Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture - 16
Solution of Macroscopic Balance Equations – I

Welcome, in this particular lecture what we shall be looking into that, after learning about the setting up of the various types of Macroscopic Balanced Equations, we also need to solve them and this solution is needed during the simulation or the designs. And perhaps the solution methodologies will not be very new to you, because you study all these methodologies under mathematics, in mathematical techniques or numerical techniques, which are used for various other disciplines.

So, in this particular lecture, I shall be highlighting a few commonly used techniques, to solve the equations you obtain after making those, energy balance, mass balance or momentum balance in a lumped parameter system.

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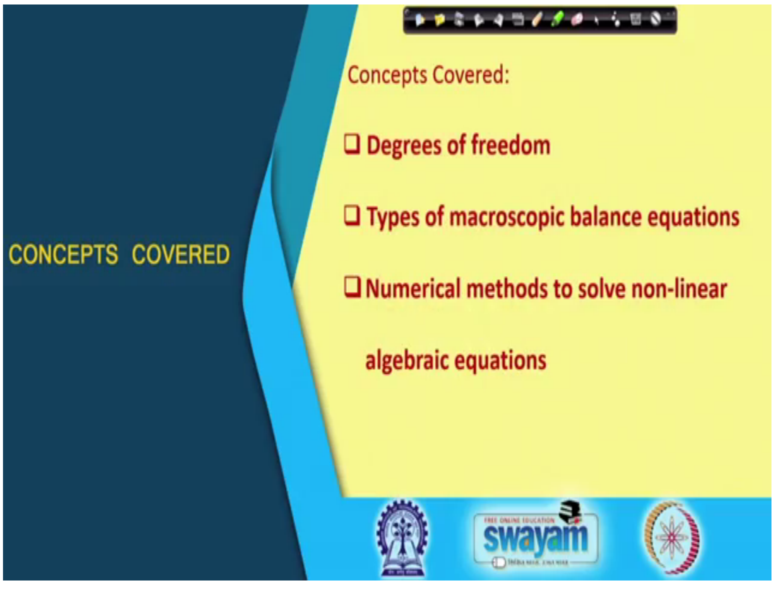

So, in this particular lecture we shall again look back to do degrees of freedom and the types of macroscopic balance equations, in this particular type what we will look into that, what are their mathematical types, not from the point of view of physics, but point of view of their mathematical nature characteristics. And next we shall be ending this lecture with a few commonly used numerical techniques, to solve the non-linear algebraic equations.

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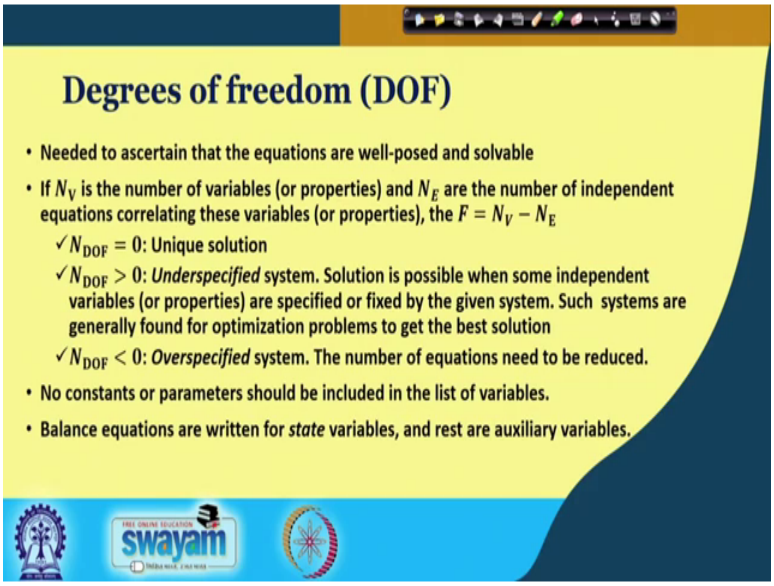

So, first let us again go back to degrees of freedom and you are seeing that this degrees of freedom is coming very often to us, because this is the one which we need to ascertain before we are going for any kind of solution. And when in case of the solution of the various equations, the degrees of freedom analysis has to be done to check whether the particular problem has been well posed or not.

