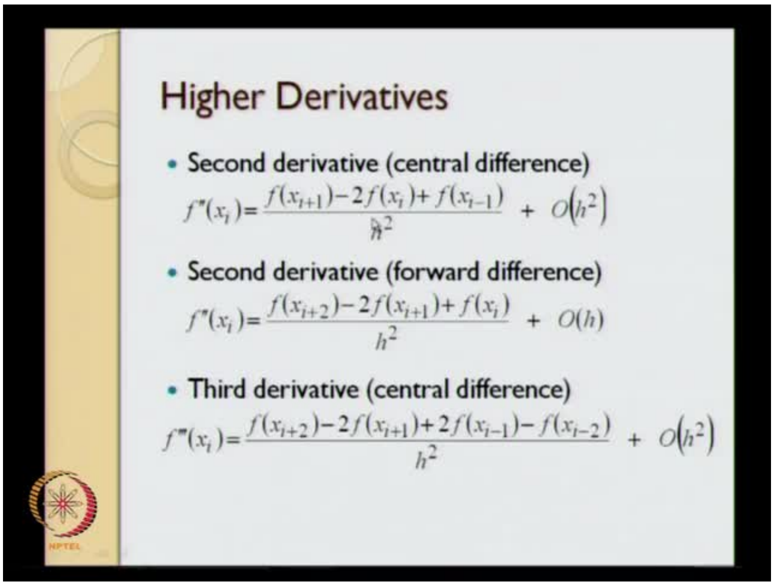

Then we also did the higher derivatives. The second derivative using central difference formula we obtained. Using the forward difference formula, can be obtained in the similar manner. We did not do third derivatives and so on mainly because they are not as used in chemical engineering. there are a few disciplines in chemical engineering, which do use the third and fourth derivatives, but for the most part we are restricted the first and second derivative. As a result, we just stopped at first and second derivatives, and this is the equation that we you can use for the central difference for numerical differentiation.

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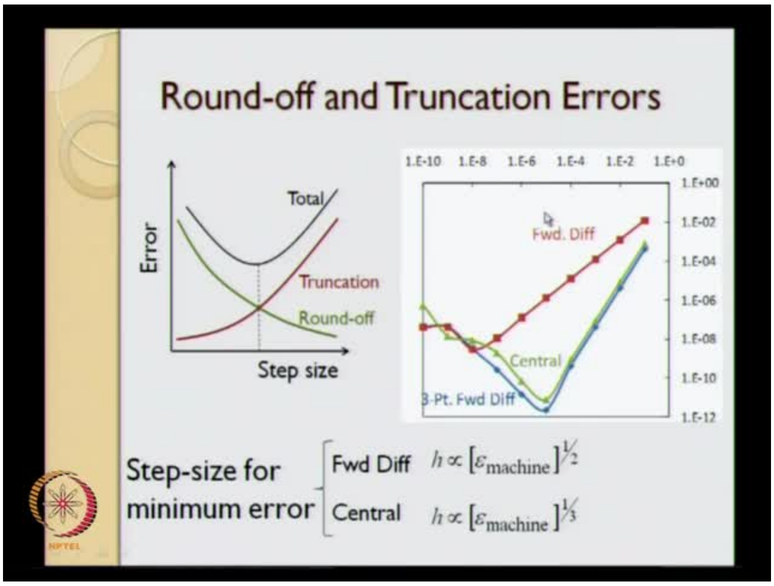

Then finally, in the numerical differentiation, we covered the trade of between round-off and truncation errors. What we have shown earlier as just the truncation error part; truncation error decreases as h is decreased. However, with respect to round-off errors, the round-off errors increase as h is increase, the red curve over here shows the truncation errors as step size is decreased, the truncation error decreases however the round-off error increases as the step sizes increased.

So, the total error goes through minima and that minimum happens at certain step size. for f dash of x, we had found that for forward difference method, h is, the best h that we get is approximately propositional to the machine precision to the power 1 by 2, and for the central difference, h is propositional to the machine precision to the power one-third.

In Microsoft excel, machine precision is 10 to the power 16, as a result h is approximately 10 to the power… sorry, machine precision is 10 to the power minus 16. So, the h that we should use for forward difference should be of the order of 10 to the power minus 8, and h that we use for central difference should be of the order of 10 to the power minus 5 to 10 to the power minus 6. So, this is the numerical result that we had obtained. this is result from the excel solving that we have done in module 3 itself, and we can see that the forward difference the errors are always larger than the errors in the central difference formula, and 10 to the power minus 8 is the best h value for forward difference, and 10 to the power minus 5 is the best h value for the central difference, as well as for the three point forward difference.

