Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture – 17
Solution of Macroscopic Balance Equations – II

Welcome. This is lecture is a continuation of my previous lecture in which I started telling you about some of the selective methods for solving non-linear algebraic equations. And this method we will be looking into a few more of these numerical methods to solve the non-linear algebraic equations.

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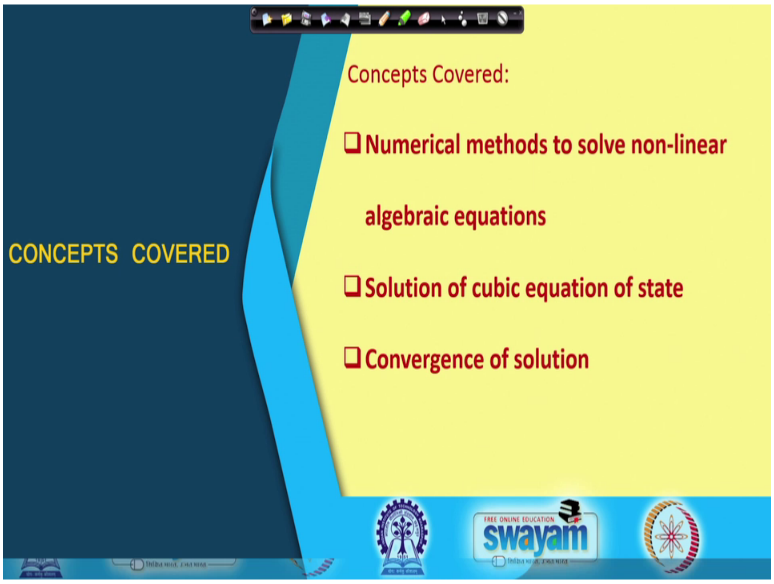

So, in this lecture we shall be studying those few more methods to solve non-linear algebraic equation, and then we shall also take a special case of solving the cubic equation of state. And then we shall be ending this lecture with some m knowledge about how to figure out the convergence of a solution.

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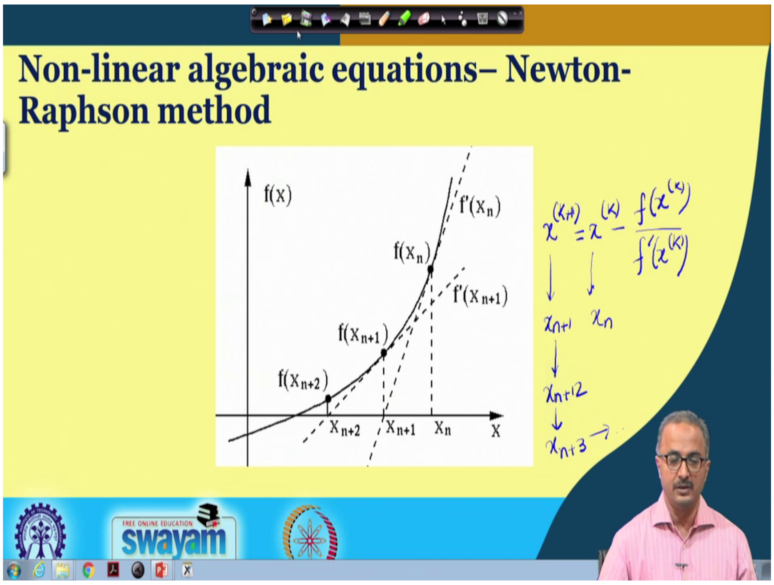

So, this particular thing it is kind of a carryover from my last lecture, in which I started with Newton Raphson method and as I told you that the Newton Raphson method is a very fast process vast method and it needs very efficient. But the only thing is this it becomes cumbersome, because at each state you have to calculate the derivative of the function at the new estimated point. And now in this figure I am just showing pictorially how the Newton Raphson method works in terms of the solution convergence.