And as we have learnt earlier, that we always want to ensure that the number of unknowns should be equal to the number of the equations or independent equations, correlating these unknowns, only then we are going to have some unique solution.

So, what I said that it is to needed to ascertain the equations are well posed and solvable. Now, if N V is the number of variables or properties and N E is the number of independent equations correlating these variables or properties, then the degrees of freedom equal to N V minus N E, this V know already. And there could be many situations like this total number of degrees of freedom may be 0 that gives us unique solution and if this total number of degrees of freedom is more than 0 then it will be under specified. More than 0 means we have, we are having more number of variables than number of equations ok.

So, in that case we shall not be able to solve for the, all the variables ok, but this kind of systems are also there when the number of variables are larger. These kind of systems are used for optimization problems, because in optimization, we need to know that which of the variables and there will be many choices of the variables, so which of the variables should be taken for optimization. So, in those cases we have sometimes this under specified system and then we have over specified system; that means, the number of equations is more than the number of variables.

So, in that case we try to reduce the number of equations. Generally, no constants or parameters should be included in the list of variables; that means what? That suppose, you are calculating the heat transfer and rate, and you need the heat transfer coefficient. So, this coefficient will come as a parameter and that should not be counted in the list of the variables, because this coefficient will in turn, depend on the temperature, flow rate, etcetera ok. So, it will be counting as you twice, I am counting the same kind of variables.

And then balance equations are written for state variables and rest are auxiliary variables. State variables means what; that those variables which are defining the state of a system. For example, we have temperature, pressure, level, then flow rate. So, all these are state variable, even composition is a state variable.

So, other than these variables we have many other variables in the equations, you will find those are auxiliary variables and generally, whenever we are writing the balanced equation we have found, that those balance equations are being written in terms of the state variable. For example, if you look at the mass balance equations there is those equations are for the composition; energy balance is for the temperature, momentum balance is for the velocities ok. All these things are the state variables.

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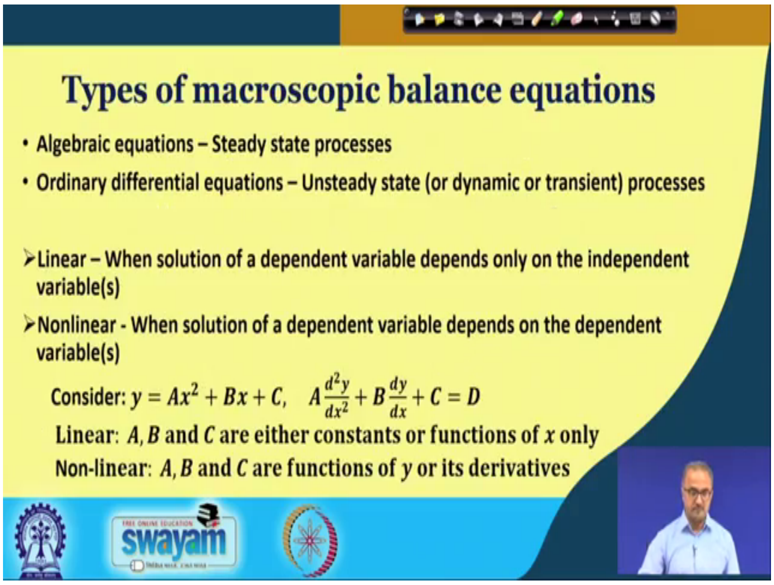

Now, when we look at those macroscopic balance equation, we find mathematically they have some different characters. So, we could have algebraic equations or we could have differential equations and algebraic when then, when we find we have the steady state; that means, there is no variation of the particular system with time and our; when do we get differential equations? When we find that it is unsteady state.

And whenever we are talking of the microscopic balance equations we are already lumping the system all the variables; that means, we are giving only one value now to the whole system. For example, we are saying that there is only one temperature or one composition to the whole system.

So, in that way we are neglecting the spatial derivatives and we are having only the derivative with respect to time; that is giving the unsteady state. So, in that case we are getting ordinary differential equations ok. Now, when we look at these equations, we may have again two types of equations; one will be linear and one will be non-linear and what we understand by these linear and non-linear equations? Let us look at these two equations; one is an algebraic equation and one is a differential equation ok.