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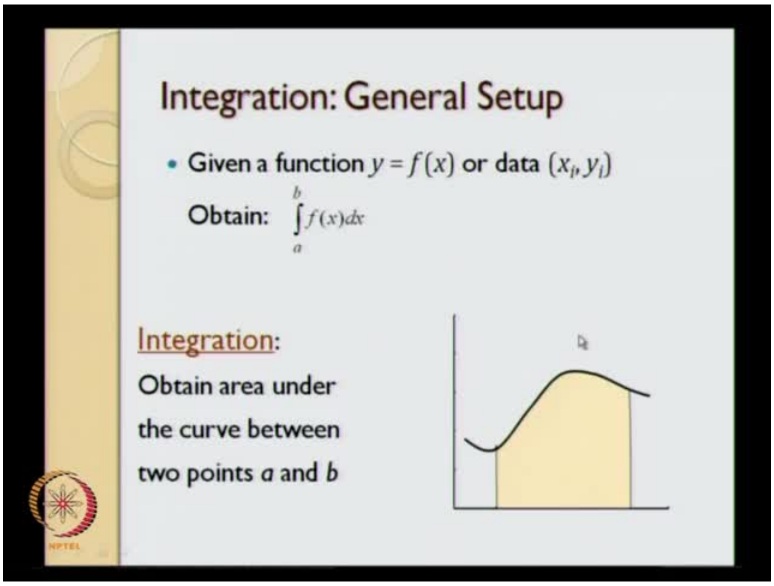

Going to numerical integration, numerical integration is nothing but, area under the curve between two points a and b.

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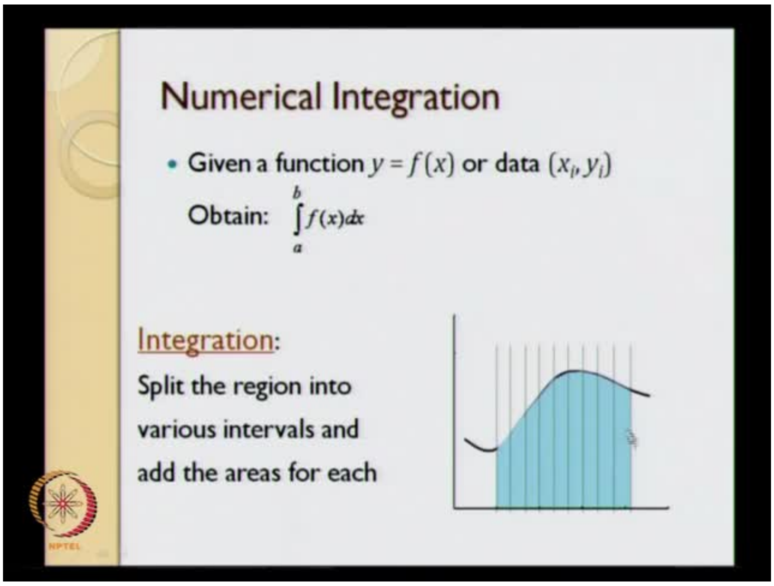

So, this area of the shaded region is what numerical integration is really all about. how we do numerical integration is that we split that area into various intervals, they may be they should preferably be equally space intervals, but there is no reason for us to choose equally spaced intervals. So, we split the region into various intervals and add the areas under each of the curve. So, for trapezoidal method, the way we will do it is we will keep calculating area for each trapezoid and progress as shown.

So, we will calculate the area for the first interval, second interval, third, fourth, fifth sixth and we will just add up those areas, as we show in this animation this plus this, plus this this this this this this, and this we will get all those areas, and we will some of the areas under the curve under individual trapezoid, and that represents area under the curve.