So, here we are choosing these two axis that if f x f x is the function which we have to for which we need to find the root and this is the independent variable. And here we have put one arbitrary function shown by this solid lines, solid black line. Now we start with some initial values say X n and this is and we have to reach this particular value, this is the solution ok. So, we will start with his guess value and at this guess value what we do? We will find the value of the function that is f X n, and by doing the derivative what we are finding basically? We are finding the slope of this tangent to this particular function at this particular value of the X n ok.

And once we find the tangent that is point and we see where the tangent is crossing this x axis ok, that is second taken to be the next updated value of the root ok. So, by doing the calculations as I shown you in my last lecture we are approaching this X n plus 1, just for your remembrance I just put the equation for you again that X k plus 1 is equal to x k minus if x k divided by f prime x k ok. So, this is the recurrence formula for the Newton Raphson method.

So, using this particular formula we are able to update the value of the root. So, here we are not taking x k, we are putting them in this particular thing is taken to be say x n and this is taken to be say x n plus 1 and from this we are going towards x n plus 2 and then x n plus 3 and so on and so forth ok. This continues until we reach convergence.

So, now we find the next best value, then again we from this x n plus 1 again we find out the value of the function and again we put the tangent over here and this f dash prime X n plus 1 is a derivative at a tangent to this and from this again we find we are going to the another updated value that is X n plus 2. And now, if we keep continuing this thing we find that from this particular guess value we are approaching the solution, and we again stop the solution when our convergence criterion is made. So, this is the pictorial representation of the Newton Raphson method.

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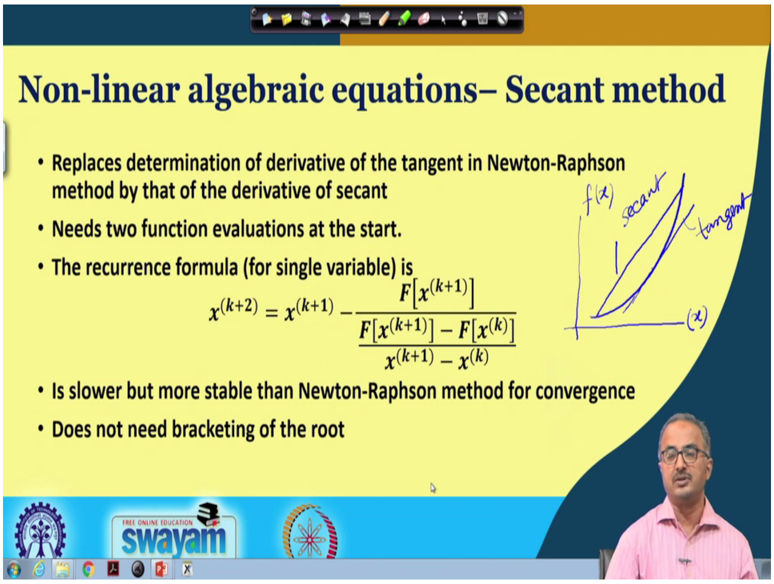

Now, we go to another method Secant method; in this method you will find that here also we need to find out the derivative of, but in a different manner ok. In this case that in the Newton Raphson method we are finding the derivative of the tangent where as in this particular method we are finding the derivative of a secant. Perhaps, you know that the difference between tangent and secant just for your remembrance; let it put it for you.

Now, suppose you consider a given curve and suppose we have some curve. So, at a given points if you are plotting this thing this is the tangent ok, but on the other end if you have some other segment of the curve so this is the secant, this is the secant and this is the tangent. So, as the name of the method suggests you that in this particular method we are considering the secant and we are going to find out the derivative of the secant.

And derivative can be found out of the secant, if I know this particular point and I know this particular point; that means, what that in case of Newton Raphson method we were using only one point ok. On the other hand for the secant method to be implemented we need two points ok, to find out the slope; that means, in case of the Newton Raphson method we need only one starting value where as in case of secant method we need two starting values ok.

