Mass, Momentum and Energy Balances in Engineering Analysis
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Lecture – 22
Numerical Solution of Macroscopic Balance Equations

Welcome, we have so far learnt the mathematical solutions of the balance equations and we have seen a few selective ways of solving the mathematical expressions like we talked about exact inexact homogenous non homogenous etcetera ok. Now many times we find in our physical systems the balance equations are quite simple, so that you can analytically solve them and as I told you any analytical solution will always give us the exact value with because there is no approximations involved as such in those another solutions ok.

And the goodness of the solution will depend on the goodness of the model equations. On the other hand, many a times we also find that the expressions for these balance equations are becoming very complex that it is not feasible for us to adopt any kind of analytical means of solving those equations. In that case, we have to go for numerical solutions and these numerical solutions maybe for differentiation maybe for integration ok.

So, in this particular lecture, what we shall see, we will take some numeral solution of the macroscopic balance equations and in this we shall be focusing more on the differentiation problems ok, where we shall be having the derivative in future we shall be looking into the integration problem.

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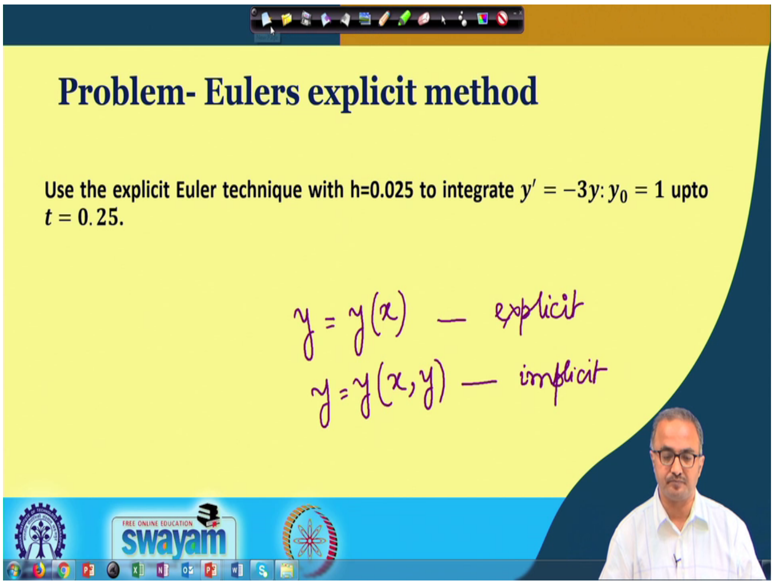

So, first I shall be talking a selectively, because in the courses and the books dedicated on the numerical techniques, you will find plenty of a methodologies have been proposed and also derived.

So, I will not be going into those derivations and all sorts of the method, but I will suggest you that you please go through the dedicated books on lectures on this numerical analysis, so that you can find out the background of the various methods and their derivation, so that you can go with some different types of numerical techniques and understand their applicability for various types of problems.

So, in this lecture I shall be dealing with only a few of the numerical techniques which are used to solve differential equations and which are very commonly used in the domain of this process analysis. So, first let us take up this Eulers explicit method. As I told you per in our previous lecture that explicit and implicit means, that if you are able to get the value of the unknown variable in terms of the independent variable, then it is called it explicit and if you find that the value of the dependent variable has to be found on the basis of not only the independent, but also the dependent variable itself, then it becomes an implicit.

So, to make it a mathematical statement, we can say if y is the dependent variable and if y can be found as a function of only the independent variable x, then we call it explicit, but if for some reason we find that this y has to be found not only based on x, but also based on the y, itself so it becomes an implicit form ok.

So, this is the way we are defined distinguish between explicit and implicit ok. So, first we shall be looking into the explicit method and here we are taking some example, that we have to solve this particular expression that y prime equal to minus 3 y and with we need whenever we are using any kind of a numerical solution method for solving some differential equation, we go step by step because what we basically want is this, we want to find out the value of the independent variable at some particular value of the dependent variable away from the initial value ok.

Now, by integration we can do that analytically we can do it very simply, but whenever we are going to the final value, so we find that in when you are going numerically then we have to take some steps.