Now, you can see that suppose, I take a quadratic equation, it could be extended to any other type of equation, but let us assume that we have a quadratic equation. Now, here we are writing a general term like y is the dependent variable, x is the independent variable. So, we can write that y is equal to Ax square plus Bx plus C and similarly, we are also writing a ordinary differential equation, in that case we have only one independent variable and suppose, this is similar kind of equation we are writing here ok.

Now, depending on the nature of this A B C or D, we will say that whether these equations are linear or non-linear. Now, when ABC and D are constants then we say these are linear equations, but if we find that ABCD, this ABCD are not constants ok, but they are dependent on the dependent variable, so in that case becomes non-linear. Similarly, when ABCD are functions of the independent variables, in that case also we have linear equation.

So, that means in this case, either this ABCD should be either constants or they are functions of the independent variable whereas, they will be non-linear, if these ABCD are the functions of the dependent variable that is their functions of y itself.

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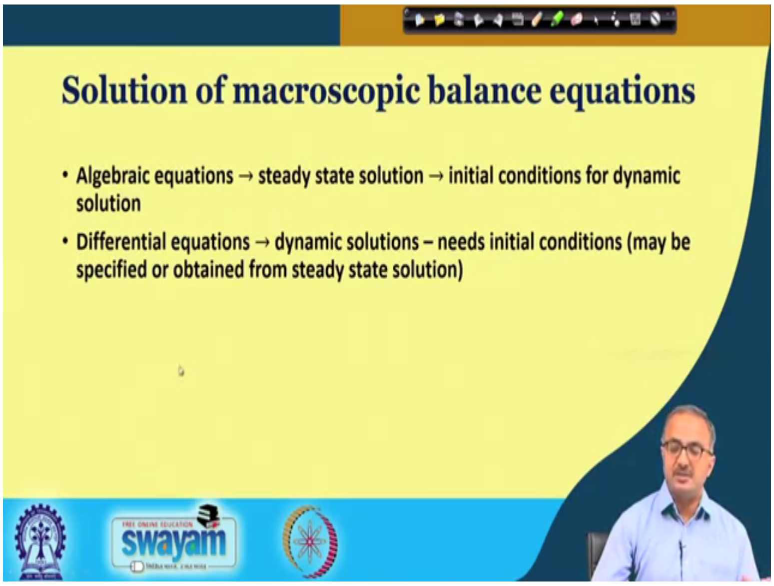

Now, coming to this, when do we go for this algebraic solutions and when do we go for this differential solutions? You know that as I told you that algebraic equations are obtained when we are talking of steady state solution and sometimes these steady state solutions provide us the initial condition or for the dynamic solution. For example suppose, we are having a flow system and suppose, we are filling up one chamber with some liquid and there is both inflow and outflow.

So, maybe initially we find that it will be steady and this inflow and outflow are balanced completely and the water level is unchanged ok. Now, suppose somebody perturbs or gives some kind of change either in the inlet water liquid flow or the outlet liquid flow or both, in that case what will find; that system will grow trying to, we will try to go to another steady state.

Mind it that it is that necessary that it can reach, but it will try to go to another steady state, in that case we will solve for the initial state that what is the level of water when the flow rates are constant. In that case we can solve a steady state equation and that solution will be the initial condition when we are going to solve for the change in the level of water due to any kind of disturbance in the inlet and outlet flow rates.

Now, the differential equations will be there to get the dynamic solutions and as I told you that whenever we are going to solve these dynamic equations, they need some initial conditions to start, the solution. And these initial conditions can be obtained either by some specifications given by the user or by solving the steady state balance equation.