And again this two starting values can be arbitrarily chosen. So, that is why you find that we need two function evaluations in instead of one function evaluation in case of Newton Raphson method. On the other end we need the derivative evaluation in Newton Raphson method that is not needed in secant method ok. Now once we chose it we start with two initial values say x k and x k plus 1.

Now, again you see that this f x k plus 1 minus f x k divided by x k plus 1 minus x k this gives us the derivative of this particular or slope of this particular secant ok. So, we are using the similar kind of formula as the Newton Raphson method only replacing the f prime x k by this particular formula. And rest of the equation rest of the solution method is saying that once we find this updated value of this x k plus 2 we replace the x k with the x k plus 1 and x k plus 1 with x k plus 2 and we find x k plus 3 ok.

And then after finding x k plus 3, we replace x k plus 1 by x k plus 2 and x k plus 2 by x k plus 3 and we get x k plus 4. So, this is the way we keep; we doing this particular thing and we go for towards the solution it is found that it is slower than the Newton Raphson, but it is more stable. By stable we mean that how robust it is in particular method is so that it does not diverge when we are choosing some arbitrary value for the roots ok.

So, it is found to be more stable, but it is slower than the Newton Raphson method and it does not need bracketing of the root; that means, we do not need as we learnt earlier in the bisection method we needed to bracket the roots between so that the root is between two range we are choosing. In this case also we do not need like Newton Raphson method we do not need to bracket the root.

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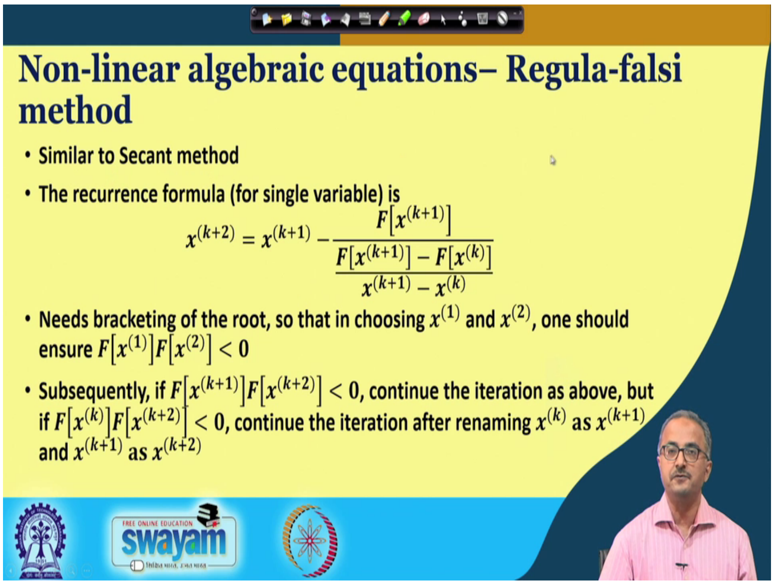

Next we to go to Regula-falsi method that is also sometimes called the method of false position, it is similar to secant method only difference is this that in this case this is the first two guesses has have to bracket the root. So, this is similar to the bisection search ok. So, in this case again we are starting with two values, but these two values will be bracketing the root ok. So, if we know the root for root we will have the idea of the root then this method should be used.

Now, in this case what happen is this that whenever we are bracketing the root and whenever we are updating this value of the root then what we find that how we are replacing the previous two values will be depending on the products or the functions at the these various points. So, first is this to bracket for bracketing criterion is this that the product of the F x 1 and F x 2 this 1 2 represent the initial two values this product should be less than 0; that means, we are bracketing and this was the same thing we were using in case of the bisection search ok.

And after this we are going to check that whether this updated value is bracketing the root or not ok, for checking that again we find out the product of the function values at this a k plus 1 and k plus 2 and k and k plus 2 ok. Depending on the sign of the product again we reassign the values of x k to either x k plus 2 or x k 1 to x k plus 2 so depending on that.