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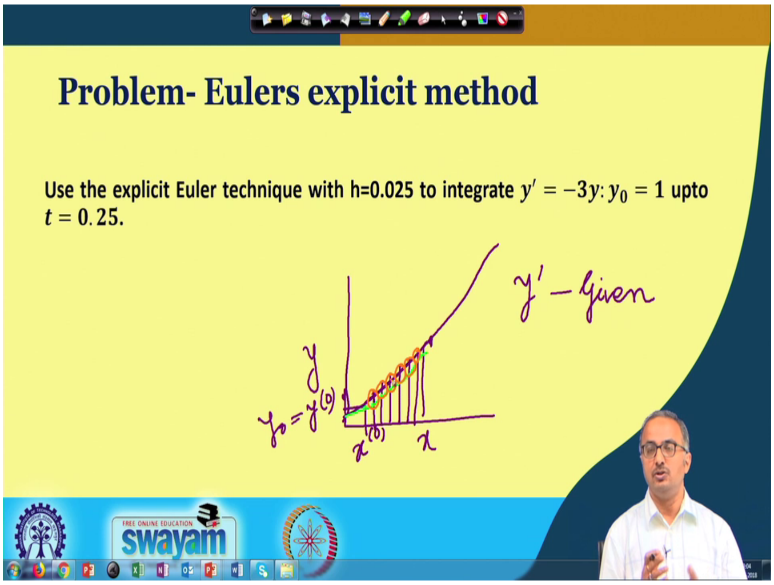

That means, suppose I have this particular y versus say x and I am given y prime and this is given, but I have to find out the value of y for different x values, suppose I am given the balance suppose this is x 0; that is and here I know the value of the y 0 ok, so suppose this is our initial condition ok. So, but suppose this is the form of the y. So, we have to find the value of y at some other x value.

So, if I know this particular expression of y then I can simply take the value of x and I can get the value of y over here, but that is for an analytical solution, but when go got go with numerical method what we do is this, we go step by step; that means, from this value we find this value then we go to this value, this value like this we go in steps and finally, we try to approach this.

Now depending on the numerical technique, we will find that we are not always following the exact function. What we are doing? We whenever we are going numerically, we are making some assumption for the particular function.

So, what happen that; even though this may be this may be the true value, what we are essentially doing is this we will be going from this we are going towards this and then moving towards this and moving towards this, then you will find that the at each of the points there is some kind of a deviation in the between the true value and the numerical value ok.

So, you can see. So, we are getting some kind of deviation at each point of the x ok; that means, we are approximating the exact solution by some assumed solution and we are taking that path ok. So, you find that whenever you are applying any numerical techniques there will be some error associated with the values of the unknown variables you are solving, because you do not know the exact nature of the particular function ok.

So, numerically we are always approximating the actual variation and then we are finding the solution. So, that what we find essential in that way we have so many numerical techniques and because every we are trying to improve upon our approximate value, we want to stay as near as possible to the exact function, but our numerical techniques are not able to do that and that is why you will find in the literature.

There are many techniques proposed to improve the solutions numerically ok. So, with understanding now what we shall do? We shall try to understand that how to find the value of y; given that this is the y 0 at 1 and we have to use this Eulers explicit method. I will not go into derivation of this method, I will simply demonstrate it by 1 example and I cannot understand that you can understand this method ok.

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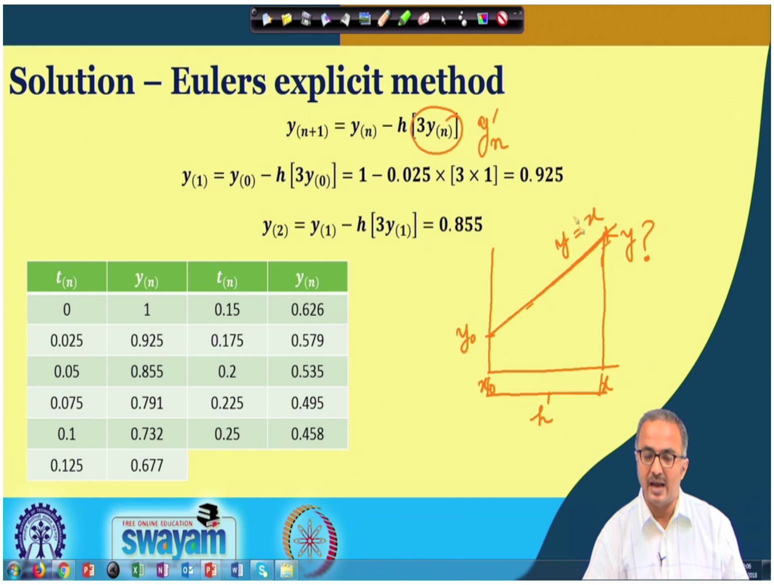

So, let us go like this. So, here this is the formula of these Eulers explicit method. Now here what we have, this is y n plus 1 is equal to y n minus h into, this is the f y n, this is basically this particular representing the given function y prime and n ok. So, this is the in general the expression for all the Eulers explicit method.

So, in this is what you are doing that, this is we are getting from the problem given problem, also we are putting this y prime y n over here and now things become very simple. You can see easily here that this is the unknown that is this is the value of y at the next time step and this value depends on the time step chosen ok.