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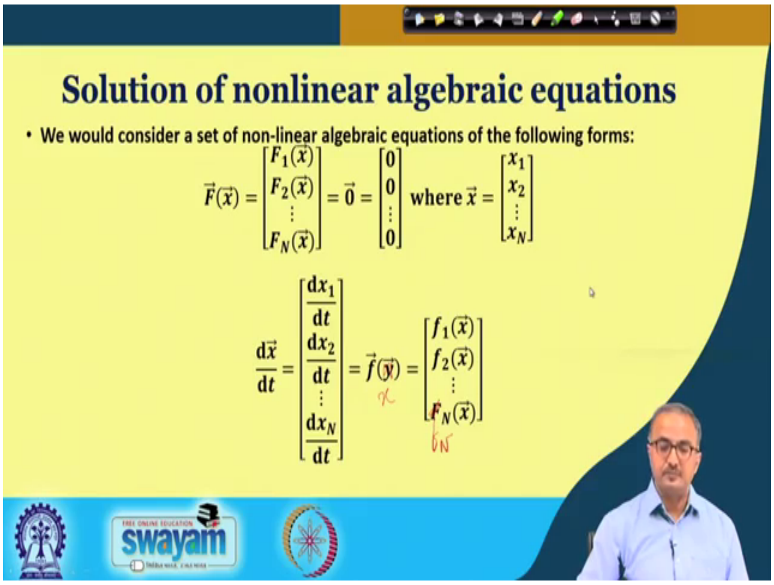

Now, let us move on to, look at the various solution strategies for the non-linear algebraic equations. As I told you, I will not be going into the detail of this, because these kind of methods are separately taught under numerical techniques and also I will not be giving any derivation of these techniques. I shall be simply giving the formula and for detail you can look into any standard numerical technique courses or any other books and a few references, I have also given you at the end of this lecture.

So, first let us consider a generalized formulation based on which we shall be going to solve these equations. So, let us define here I am talking about multivariable system; that means, we have many processes going on simultaneously and we have more than one variables ok.

So, here we have something like this, we are defining a set of variables and these are in terms of vectors and these x represents the independent variables. For example, in the real life process, they could be the temperature, pressure, flow rates, etcetera and this F can represents the various dependent variable like; heat transfer, mass transfer it, all these things they can be, they will be like this.

So, now we are this vector can be put in terms of like this we have F 1 F 2 up like that to N, there could be N number of systems ok, which are getting affected by the same set of independent variables and which this is equal to 0 and here 0 is a vector with. That means, F 1 x equal to 0 F 2 x equal to 0 like that F and x equal to 0 that is why we have a vector over here and as I told you this x vector comprises all the individual components or in our cases individual properties or the some variables of the system.

Similarly, we can also pose these problems for the differential equations like this that dx by dt equal to dx 1 by dt dx 2 by dt like this. We can also pose the problem and here also we have something on the right hand side, it is not always 0. It is having some kind of for, this will not be. This is not be y, it will be x, it will be x. So, this if I will be again having some various components like f 1 x f 2 x like that to f N x this should be f N ok.

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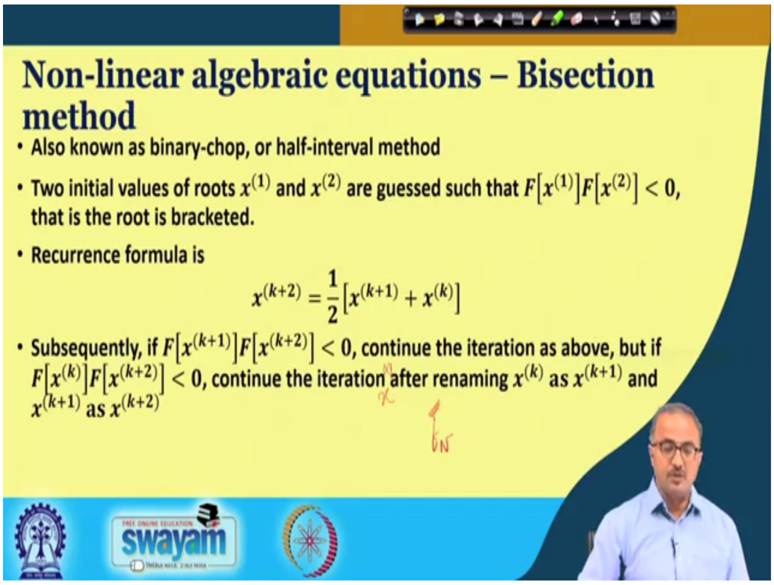

Now, what in this particular lecture what we shall do? We shall be focusing only on the algebraic equation. So, first I go to one very simple way of solving, that is the bisection search this particular name is also known as by binary chop or half interval method. As the name suggests, that in this particular method we are trying to half or make the divide in particular interval, to find the root of the equation in a equal parts ok.