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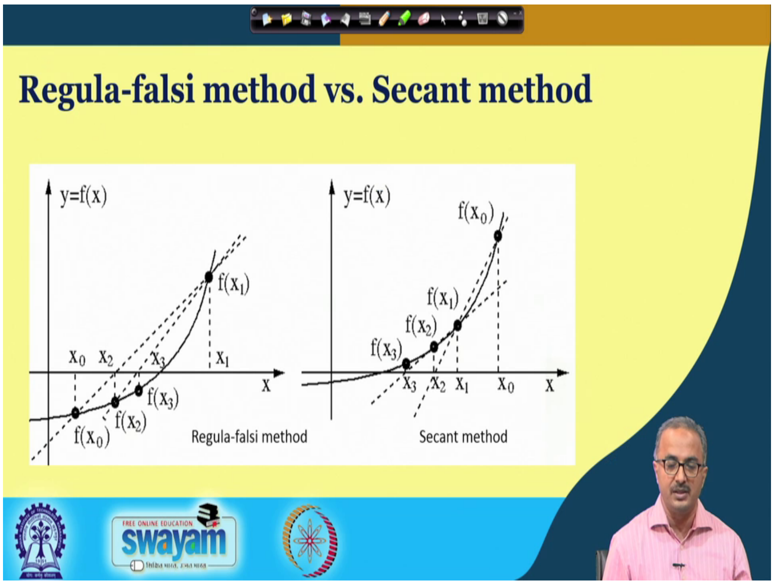

So, let us look pictorially in this particular thing that in case of Regula-falsi what we are finding that initially we start with the bracketing of root, suppose x 0 and x 1 other 2 initial values and we can find see that at x 1 f x 1 is here and x 0 f x 0 is here. So, when we take the product of these two we find this is come to negative, that shows that the root is bracketed between x 0 and x 1 and you can see here also the rooted somewhere here.

Then what we do after application of the formula we get the value of x 2. Now again we take the product of f x 2 with f x 1; now you can see here that f x 2 and interface 0 will give you a positive ok, but f x 2 into f x 1 give you negative. So, we should replace x 0 with x 2 and again find out the next root as x 3, now again you can see here that f x 3 and f x 2 is giving you positive.

Whereas f x 3 into f x 1 giving negative. So, again for next two should be with this x 3 and x 1 ok. So, this is the way you can see that we are able to approach the solution on the other hand if you look at a secant method you can see that here the root is somewhere here. Whereas we are starting arbitrary away from the root and you can see both the roots are on the higher side of this actual value ok.

But it does not matter again we are finding this two will function values and even with this we are finding that we are approaching the roots. So, we are getting x 2 here again with x 2 x 1 we are finding x 3 here with x 3 x 2 we can again find the x 2 here and like that we are able to approach the solution ok. So, these are the basic differences between Regula-falsi and the secant method.

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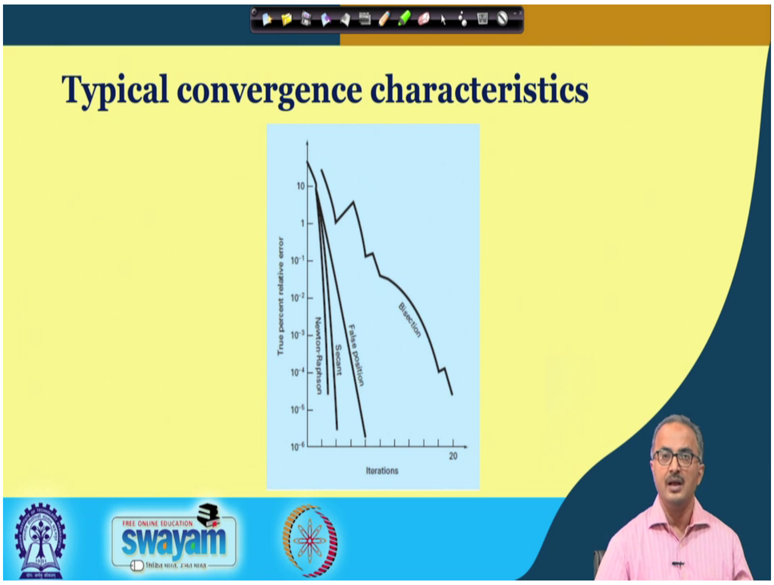