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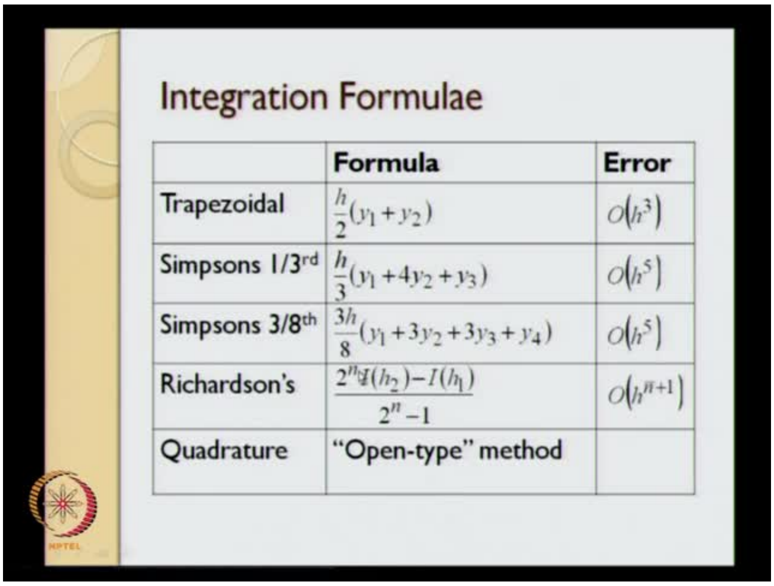

Integration Formulae

	Formula	Error
Trapezoidal	$\frac{h}{2}(y_1 + y_2)$	$O(h^3)$
Simpsons 1/3rd	$\frac{h}{3}(y_1 + 4y_2 + y_3)$	$O(h^5)$
Simpsons 3/8th	$\frac{3h}{8}(y_1 + 3y_2 + 3y_3 + y_4)$	$O(h^5)$
Richardson's	$\frac{2^n I(h_2) - I(h_1)}{2^n - 1}$	$O(h^{n+1})$
Quadrature	"Open-type" method	

We used three different methods, the trapezoidal rules, Simpson's one-third rule and the Simpson's three-eighth rule, in order to compute the interval. The Richardson's method, we said was for trapezoidal rule it is 2 to the power 2 minus 1, divided by 2 to the power 2 minus 1, that was the for trapezoidal rule. For both Simpson's one-third and three eighth rules, it is going to be 2 to the power 4, in this particular case. And the order of accuracy is h cubed for the trapezoidal rule, whereas, h to the power 4 for Richardson's rule using the trapezoidal solutions.

Whereas, when we apply the Richardson's rule for Simpson's one-third, we will get x to the power 6 accurate. Simpson's three eight, also will lead us to h to the power 6 accurate and this should have been n bar rather than n, where n bar is the value that we see over here. So, it is 2 to the power n bar minus 1 and not 2 to the power n bar over here.

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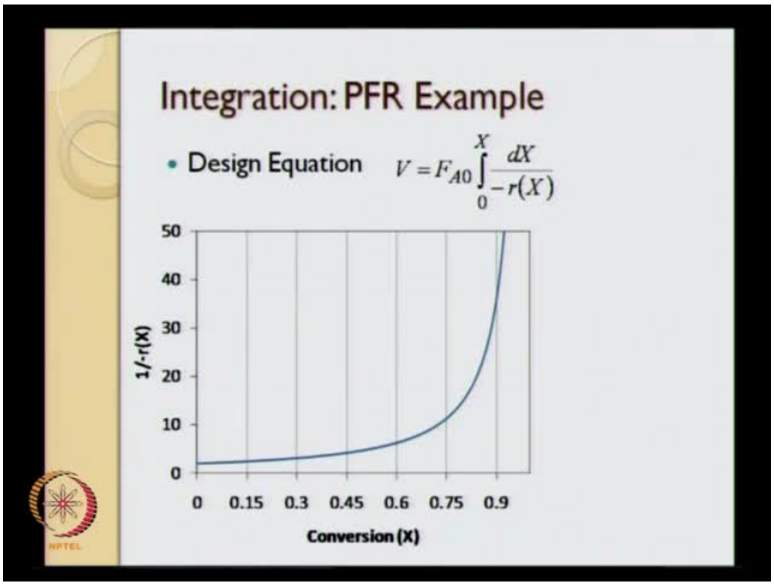