So, what we do that to start this particular type of method, what we need? We need two initial guess values ok. Now, by x 1 and x 2, I am meaning that there the initial guess values and I am putting them in parentheses to signify that without the parentheses, they would mean as if I am taking some root of them. Like, if I do not put the parenthesis, it could mean x square, but this is not x square, this is just showing the iteration level ok.

So, we are putting parentheses. So, x 1 and x 2 are the two initial guess values, which are needed to do this particular method and how do we select this x 1 and x 2; that these x 1 x 2 should be bracketing the actual root ok; that means, the root must fall within this particular range ah; that means, for that we want to make sure that the function is monotonic in this particular zone. That means, it should have either it should be increasing or it should be only decreasing, it should not be kind of fluctuating ok.

So, with those kind of conditions we make sure that we are choosing x 1 x 2 in such a manner that Fx 1 into Fx 2 is less than 0. What it means is this; that means, if on one side, we have the Fx 1 is on one side, Fx 2 is the other side we can check thatif this product of Fx 1 and Fx 2 is coming to 0. It would mean that these the two values are bracketing the actual root, because at the actual root the value of F will, it is supposed to be 0 ok.

So, if it is positive or negative. So, it means that in between this positive negative values we have the 0 value somewhere ok. So, that is the meaning of this particular condition and this is the recurrence formula. Recurrence formula means how to proceed with the root finding some method. So, once I know these two values then I just simply half that particular zone and at this new value I again calculate the value of F x, once I calculate the value of F x. Now, what what I do?

Again, I take the product of F x k plus 1 and F x k plus 2 and if you find that this is now, coming less than 0; that means, the new range should be between this x x k 1 and x k 2 and we can again keep on proceeding with this particular method, but if we find that we also take the product of F x k and F x k plus 2 and we find it to be 0 then what we find? We continue the iteration, but now we have to rename the x k and as x k plus 1. This I will tell you a pictorially it will be easier for you to comprehend the method.

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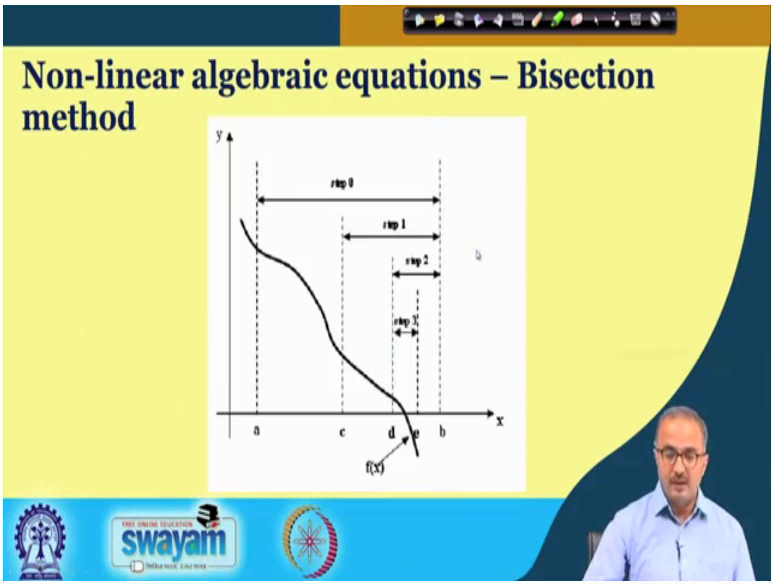

Now, you see here, that initially I having this a and b ok. So, this is step 0. So, here I have some y and some x. So, I am, what I am doing that the, and you can see these monotonically it is decreasing ok. So, initially and my root is somewhere here ok. So, here I want to approach. So, what I am doing? That I am assuming some value initially this here and this particular value here and you can see that this value, at this value you now, you see that if this can be extended downward, you can see that the value of this f x will be coming down ok. It will be negative on the other hand, this is positive ok.

So, if I take the product of this value and this value, I will get a negative value; that means, that the root must be between these two initial guesses. Now, what I do? I now bisect it; that means, I take the midpoint of these two, again I find the value of the f x here ok. Now, what I do? I can, if I take the multi product of these f x and these f x. This will be positive ok; that means, the root does not lie here.