Now, you can see this particular h value tells us that how closely we are following the actual solution. So, it may be so that if the problem is very very non-linear, then you can see that this value will matter a lot and the linearity of the problem and this particular expression is you can see this is the linear expression linear expression in h.

So, what it means basically is this, that suppose I have a very linear solution, it is suppose this is y equal to x, then you can see even if I start suppose this is the y naught at x naught, this is given to us ok. Now in this case I can check that suppose I want the value of the x over here at this particular x, I want the value of y. So, here I want the value of y ok.

Now, because it is linear, I can choose a big h the step size h and because this is a linear I can quickly go to this particular value. Now consider another situation when I have a very non-linear variation of y with x.

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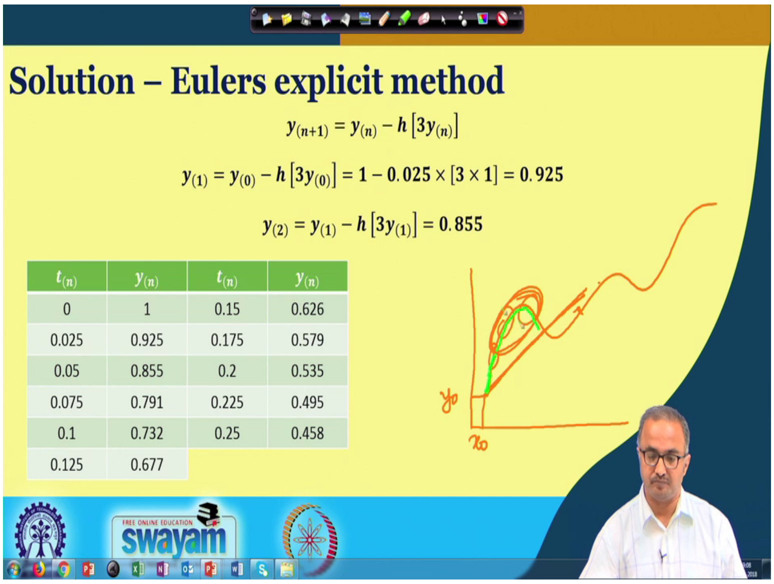

Now, suppose again I am that is non-linear thing non-linear ok. Now you can see that suppose this is the again the value of y naught at x naught.

Now, suppose I want to take the value over here, now you can see if I choose the same big h, then what I find that I may be going like this and in that I will missing the y values over here. In this region I will not be able to predict the values properly, because I am going in this particular fashion ok.

So, in that case what I need to do is, this then I need to take some other value of the h, so to try this thing I will take a smaller h. So, I will go like this, I will take small small steps and I will tried to move like this ok. So, that I can stay near the actual variation and you can see that the smaller the value of h we take, the closer we can stay along the actual nature of the variation of the particular dependant variable. So, that is how this step size plays a great role in deciding the accuracy of the solution and whenever you are solving numerically, you should be aware that how to get this particular step size.

Now just come back to this problem, now you can see that by the given step size, what we are doing now, we are now trying to predict the values of the y for the future time instance. So, here we can simply write that, at we put the value of time and we put the value various values of the y n which year predicting by this particular method. So, we have these are the different values of the y and now you can check that how good these values are.

Instantly for this particular problem you can see that in this problem the analytical solution can be found very easily.

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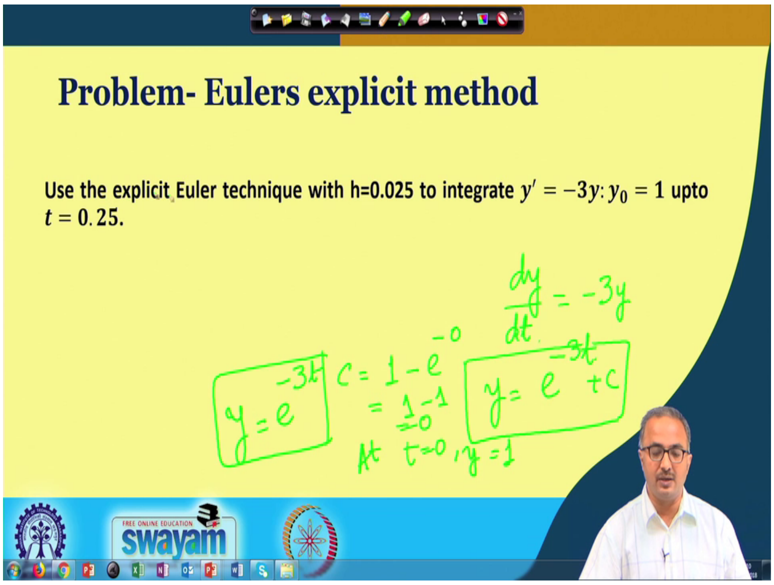

So, you can see that it is dy by dx equal to minus 3 y and you can see that y is equal to e to the power minus 3 x plus c. So, this is the exact value of the particular thing. So, here I will put this in terms of t. So, let me put this in terms of t, this is not x ok. So, this will be t this will be t here and here also it is not x, it will be t here ok.