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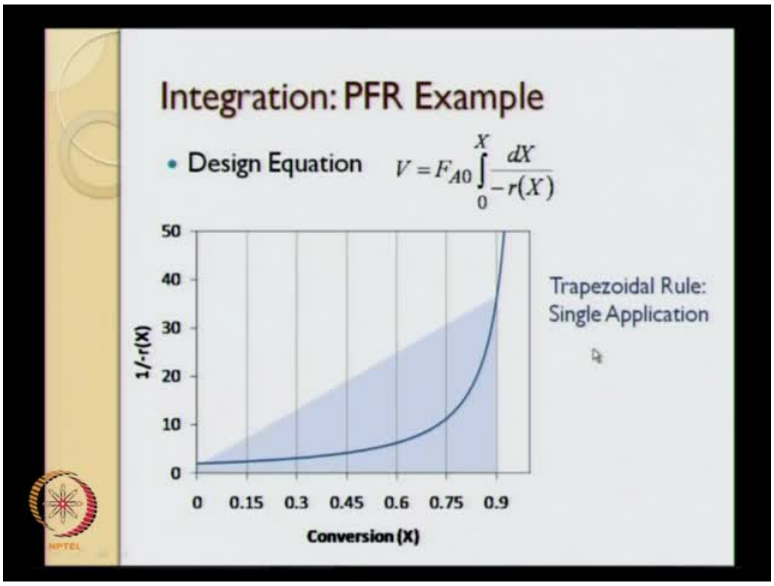

So, that is the integration formula that we get using trapezoidal, the Simpson's rule, the Richardson's rule and the implementation of trapezoidal rule for the PFR example that we had seen, the single implementation of the trapezoidal rule is to find the area under this particular trapezoid when we wanted to integrate from 0 to 0.9 d x divided by minus r of x.

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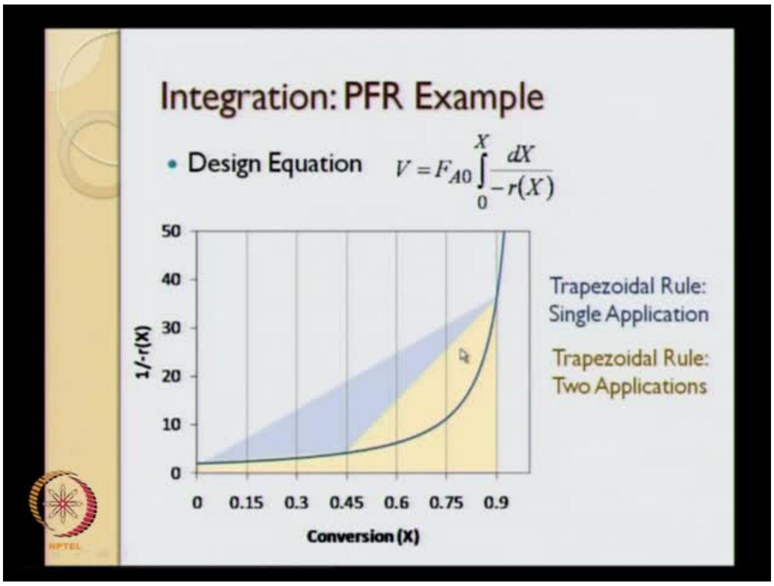

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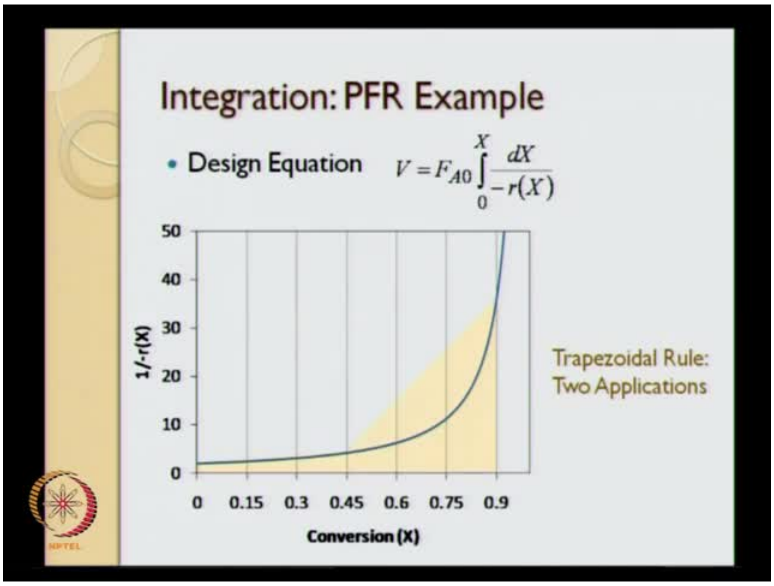

Two implementation of trapezoidal rule was area under the orange curve. Clearly, we can see area under this particular a pink or orange curve is significantly better than area under this light blue curve, as the approximation for the true area. The two applications of the trapezoidal rule will lead us to this particular area plus this particular area.