Now, if I take the product of this f x and again the same f x, I will find this is negative; that means, the root is now between this new value c and the new value at b ok. So, what I should do? I should reassign this particular x to this x ok. Again, I will now that; that means, I have shrunk the my region has been shrunk ok.

Now, after this shrinking of this region again, I take a midpoint of these two, again you see that I can find the value of f x here and again I find that between this f x and this even f x if I take a product, this will come out to be positive. But if I take between this and this value again, I will see that it is coming out to be negative ok; that means, now I have again shrunk my region of search between this point and this point. Again, I take another half value over here.

Now, I find that if I take the fx value over here and now, if I take the product of this value with this value, it will come to be positive, but if I take the product of this value with this value, this come to be negative; that means, now the, this b should not be left anymore. Now, these values should be shifted to this again, I will now, next time I will shrink this region between d and e.

Now, you can see that it is a very systematic way of slowly and slowly shrinking the zone of our search. And how long will you continue? You will continue until you reach some particular convergence specified by the user. It is not that you are going to reach exactly 0, because in generally we are not always bothered to reach, I mean reach 0 value and in practice we also do not get the actual value, that does not really matter to us. We should be nearby that particular state ok.

So, it will be depending on the users choice, what I can do that I can take again the, new value of x and at that point again I find the fx value. Now, if I see that fx value is less than or equal to some user specified convergence criterion ok; that means, if I put it mathematically, it would look like this.

If f x, is less than equal to some user, user defined convergence, then I will stop this particular solution that that I will take as my solution. So, it is you can see that it is a very straightforward and very easy way to implement this bisection method for this non-linear algebraic equations.

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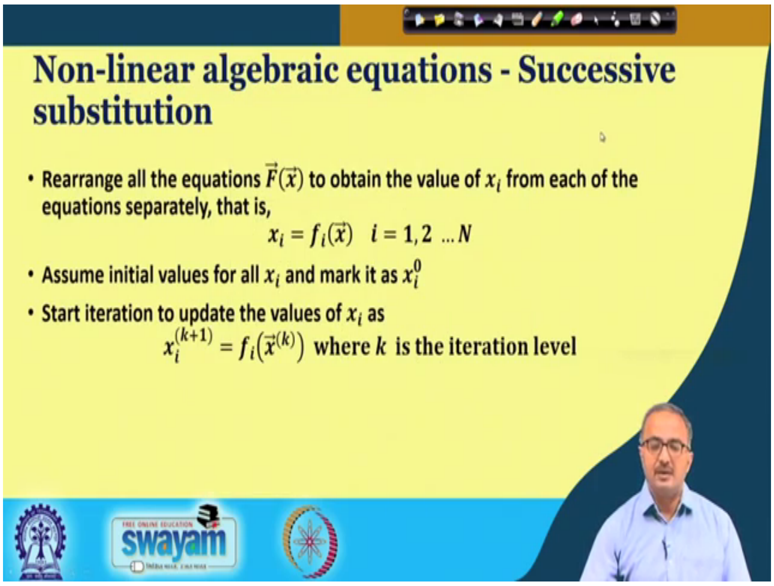

Now, next we come to another method that is what we call the successive substitution. As the name suggests, what it means that we are successively substituting some values over here. Now, what are these things? Let us go by this example first, let us rearrange, we can always rearrange the equations in such a manner that we can separate out the dependent, represent the roots in terms of the other roots ok, I will give by some example.

So, suppose I have the some x i; that means, there could be N number of independent variables. So, we are for each of the independent variables, we are rearranging the given equations in certain manner so that the each N number of equations will give rise to N number of independent variables. And then what we are doing we are again taking some initial value guess value as x i naught and then we are updating this value by putting them back into this equation.

So, we are getting the initial the values of the x at the present level, to get the values of the x at the next iteration level and this way we continue till we find that even this fx values are coming to some kind of a converged value.

