## Mass, Momentum and Energy Balances in Engineering Analysis Prof. Pavithra Sandilya Cryogenics Engineering Center Indian Institute of Technology, Kharagpur

# Lecture - 23 Numerical Evaluation of Integrations in Macroscopic Balance Equations

Welcome, till now what we have done is that we have a written the Macroscopic Balance Equations and in the both steady state and unsteady state. And we have looked into the solution procedure for them. And we have seen that how to do the solution for the differential equations we have and during that we found that at times we need to carry out some numerical integrations also.

So, today what I shall see that, how to make the numerical integration taking up a few commonly used methods for integration. Please understand there are many equations available in the literature for which you can look into dedicated books or the numerical techniques I shall be looking into only a few of the commonly used ones.

So, this lecture pertains to numerical evaluation of integrations that appear in the macroscopic balanced equations.

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So, first let us understand what is meant by numerical integration. So, it is basically by integration we want to find the area under a given curve representing a given process that

is a meaning of integration ok. So, and its evaluated as a weighted sum of the function evaluations within the domain of interest; that means, that whenever we are trying to carry out this integration like this that between two limits a and b we are trying to integrate F x dx ok.

So, let us assume that this is the some kind of function F x and here we have one a point what we are calling it x 0 and we have b point, we are calling it x n ok. And by this particular thing we mean we want to find out the area enclosed within this particular domain within the domain by this particular curve ok.

Now, this is the, what we do analytically? When we try to do the things numerically? What we do that we put this whole domain is divided into intervals ok? The domain of integration is further subdivided into intervals and let us call this intervals as h i that width of each of the intervals is h i. And h i may be found like I can just subtract the values of x at two consecutive points to find out the value of the h i or the interval or sometimes we call it step sizes ok.

So, once we do this and then we evaluate the values of the functions at this designated things designated values of x ok. So, we evaluate this values are designated values of x and then we try to evaluate some kind of formula we explore to how to get the value of the integration? Now, here you see that whenever we are integrating it we are summing up these particular values of the function at some points x i with some weightage factor.

Now, depending on the weightage factor associated with this particular function value we get different types of formulae for the integration. And all these formulae will have different levels of accuracy and it is also important for us to select this weightage factor as well as this width of the intervals. So, all these things you come into picture I will not go into a detail of those derivations what I will simply show by some example that how to implement a few of the integration methods numerically.

So, let us see the first here I just want to explain one thing that here there is a small gap you find it is just to show that there could be many number of intervals. So, here we have taken a gap from x 3 to x n minus 1. So, it is not a really break in this function it is just a break from F 3 to F n minus 1 ok. So, it is just to show that otherwise its a continuous function.

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Now, let us considered a practical problem like this a eleven meter beam is subjected to a load and the shear force a follows the following equation. So, whenever you are loading any kind of beam or any kind of material for that matter you know that there could be different types of loads it could be under compression, it could be under tension, it could be under shear and this kind of loading of the beam have to be studied, whenever we are trying to design any kind of support, structure, like bridges like some towers everywhere we need this kind of solutions.

So, here in this particular problem we are given a term for the shear force acting on this beam under some load. And here this x is the length in from the along the beam. So, length you can be again represented in various units and depending on the units this value of the, this unit of this F will also changed. So, here we are not concerned with the unit of the F for x here, we are just trying to figure out the it is or now we are just trying to figure out how to carry out the integration.

So, here we have the this F is equal to dM by dx and M is the bending moment and integration yields this relationship ok. Now incidentally it is given that the total length of the beam is in meters, but here we are not really concerned about the things because we are basically focusing on the solution of this equation. So, let us assume that we have the appropriate units for this particular equation.

Now, you see that the integration of this equation yields the; if you integrate this equation you can get this particular equation to find out the moment at any position x. So, 0 is the initial value of the x ok. So, it is a simply analytical way of doing this particular integration. Now here you see that we are having this F dx that is to be done. Now incidentally in this expression, we have taken a simple quadratic equation to demonstrate the comparison between the numerical solution and the analytical solution.