Now, for a typical problem you can see that how the typically this four methods differ in their convergence characteristics, that means how fast they converted how many iterations they will take to converge. So, here you can see that bisection method is giving it is also converging, but with an fluctuations. That means it is not converging monotonically.

Sometimes it is decreasing this error is decreasing again increasing again fluctuating this if it is going to convergence and it is taking say about say two into iterations. Now when you go to measure of false position even though you are bracketing the root that is a Regula-falsi method you say that it is also converging monotonically and it is better than bisection method ok. That means, in both Regula-falsi method and bisection search even though there is bracketing.

But the bracketing is not really increases the speed on the contrary if you look at secant method or the Newton Raphson method we did not try to bracket the root here we are finding the convergence is much faster. The secant method is giving faster convergence even than the Regula Falsi and Newton Raphson method gives us the fastest convergence. So, this is a typical convergent characteristics of these four methods.

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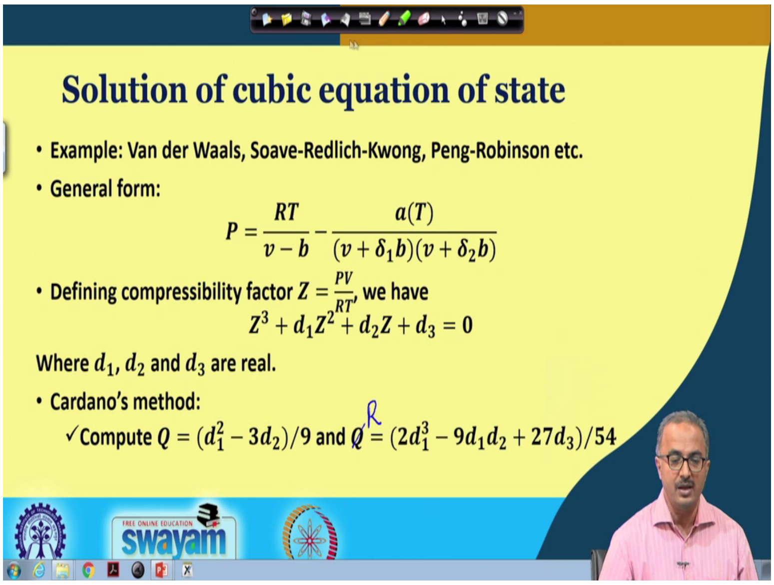

After knowing this what we can do that now we shall go to another the special situation that is of a cubic equation of state.

Now, even though its cubic and we have learnt all this methods to solve the non-linear algebraic equation, but is a special case because in this cubic equation of state we are basically try to figure out the properties of the two faces, that is vapour and liquid that maybe coexisting. And event to ascertain whether the particular at the particular temperature pressure we are having only 1 phase or 2 phase all these things. So, for this we are adopting some special method and cubic equation of state there are many of them Van der Waal force is the first one which was proposed and later many such kind of things came Soave-Redlich-Kwong these name of names of three scientists, then Peng-Robinson the names of two scientists.

So, by their name also we have many cubic equation of state and the general form you will find that these are the general form of the any cubic equation of state, and what will be difference is this the value of this delta upon delta 2 a and b and this b this b delta 1 delta 2 will be changing for, and this is a value will be changing for the various equations of state.