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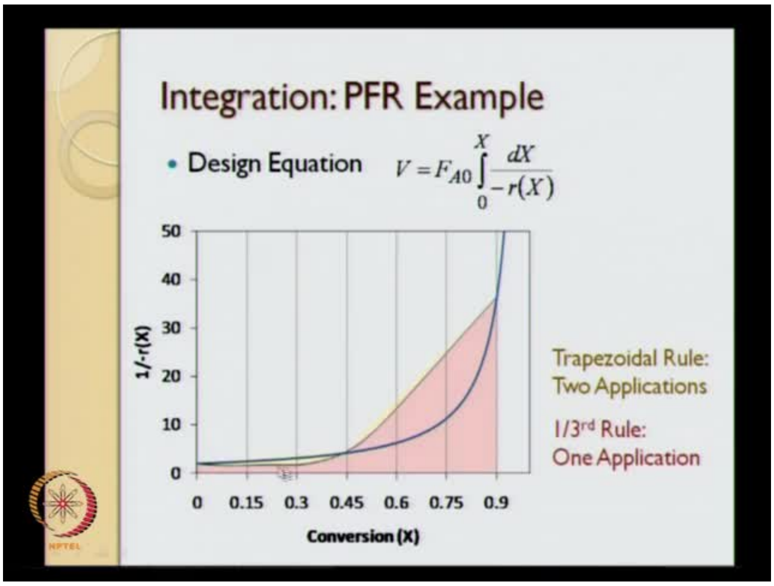

As against that we have the single application of Simpson's one-third rule, we are going to fit a second order curve. This particular curve is a second order curve and that is fitted to these three data points and area under the second order curve is what we get form a single application of the Simpson's one-third rule.

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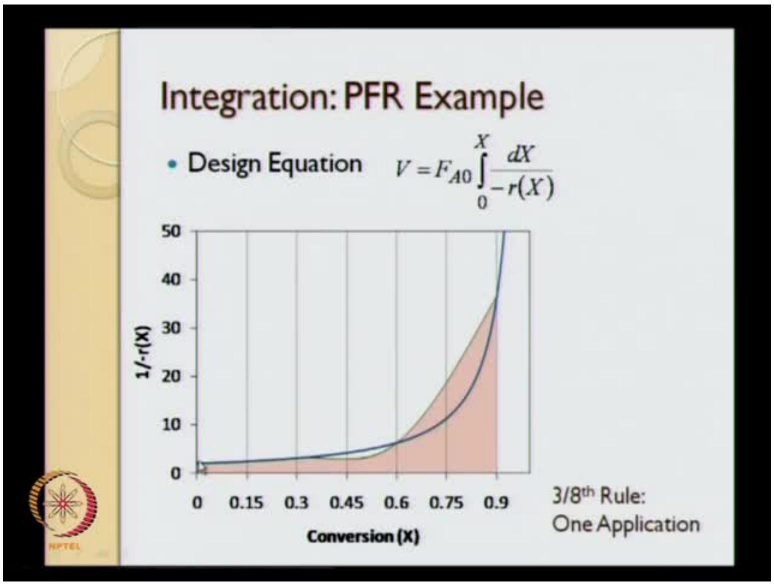

Finally Simpsons' three-eighth rule is going to give us area under a third order polynomial and that is fitted to this point, this point, this point and this point. So, this is the third order polynomial that that we fit and area under the third order polynomial is the result of single application of the Simpsons' three-eighth rule.