In practice you may find that you may not be having such simple form of the equation that is first and any and also it may. So, happen that you do not know the functionality of the dependence variable then what you do that you might be having some experimental values of the dependent variable at some specific points like for example; you may be given the density or some other property at some specific values of temperature.

So, you do not have really any particular equation or functionality between these two variables in that case also you can use such kind of numerical methods for integration. So, here we have this particular expression which can be easily found integrated analytically.

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So, first let us see the problem statement in this we have told that if M naught is 0 and x equal to 11 meter determine M analytically and numerically. So, these are the two things we have to do and instantly it is given that we have to find out the value of the moment at the end of the particular being it could be some other value two.

Here I have listed three of the very common ways of doing numerical integration and we shall be looking into these three and there we shall compare their result.

Solution  $F(x) = 5 + 0.25x^{2}$ Since  $M_{0} = 0$   $M = M_{0} + \int_{0}^{x} F dx = \int_{0}^{x} F dx \equiv I$   $I = \int_{0}^{x} F dx$ a) Analytical method  $I = \int_{0}^{x} F dx = 5x + \frac{0.25}{3}x^{3}$   $I = \int_{0}^{x} (5 + 0.25x^{2}) dx \approx 165.9$  M = I = 165.9 Nm

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So, first let us go with the analytical solution. So, here we have this F x equal to this particular value and now you can easily see that if you put this particular F d x as some kind of integrand I, then I is equal to this 0 to x F d x and M 0 value is 0 as given in the problem. So, analytically if you do this you find that this will give you 5 x and this will give you 0.25 x cube and then if you put this limits from 0 x you will take as 11 here.

So, if you take this x as 11 then you find that this will be the in this case you can put the value 11 and in this case you will find this is the value you will get ok. For your convenience sake I am just writing this thing this will be 5 x plus 0.25 by 3 x cube.

And this has to be integrate put between 0 and 11. So, if you do this you will get this particular result ok. So, this is the very simple way you can see. Now, let us go to the numerical manner to solve this particular problem.

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So, here we have this particular integrand. So, first let us consider the six equal intervals and as I showed you earlier that if you have equal intervals then we can simply get the step size like this that h i equal to a minus b divided by n. So, in this particular problem we are choosing the n to be 6. So, with that we get this particular value of the h. So, please understand this six is arbitrary number, you if you vary this number of intervals you will find you are getting different accuracies ok. So, let us arbitrarily we choose six for demonstration purpose.

So, you can see that b is 11 a is 0 so, divided by 6 you will get this particular value for h and in this particular case because the in length is given in meters. So, naturally this particular h will also be in meter; that means, we are finding the function value at an interval of 1.83 meters. Next we come to this particular table in this table what we are showing is this how we evaluate the value of the x at all this points.

Now you see that x will be 0 and 0 we are finding the value of the function as given and then we are getting the value of x as 0.3. So, this is the function value then we have the value of x as 1.83 plus 1.83. So, we are getting 3.66 and then we are putting this as. So, this is one point this is 1.83 into 2 you can say this is 1.83 into 3 you can say so on and so forth. So, that is how you are getting the values of the x ok.

And then also know the value of x you can find for each value of x you can find the value of the functions for the given relationship. After obtaining this particular this values let us see how do we carry out the integration.



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Now, first we shall go with the trapezoidal rule. So, here you see that we are constraint some kind of function and we have some domain of interest and this is the total width within which we have to find out the area under the particular curve ok. And in trapezoidal rule what is done that you know trapezoid the trapezoid is word that its a quadrilateral in which two of the opposite sides are parallel other two sides are not parallel so, that is a trapezoid.

So, with that geometric interpretation we see that here we have the domain. So, we are making a trapezoid like this that these a function value at this, then you can say that this is the value of the a and suppose this is the value of the b ok.

So, with these two values we are trying that we are fit is this we have made a straight line between the two points this is the width. So, you can easily see that how you find the area of a trapezoid. So, this is this f a is shown here f b shown here and this is the shaded portion is the one we are interested in. So, this I the integral value is width into the average height and average height is simply we can say this height plus this height divided by 2; that means, f a is the height f b is the height here. So, f a plus f b divided 2 is the average height ok. So, this simple principle has been taken into this trapezoidal rule and here we have what we do that we divide the whole domain into small small trapezoids ok.