Now, once you have this particular analytical solution and you can find also the value of the c from this particular given thing, you can see that for y naught; that means, at t equal to 0 at t equal to 0 y equal to given as 1. So, you can put this value you can see that c is equal to then this is 1 minus e to the power minus 0; that is, 1 minus 1 equal to 0, that means, your solution is e to the power minus 3 t ok. So, this is the exact solution ok.

Now how to check that whether you have chosen this particular h value correctly or not what you can do is this, you can now put another column here and you can start finding the value of e to the power minus 3 t and put it and then you can check that how well or how badly these numerical values are approximating the actual solution and you can easily also check like by varying this value of the h or the steps size, you will see that these prediction values will also keep changing and you can find out also that how well or what is the optimum value of h which will be able to give us the best result, by optimize mean that at after as you keep changing the x you will find that after you change the x; in fact, it will not be much of change in the predicted values.

So, you can take that to be the h means, when you keep decreasing the h value for any kind of non-linear problems it is a non-linear problem, so you find that the h decreasing h will also keep the numerical solution near the exact solution, but what we will find that as you keep decreasing h after a certain h will find there is not much change in the value of the predicted values; that means, you are reaching a precise value. So, after reaching a precise value you can also check about the accuracy of the value by comparing it with the true solution ok.

So, you will find that whatever, whenever you are getting the precise value and the precise value is also becoming accurate value, then you should stop changing the h and if you find suppose, you take the 2 h value a step sizes h 1 and h 2 and in that case use find that h 1 and h 1 is more than h 2, but the precision you will find that they are reaching the precision ok. So, what you should do, that you should choose the higher value of the step size, because if you choose the higher value of the step size then your the time for computation will get reduced ok.

So, that is how we choose the step size for the numerical solution, we want to be precise accurate at the same time fast. So, all these 3 things it has to be they have to be taken into account to decide this numerical method as well as the step size to be chosen.

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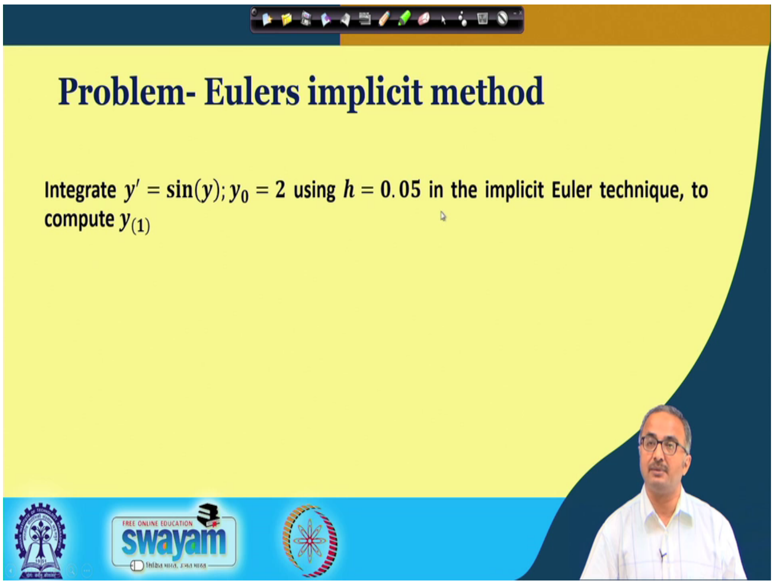

Now, we come to another problem, here we have a integration problem to for this ye sin y and here again we have to predict the value of this y at some other value and here we have to use the implicit Euler technique ok. Let us see how the technique looks like.

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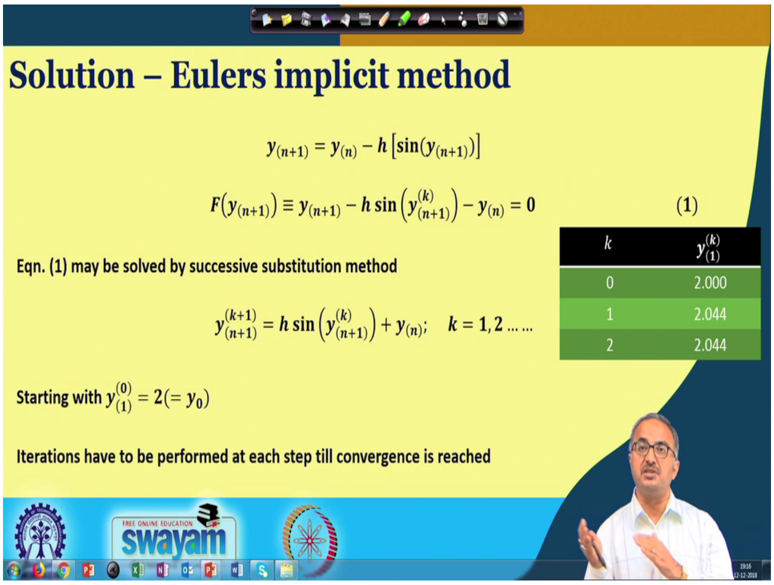