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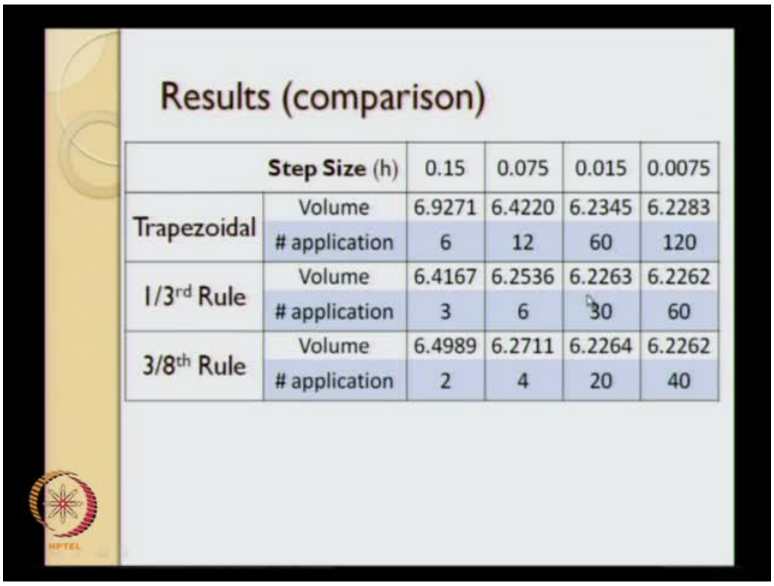

Results (comparison)

	Step Size (h)	0.15	0.075	0.015	0.0075
Trapezoidal	Volume	6.9271	6.4220	6.2345	6.2283
	# application	6	12	60	120
1/3rd Rule	Volume	6.4167	6.2536	6.2263	6.2262
	# application	3	6	30	60
3/8th Rule	Volume	6.4989	6.2711	6.2264	6.2262
	# application	2	4	20	40

These were the comparisons that we had made in the previous lecture of this particular module; the volume of the CSTR, in each column, we have the result using a single step size and what we see is that the step size of 0.15, leads to six applications of the trapezoidal rule, to get so from 0 to 0.15 from 0.15 to 0.3, 0.3 to 0.45, so on up to 0.9.

So, six applications of trapezoidal rule, three applications of one-third rule or two application of three-eighth rule, will give you these areas. The actual area is 6.226; the trapezoidal rule is further away from the true area, compared to the one-third and the three eighth rule. In this particular example, one-third rule is actually giving us better results than the three-eighth rule.

Keep in mind three-eighth rule is actually slightly more accurate than the Simpson's one-third rule but, the order of accuracy is the same, and we can see that h equal to 0.15, is already good enough for Simpson's one-third rule and the Simpson's three-eighth rule but, it still not good enough for the trapezoidal rule. We need to go for one more step of the trapezoidal rule in order to get accurate results.

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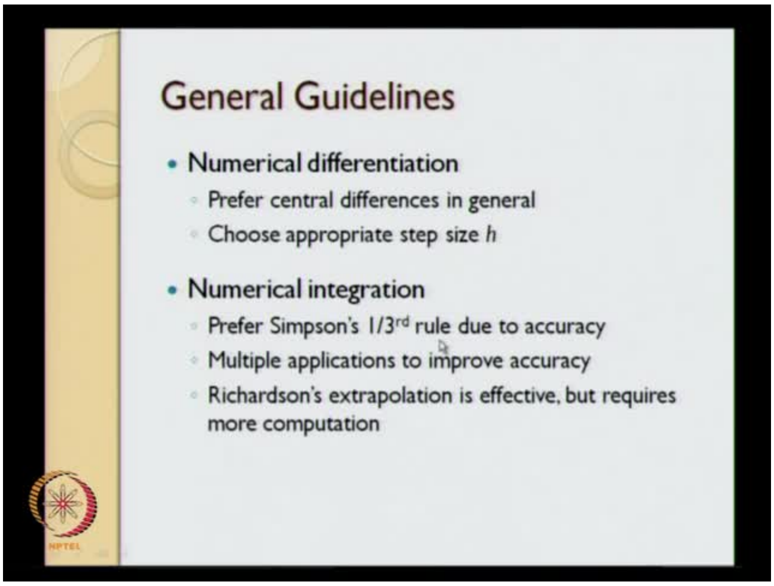

So, that is essentially what we have observed and based on all these observations, these are the overall general guidelines for numerical differentiation and numerical integration. for numerical differentiation, this is what I do as long as possible, I prefer to use the central difference method in general. As long as possible, I say, because in certain cases it is may not be easy or possible to use central difference rule and choose the appropriate step size of h.

So, the central difference rule for f dash of x, I will choose h as approximately 10 to the power minus 6. Central difference for f double dash of x, I will choose h as approximately 10 to the power minus 4, which is epsilon to the power one-fourth.