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So, what it what it means is this that we take the domain like this suppose this is the domain. So, we make small small trapezoids like this we make. So, that is a suppose this called  $x \ 0$  this  $x \ 1$  and  $x \ 2$  like and so on and so forth for each of these things. So, we every time we are making, I am going to straight line. So, you can see there is a slight difference you can see that is we will slight error in the actual value this error will be given by this particular shaded portion this is the error in our calculation ok.

So, this so, you can see that the closer we take this points ok. So, we shall be moving more towards the function and we shall be getting less and less error. On the other hand if you make too small intervals you find that the, it will take longer time to carry out the integration. And not only that you may find that after certain number of the inter number of intervals you are not getting much of a difference between the results of the two consecutive set of intervals.

So, in that case you can say that you are reaching some precision value and also it is the you are reaching some accuracy also. So, in that respect you have to choose this number of intervals judiciously. So, once you do this kind of thing and you keep applying the trapezoidal rule for each of the subdomains for this domain this domain this like I call it

one two like this if you make many subdomains in this and then you put the add them together you will land up with this particular expression ok.

So, in this expression you see that the function of values at the two endpoints are taken the same manner and rest of the things are taken like this ok. Now you see that if we rearrange the equation putting the value of the h here we get this particular formula and h is given by this b minus a by n.

So, in this kind of trapezoidal rule we have equal intervals this is not for unequal intervals. Now after this, what we can see is this that as I say that this is the width of the domain total width and this whole thing is the average height. And now what we do that we have all these values of the function at all this six points, we put these all these things in this expression. Like for example, for F x 0 we shall put 5 for F x n we shall put 35.250 and in between we shall be putting all this values ok. So, we shall put these values over here.

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And after this we find that after inputting all those values we are getting the value of the I or the moment like this.

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Next we go to the other method. Here we have the Simpson's one third rule, here you see that here we are choosing three points we were choosing two points in trapezoidal rule here we choosing three points and these are also chosen arbitrarily ok. And you can see that if you join this three points by some kind of curve, you find this is the area and this area is again an approximation of the actual area, which is having this here; here you can see that this up to this up to this portion we have the area is less than the actual area.

On the other hand between these two portions you see the area is more than the actual area, on the other hand again you see on the other side this actual area is more than the assumed area.

So, you can see overall you can see that some of these excess and this diminished areas will be cancelling them of and we may be approaching the exact area under the curve. Again you can see here we have the width and we may have different heights and again we shall be doing we shall be again evaluating how to find the value of the average height width is going to be even constant.

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So, here you can see without deriving the equations you can see that this is the particular expression we are getting in this particular expression again you can see that this is the width and this is the average height. Please note that what is happening these within the intervals these values are a bit changing from trapezoidal and again you can see that if you go back to of the original formula where I said that the integrand is that w i into F x i.

Now, you can see this w i when x equal to i equal to 1 then w i is equal to 1 when i is equal to n then w i is equal to 1 ok, but in between you can see that for say w i equal to 2 or so, this w this is maybe equal to 2. So, it is either 2 or 4 when I can say this way that when i is between 1 and n. So, it the weightage factor is changing for different points ok. So, this is how again we can see that how you can write this generalized equation same thing you can also find for the trapezoidal rule.

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	No of intervals	0	1	2	3	4	5	6		
	F(x)	5.000	5.837	8.349	12.563	18.432	25.976	35.250	-00	
	x	0	1.83	3.66	5.50	7.33	9.16	11		
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Now, we evaluate that function values at all these intervals as previously we have done looks for the all the seven points here.

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And now we implement that formula for the one third Sampson's rule and we get this particular value of the moment.

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Next we come to another popular method that is three eight Sampson's rule and the whole here you see that in this Sampson's 3 8 rule we find that we are taking four points at a time ok. Now in that case also we kind of put some curve through this particular points again as I explained earlier there could be some over estimation and sometimes under estimation of the area so, that the overall things will get cancelled out ok. So, again we have the area under the curve as width into some average height widths on the four points.