So, here you see this is the Euler technique this is the expression for the implicit Euler technique. So, here you can see that is basically this is basically the know y prime value which is coming from the given expression ok. So, now, this y prime is put in terms of the future value that is to be predicted ok.

So, that is how, if I put this y n plus 1 as y n, it becomes explicit, if I make this thing y n plus 1, this because implicit ok. So, this is a small difference in this implicit explicit, but actually this is y n plus 1 equal to y n minus h into y prime ok. So, this is as actual expression for the various implicit method. Now, now once you put this value ok, now you find that on the both the sides nearby n plus 1 and this gives rise to you cannot have it this is the straight forward manner for the y n plus 1.

And here again you see that this is an non-linear equation you are having and for non-linear equation you should adopt some non-linear technique of solution as I have described in the in the earlier lecture where you can have secant method you can Regula Falsi, Bisection, Newton Raphson, so all these methods may be used to find out the roots of the equation ok.

To solve these equations, so what we are doing that we can we are using this particular method by a successfully substituting it. So, we are putting the next value in terms of this particular value ok. As I told you in my earlier lecture this is not the unique choice for y n plus 1 k plus 1, you can choose any other ways of finding the y ok. So, if you choose this particular thing and you can see the starting with his initial value and if we have to find this by iteratively for at each step at each step you have to do iteration to converge ok.

So, whenever you want to trace the transient face of the particular function of variation, you must be by this method you are you have to keep an iterating at even step to get the solution. Now please understand this that if we are not interested in tracing the transient, then the number of iterations to for convergence will be reduced because our n is for a steady state solutions.

So, you can see that earlier what I have shown you that from transient solution also I can get the steady state solution and this is often done in the process analysis in CFD, that we do not solve a steady state equation, but we solve a transient equation to get the solution of steady state. So, in this case also depending on whether you want or do not want to trace the transient of the process, you have to keep converging or you have to decide the convergence criterion at each particular step ok. So, here we are just doing this and we have shown you the final results for the particular problem.

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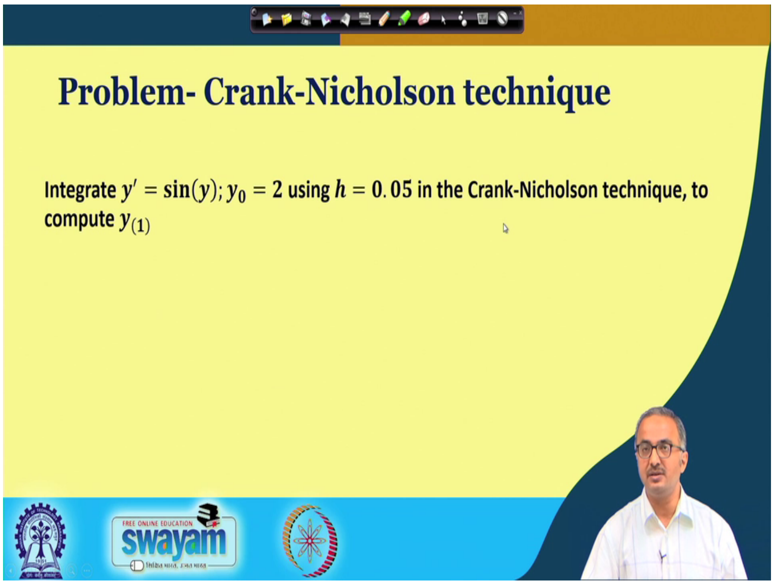

Coming to another technique, that is the Crank Nicolson, this particular technique we call it semi implicit or semi explicit method. What it does is this in the explicit methods are fast, because we do not have to iterate ok, but they have the problem stability; that means, converge all they are getting the right value ok.

On the other hand, when they go with implicit methods what you find that they are slower than the explicit method, but they are insured more stability to the solution then the explicit methods ok. Now both of them have the pros and cons. Now when we adopt any kind of semi explicit or semi implicit method, what we are trying to do is this we are trying to take the advantage of both these types of methods; that means we want to make them faster as well as, we want to make them more stable ok.