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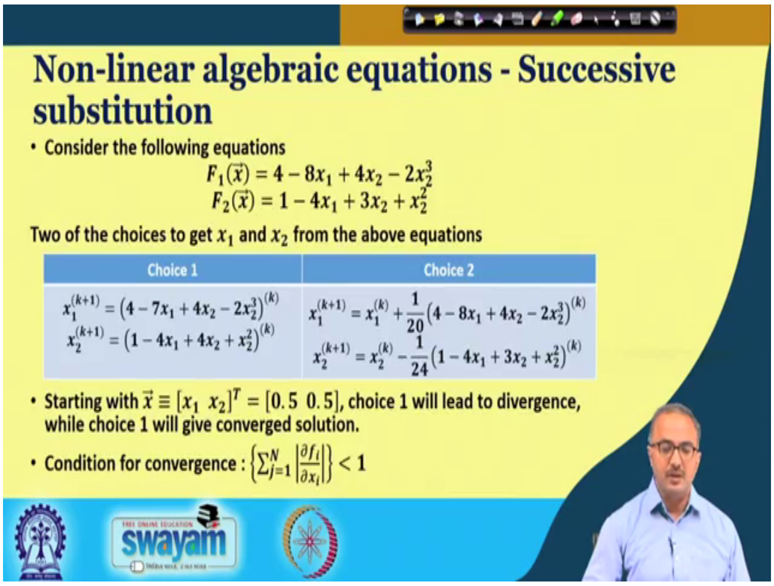

So, here I have just given some example to without solving it for you. Just suppose, I have two functions given to me and these both the functions are taken to be 0 and which you have to solve for x 1 and x 2, these are the unknowns. So, you can see that I can get the x 1 x 2 value from these two equations; I can have multiple ways of getting the x 1 x 2 value ok.

So, I have just shown you two of the choices to get the x 1 and x 2 values and this is the one way of putting the x 1 x 2 and this is another way of x 1 x 2 and you can do it easily from by looking at the equation. And you will find that suppose, we start with initial guess value of 0.5 0.5, then you will find that if you choose this particular way of representation of x 1 x 2, you are not going to the solution.

But on the other hand, if you take this particular representation then you will find that you are able to get the solution. So, that means the choice of this x 1 x 2 the expression would determine the convergence of the particular system of equations and without going into again, into the derivation of the condition for the convergence here, I simply mention that you should have this particular criterion satisfied to get the convergence.

Here, we have shown that there absolute value of the partial derivatives of the function with respect to each of the variables and sum it over here it should be less than 1. So, if you can ensure for each of the equations, you are getting this particular condition satisfied then you can miss for the particular choice of the x then you can say that you are going to get a converged result.

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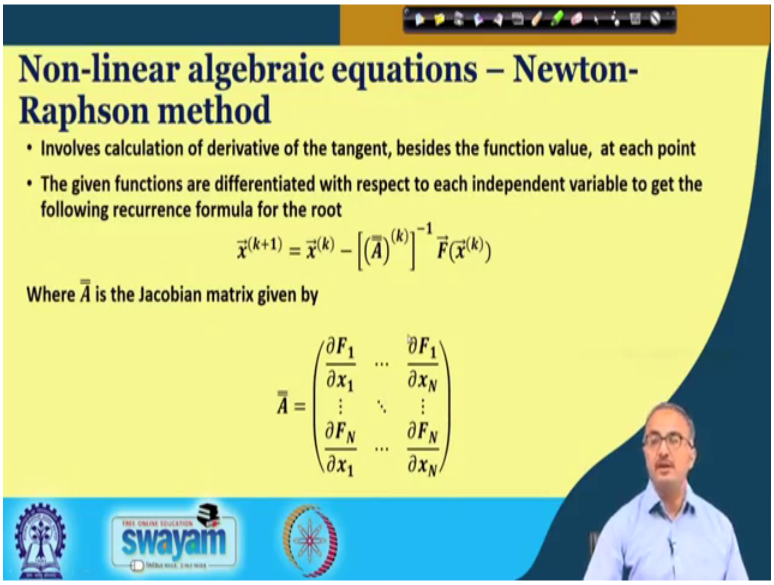

Next, we come to a very common and popular method that is Newton Raphson method. It is very common, because it has very fast convergence. So, it is very common method and involves, it involves calculation of derivative of tangent, besides the function value. So, far we have been only talking about the function values, but in Newton Raphson, first time we are finding that we have to find out the derivative to get the tangent.

So, here we find that, this is the recurrence formula again. For this particular method again, I am not going to details of it, this A is a Jacobian, because Jacobian matrix and this Jacobian matrix is nothing, but a matrix of partial derivatives of each of the functions with respect to each of the independent variables. So, I have shown you how this particular Jacobian looks like ok.