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So, this is the kind of formula you get for this and here you can see that again that all the points having are not having same weightage some have weightage of 3 and some have weightage of only olne ok. And here again you see that this particular b minus a is a width and this whole thing may be taken to the average height between the curves.

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So	lutio	n (C	ontd	)					
	No of sub- intervals	0	1	2	3	4	5	6	
	F(x)	5.000	5.837	8.349	12.563	18.432	25.976	35.250	
	x	0	1.83	3.66	5.50	7.33	9.16	11	
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So, after putting the values of the F at different values of x we simply plug it in this particular formula and we get this value of the moment.

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Now, next what we do is that we make a table for comparison of the results from the three methods with the analytical method solution because, the analytical solution is supposed to be the real value.

So, here we have put those things that this is the analytical value and these are the values with all these three methods. And here you can see that how this particular errors are changing and you can see here that 3 8 rule gives us the best result ok. So, in this way you can decide that which kind of method you should take and how you should implement them because even though the Simpson 3 8 rule is giving the best result out of these.

But, when you are doing coding or something we may find this make maybe bit more involved in the coding or during a manual calculation, but none the less if you find that you have to have some kind of accuracy in your result. So, you should choose the appropriate method without really bothering about its the time taken by that particular method.

Now, here we have discussed all the methods based on the assumption that the interval remains the same in the domain.

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Next we take a problem in which we are going to check that if the domain intervals are not the same. So, here I am taking one example using the trapezoidal rule only you can easily find out the equivalent terms for the other Sampson's rule and whether 3 8 or one third one thing we understand that as the, if the number of intervals becomes different then, it takes longer time for us to do this calculations. Because, you will find that it is not possible to then get a simple a very simple expression for the integration ok, but none the less you can use it with unequally intervals.

So, here we are given some kind of polynomial this is the fifth order polynomial again analytical solution is a very much possible you can find the analytical solution versus polynomial. So, but you have to find out the value in a numerically and here you are given the f x value at some values of x. And you can see here that the intervals are not the same like for example, you can see that for this particular between these two points this interval is 0.12 between these two points this interval is 0.10 and so on and so forth and here it is 0.14 ok.

So, like that you see now as I was telling you this might. So, happen that these are the experimental results for you and you might be fitting some kind of curve through this or this is for mistake here this should be 0.04 0.4.

So, you as I was telling you that these experimental results and you might be fitting some kind of curve through these results to obtain this kind of an equation and then you can go for the implementation of those rules. But even you even if you do not have this equation with you can still go ahead with the numerical integration based on these results ok. So, let us see how.

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Solution	x	<b>f</b> ( <b>x</b> )	h <sub>i</sub>	
Solution	0.0	0.200000	0.12-0.0=0.12	
	<b>0</b> .12	1.309729	0.10	
For successful and a data we lot a the Transmitted	0.22	1.305241	0.10	
For unequally spaced data points the Trapezoidal	0.32	1.743393	0.04	
method may be modified as	0.36	2.074903	0.04	
Ι	0.40	2.456000	0.04	
$h_1$ $h_2$ $h_3$	0.44	2.842985	0.10	
$= \frac{1}{2} f(x_0) + f(x_1)  + \frac{1}{2} f(x_1) + f(x_2)  + \cdots$	0.54	3.507297	0.10	
$h_n$	0.64	3.181929	0.06	
$+\frac{1}{2} f(x_{n-1})+f(x_n) $	0.70	2.363000	0.10	
	0.80	0.232000	-	DO.
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So, here for the unequally spaced data points we have the trapezoidal rule it is written like this and now what you see that we are not able to club each of this domains subdomains together. So, that is why you find that were each subdomain we are making this kind of the area under the curve.

So, it is between x 0 x 1 this is between x 1 x 2 and so on and so forth. So, now, putting this things we know the values of the h 1 h 2 from these differences ok. So, we put those differences between two consecutive points and we take the function values at the 2 x values ok.

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So, now you can see that for all those things we are putting this values of h and the f x and we will getting this particular value.

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So, these are the some of the reference books you may consult. So, the first two books will give you on the mathematical as well as numerical things and these two books will be generally dedicated to numerical analysis.

Thank you.