So, in one of these formulations we have Crank Nicolson, is a very popular technique in numerical methods ok. So, I am discussing only this particular method and please understand there are many other such kind of methods in the literature.

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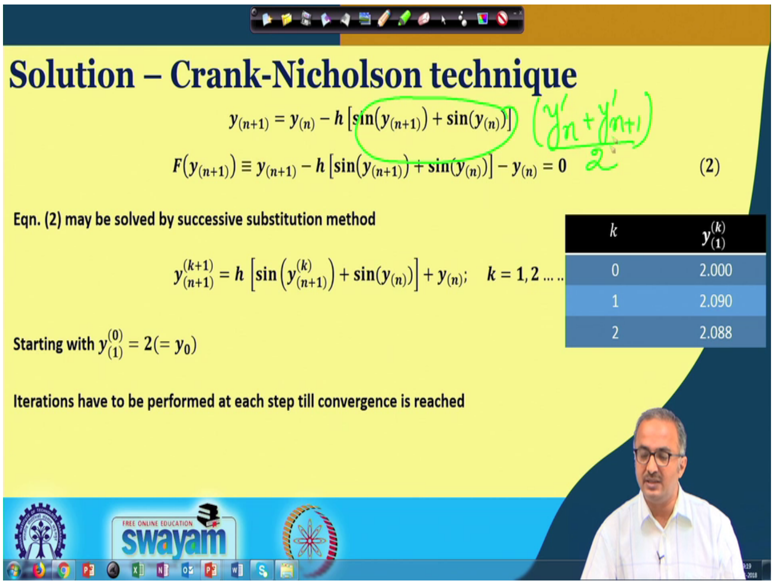

So, here we have this particular given expression here and what we are going to do is this, we will not be going over the. So, here what we are basically doing is this, this particular thing this right hand side what basically represent is, this is representing that y prime at n y prime n plus 1 and we are taking the average of this; that means, we are giving weightage to the values at the previous time step or the previous value of the dependent independent variable and the present value of the independent variable that is how this become semi implicit explicit or implicit ok.

Now with this particular understanding what we are now doing is this, we are getting this particular expression and you can see in this we have both sign yn and sign yn plus 1. And you can see that we again we have to solve because of this implicit nature, again we have to do iteration to get convergence at each successive value of x or the time.

So, we can again perform this thing and we find that these are the solutions. Now if you compare this solution with the earlier solution, you can find that if you can count the number of iterations involved to get the convergence and also stability you will find this Crank Nicolson it is generally working better than the implicit methods, but it is not so fast as expressed method, but it is at least ensuring the stability which is not there in the explicit method of solution ok. So, this is a very very popular method of solution of the differential equations.

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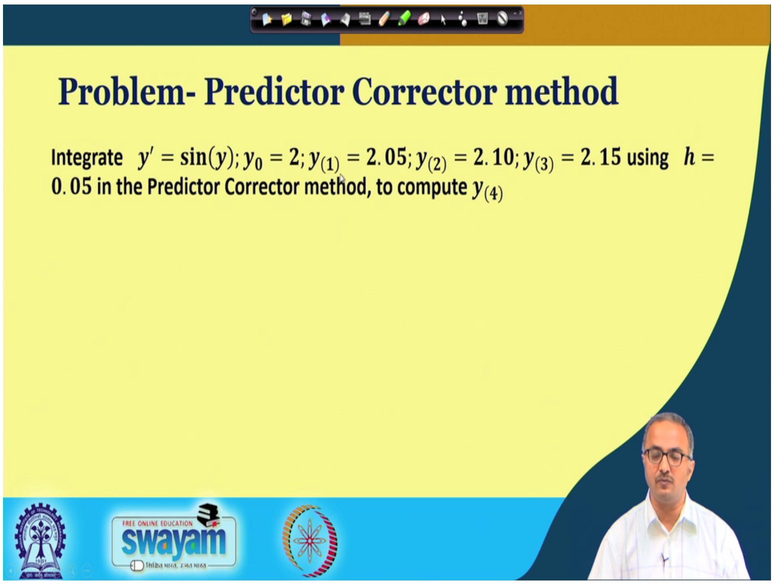

Another method is very popular, that is Predictor Corrector. It is something somewhat like the combination of the implicit and the explicit methods. Now here we shall again see how this is done. So, here we are taking this same function we are taking and what we are doing that this particular method need more than 1 value to start up ok. In earlier methods be needed only 1 value of y for some value of x, but here we need more than that.

So, here we have 1, 2 and 3 and these many values are needed and understand one thing, there are many types of these predictor corrector methods in the literature. I am showing only one of them to you and if you check the literature we will obtain, you will see there are other methods and you can adopt the particular method depending on the problem at hand; that means, we have to decide case by case basis which method is going to work best for your system ok.