So, without bothering about what exact form of this a b delta 1 delta 2 are we can still evolve some general method of solution for this equation of state. So, if we define the composite factor as Z with PV by RT then we can reduce this particular equation in this type of cubic polynomial and in this we shall be having this d 1, d 2 d 3 as real values ok. So, there will not be the imaginary values of these coefficients; however please mind it because X may go imaginary.

Now, there is one method one of the methods are several methods proposed in the literature this is one of the methods I am showing you. So, here this Cardano's method and what he said that we put we find some this thing this will be R ok. Now we have these two parameters again we define in terms of the d 1 d 2 and d 3. So, these are the two parameters we define in these two terms and based on these two parameter values we shall be finding the roots ok. So, without going into the derivation of this we shall be going to the final solution.

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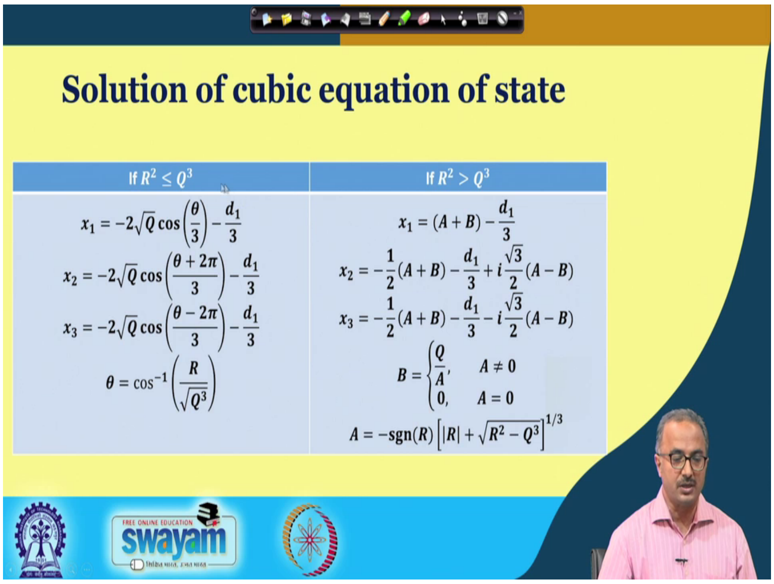

So, here it is that if R square is less than Q cube Cardano proposed these are the three roots of the equation. And here it has been defined in terms of q and d 1 and we have to theta here theta is defined in terms of R and q ok. So, this is for the case when R square is less than or equal to q cube and if alpha is more than q cube then we have this set of solutions for the x 1 x 2 x 3 again here we find we have A and B and this A and B have been defined here ok.

So, we can straight away use this set of solutions for the cubic equation of state however, I must mention that this is one of the previous methods. Later on many modifications were done for this method. And here I just want to mention one thing that shows the sign ok. So, this whatever value of R you get you have to pick up the sign of R this is the meaning of this particular operator.

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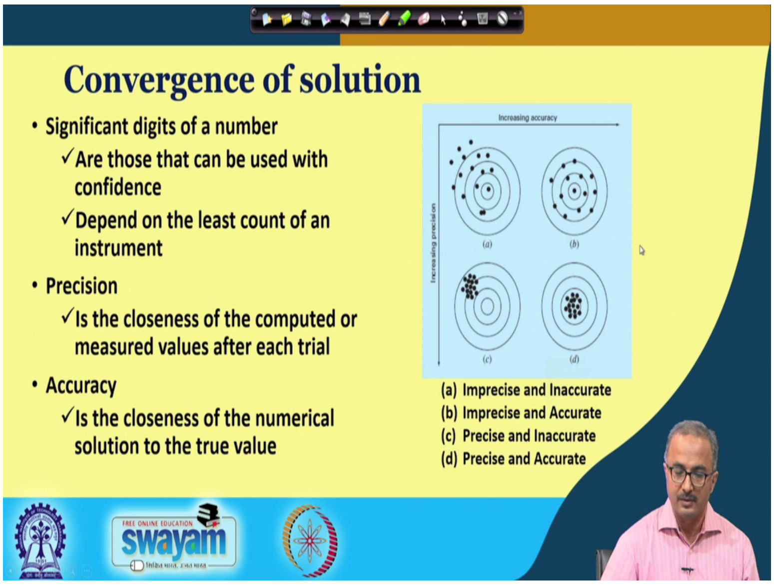