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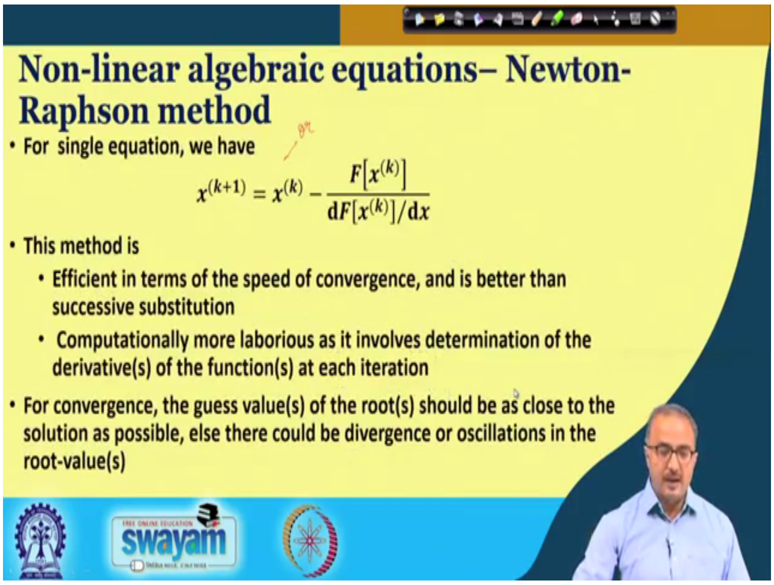

Here, it would be a bit of correction to be or ok, so we have this is for a multivariable system. And you will find that this is the, if I talk of single variable, the same equation may be reduced to this particular form. In this set you see that x k plus 1 that is the new value, updated value of the root will be equal to the represent level of the root and the function value divided by the derivative of the function.

And this method is very efficient in terms of speed of convergence and is better than the successive substitution ok, but it is computationally more laborious, because we find that we have to always find out the derivative of the function and especially, these derivatives becomes difficult to find out, if we have a very complex set of equations ok. So, that becomes a very computationally intensive job. So, even though it is a very, it gives fast convergence, but it has this particular I would say drawback, but its particular feature which, which sometimes makes it difficult to implement.

On the other hand, this particular method needs a very good choice of the initial guess, because the convergence or divergence or by this particular method depends on the choice of the initial guess. It may so happen that if our initial guess is far from the actual root, then we may diverge or our solution may oscillate ok. So, we have to be careful about this method, but despite all these shortcomings, this Newton Raphson method is very popular, because it ensures a faster convergence rate.

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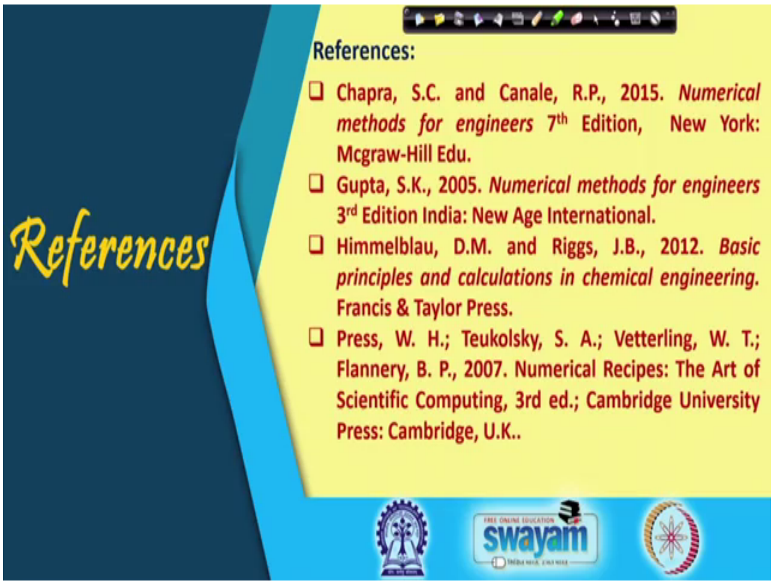

So, we have covered two of the methods and here are some references which you can refer to get more insight into these methods and I shall be talking of a few more methods for this solution of the non-algebraic equations.

Thank you.