So, here I have shown one and for that we find that we have plenty of values to start with y 0, y 1, y 2, y 3 and to get the value of y 4 ok. Let us see how we do that..

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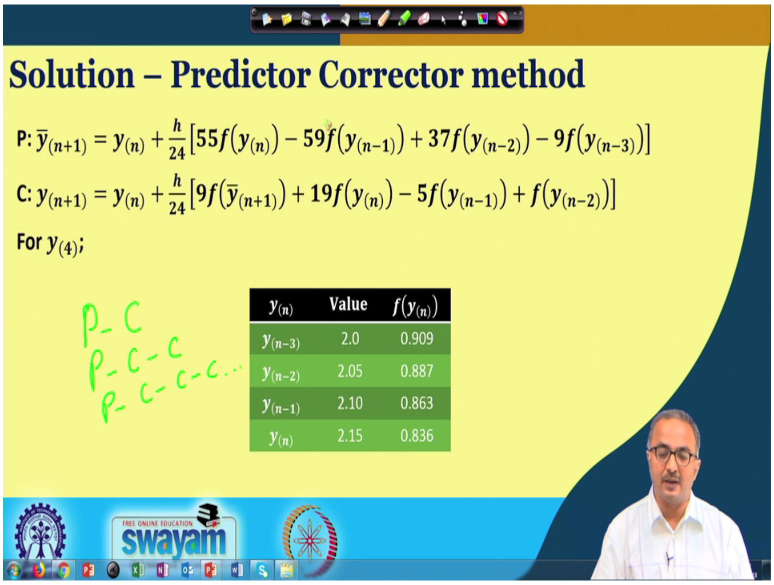

So, here we have this 2. So, here by P, we mean predictor and by C been corrector. Now you can see that these two formulations are a bit different. Now first formulation you can see that y n plus 1 is put in terms of or the previous value of iron which are known or which are supposed to be known ok.

And you can see this that means, we are having an explicit way of finding the value of y n plus 1 in terms of the previous values ok. Now here you find this is coming putting as over bar and once we know this value then this value is taken for the corrected method, which we can see this is an implicit in my n plus 1. So, here my n plus 1, this corrected value and this is the y over bar n plus 1, which is obtained from the explicit expression. So, this a corrected equation they are predicted equation ok.

Now, the thing is this, once you have given some value of the previous time previous steps, so what you can do? You can find easily this particular value of y bar. Once you get this value of I over bar, then you can come to the corrector method and then you can update the value of y n plus 1, but was the you must understand, that there is no need to stop at one application of piece this corrector equation, you can apply the corrector equation many times.

Once you do this predictor method, then you can apply the corrector method multiple times to get updates of this y value and till you get convergence; that means, if I write in these terms, what I can write this, I can have one predictor, one corrector. I can have 1 predictor and 2 corrector and then I can have one predictor 3 is corrector. So, you can see that this can go to many many numbers ok, depending on the kind of accuracy you need in your solution ok. This is pretty straight forward, you do not have to solve any kind of differential equation or do not have to solve any kind of integration, simply by an algebraic expression you are able to get the solution ok.

And now the another issue comes in this particular solution is this when how to start this one, because initially we may note this y n, but what about these y n minus 1, y n minus 2, y n minus 3. So, for this, what is suggested is this that because this PC methods are supposed to be better than the Eulers method, then what you can do is this initially you take smaller step size and use the Eulers method either explicit or implicit to generate this few values ok.

So, suppose you want the value of y 4 ok, so y 4 should dependent on y 3, but to get the value of y 3 what you do, you can start with y 0, get the values of the y y 1, y 2 and y 3 by applying the Eulers method ok. And after you obtain that then you switch over to this predictor corrector method now, so that you can now take a bigger step size and so that you can go the to the convergence faster ok.

So, that is how we say that the starting problem which is encountered in this kind of methods may be overcome by putting some other method; that means, we are hybridizing the methods ok, that is how we apply the predictor corrector method and here I have shown you the values of the yn ok, why is that is required in this particular problem.