For numerical integration, what we said is we would prefer Simpson's one-third rule, because the accuracy of Simpson's one-third rule is h to the power 5. We will use multiple applications of Simpson's one-third rule to improve the accuracy, and we will use Richardson's extrapolation, it requires more computation but, it is effective. Usually, I have found Simpson's one-third rule to be good enough for most particle examples of our interest. We choose smaller and smaller h values in order to get more accurate Simpson's one-third rule.

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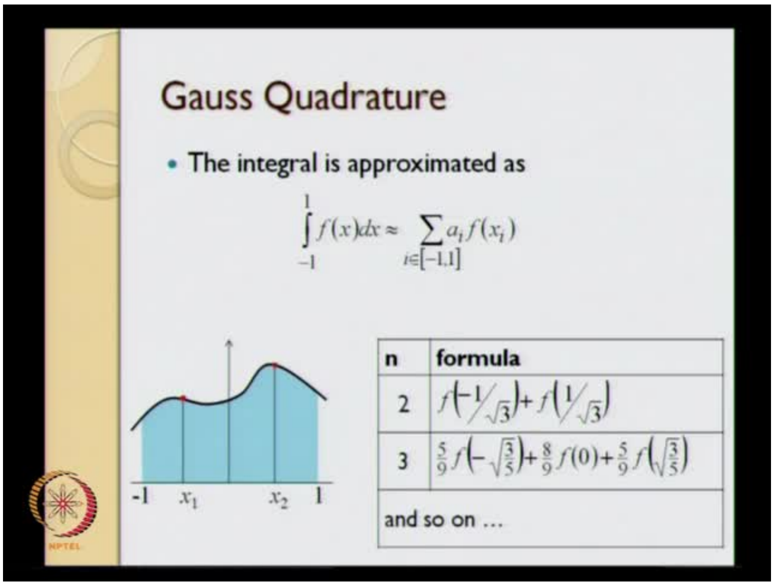

And finally, Gauss Quadrature is an open method. In case of n equal to 2, we find the integral form minus 1 to 1, that is integral under this blue shaded region, we will use that as a weighted average of f of x 1 plus f of x 2. For n equal to 2, we will get the value to be f of minus 1 by root 3, plus f of 1 by root 3. For n equal to 2, we will get 5 by 9 multiplied by f of minus root 3 by 5 plus 8 by 9 multiplied by f of 0 plus 5 by 9 multiplied by f of root 3 by 5.

So, this is the result for Gauss Quadrature. The advantage of Gauss Quadrature is it is very easy to implement and it gives a fairly high order of accuracy. The disadvantage of Gauss Quadrature is that it cannot be straight forwardly applied, if we want to use multiple intervals for applying the Gauss Quadrature.

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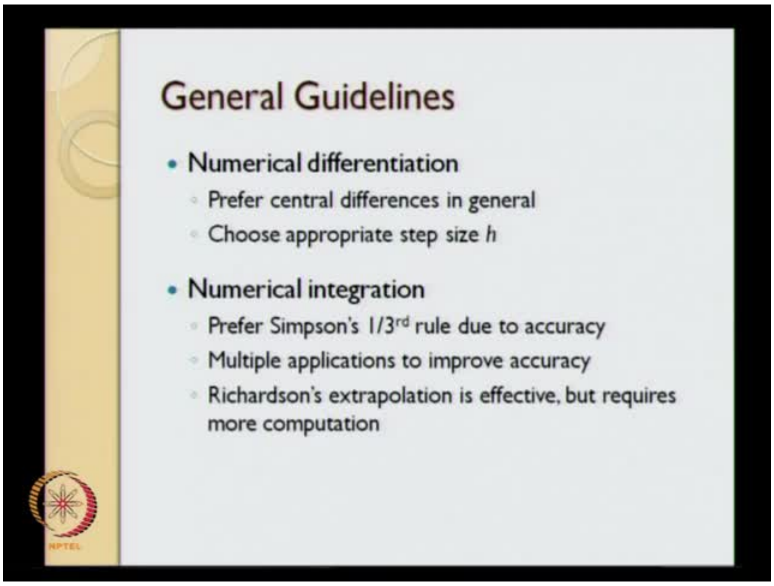

However, it is a very good formula and we have formula that is h to the power 12 accurate and h to the power 16 accurate also that have already been recomputed and a standard text book will give you these results. For example, Chapra and Canale, has the results available for n equal to 2, 3, 4, 5 and 6, I believe. You can read up that the text book to get the idea of higher order Gauss Quadrature.

I will leave you with the general guidelines that we have developed in this particular lecture thank you.