Next, we come to the convergence of the solution. Now for convergence whenever we are doing this again I am giving you any very briefly some idea of the convergence first you have to know the significant digits of the solution. Now, what it means what it means that these are those values that can be used with confidence, and generally it depends on the least count of the instrument when you are some doing some measurement.

Now, we have to see that whenever you are solving some problem you do you should be understanding that when you report any result that those result they should make some physical meaning ok. Now suppose you are measuring temperature with a thermometer. Now if the thermometer if you are talking about the thermometer which we use in our at our home to measure the fever, in that case what you find that the thermometer has a least count of point two degree Fahrenheit ok.

You will measure like 98, 98.2, 98.4 like that you measure. That means, what whenever you are reporting or you are calculating the temperature of our body you should not mention it like ninny 98.4675. Now, this after 98.4 6 7 5 these are immaterial because this 675 cannot be verified by your thermometer. So, in that case you should better restrict yourself only to one significant digit that we call this 98.4; we called it only these three are the significant digits for the solution or whatever you are reporting ok.

So, this is what I said that by; what I meant by saying that it depends on the least count of the instrument. So, as you keep on increasing the least count of the instrument; that means, you are increasing the accuracy of the instrument you find the number of significant digits also starts increasing ok. Next is precision one is precision one is accuracy that is precision.

What you mean by precision means that whenever we are computing the values in the iteration we should see that each consecutive value whether this consecutive values are nearly equal or not ok. Now if they are very equal; that means, after each iteration when I am checking the closeness of the consecutive values if I find that they are very close then we can say that we are approaching the precise result. On the other hand we have accuracy; now accuracy tells us that how close we are to the true value actual value now it may be. So, that we are having precise solution. That means, after each consecutive iterations the values are very close, but these closed values need not mean that they are also the true values ok.

So, that is the difference between the precision and accuracy. And let us see by this particular diagram here we have shown for those games we play that where we have to either with the rifle or pistol we have to hit some target. So, let us assume here that the centre of this particular thing the bull's eye we call it. So, the centre is the where you want to hit it ok, now we have shown you four cases. Now here you can see in the first case you can see that most of the things are away from the actual the centre of this thing ok.

This one is near the centre, but it is not exactly at the centre. So, we can say this all this solution is are imprecise as well as inaccurate ok. On the other hand when you come to this one what you find out here that at least one of them has hit the exact centre of the bulls eye ok; that means, our solution is accurate, but imprecise because other things are very scattered.

Now, you look at the third one, in third one what you find that all these solutions are consecutive solutions are almost nearby they are clustering nearby. So that, but all those things are very much away from the exact solution, but that that the on the centre ok. So, this we call they are precise, but not accurate. On the other end you look at this we find that the solution we are reaching solution of one thing and second thing is this all the consecutive values of the roots we are finding or they are very much close to the actual solution.

So, we say this is precise as well as accurate. So, this is the way you can look at precision and accuracy of the solutions.

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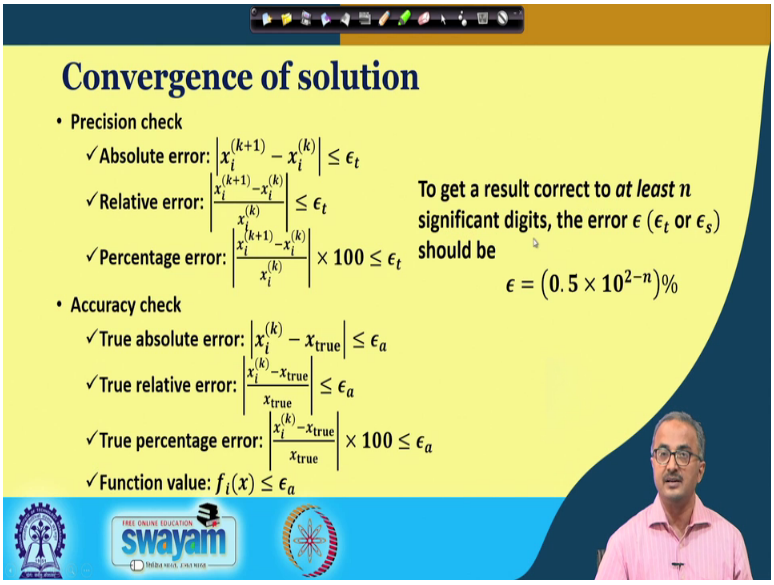

And here I show some commonly converged the criteria of convergence for precision check; that means, when you do not know the true value of the solution. So, we take a precision. And then you can also stop your solution, means you can say that converging. So, if something can be absolute error; that means, you take since the difference between the two consecutive values of the root ok.

And here I am saying x i because there could be more than one equation you are solving for ok. So, it should be applicable for all the equations. Next will be relative error and this is means that the absolute error divided by the value in the previous where iteration available ok. So, this is the relative error and then we have percentage error it is the relative error into 100 and here I have put the convergence criterion that is user defined and this t shows it is the for the approximate values and here we have the for the accuracy check. Now here we are putting if I got true value; if you know true value then what I should do I should always check, this is the two consecutive values we can check always with the true value, it is similar to this one and again we say have some kind of a problem user defined criterion and these are the same as this one ok.

Only thing is this here we can have another one that is we check the value with respect to the function. So, if even we can put for accuracy we can also put a convergence criterion for the function ok. So, each time we are finding some new value what we do we put the value in the function here and check whether the function value ideally should be 0, but whether how much near to the value of the function we are approaching. So, that is the way we are putting this accuracy check.

So, these are the general methods of locating the convergence of a given solution technique. So, for it is given that to get a result correct at least up for n significant digits this is the criterion that has been prescribed in the literature for these particular values of epsilon.

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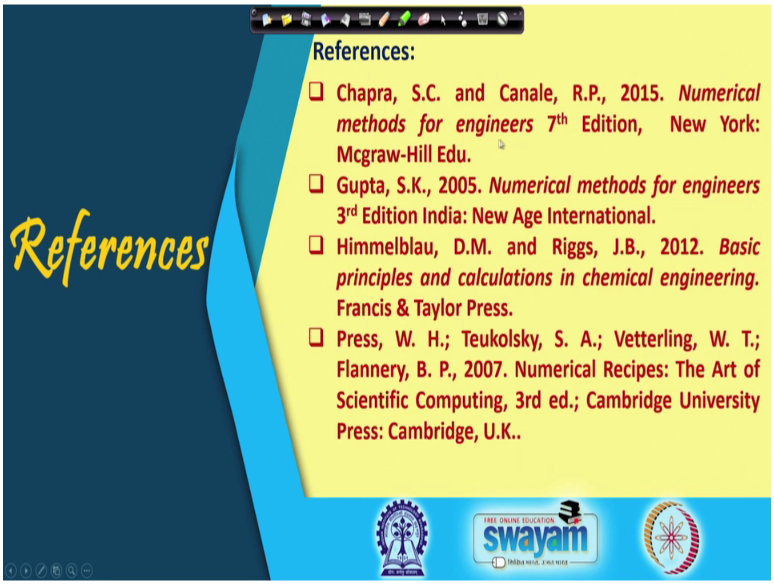

So, more of this you can find out in these references.

Thank you.