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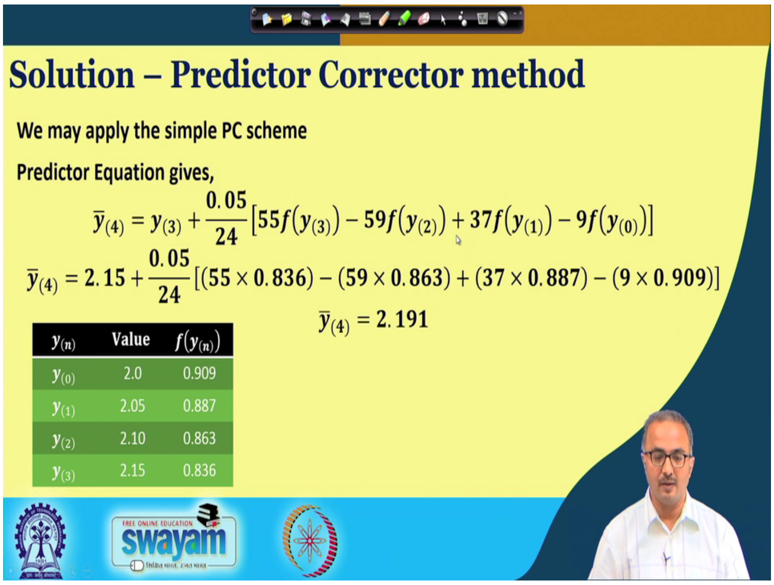

So, here you can see that we have applied this thing and we are showing the results to you.

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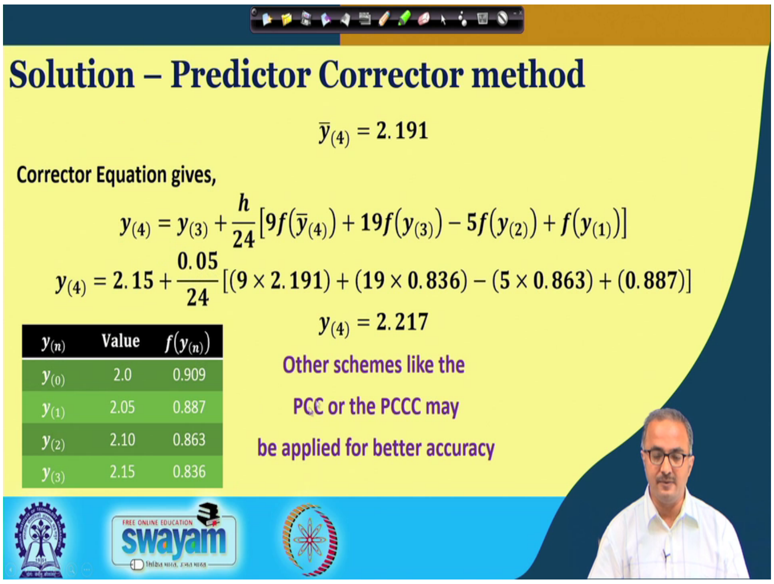

So, I will not going to the detail of these things you can solve easily these values, so first we are predicting and then correcting and as I told you that they could be multiple number of corrector name for better accuracy of the particular problem.

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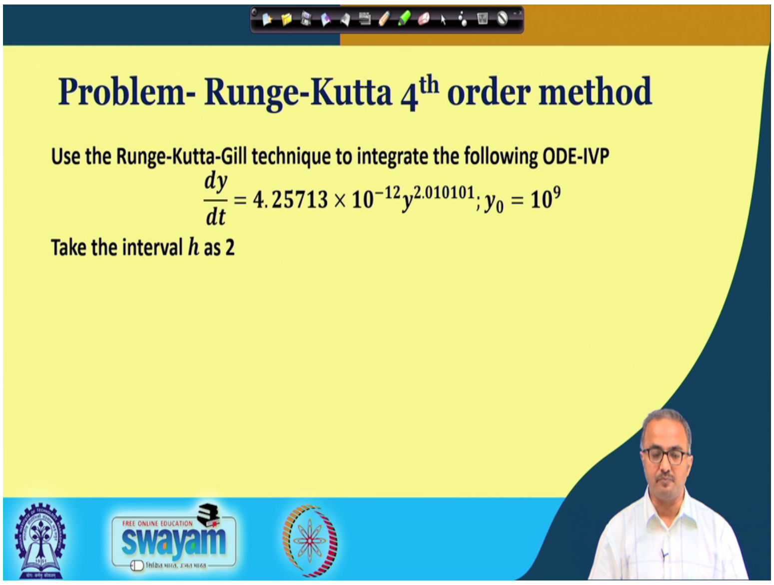

And next week come to another very popular method that Runge Kutta method and this method has also its many variations. So, I am talking about one of the Runge Kutta methods, this is kind of a family of methods you can say ok. So, it has depending on the order of aberration needed, we have first order second order like this. So, this fourth order Runge Kutta is very popular.

Even in fourth order you will find there are many variations in the literature ok. So, I will just give you the expressions to find out the value of the y for the fourth order Runge Kutta gives technique that give improvised upon Runge Kutta method to get this particular solution technique ok.

So, here we have this particular expression for the dy by dt and this is the initial value of y naught and we have to with this h we have to find the value of the y.

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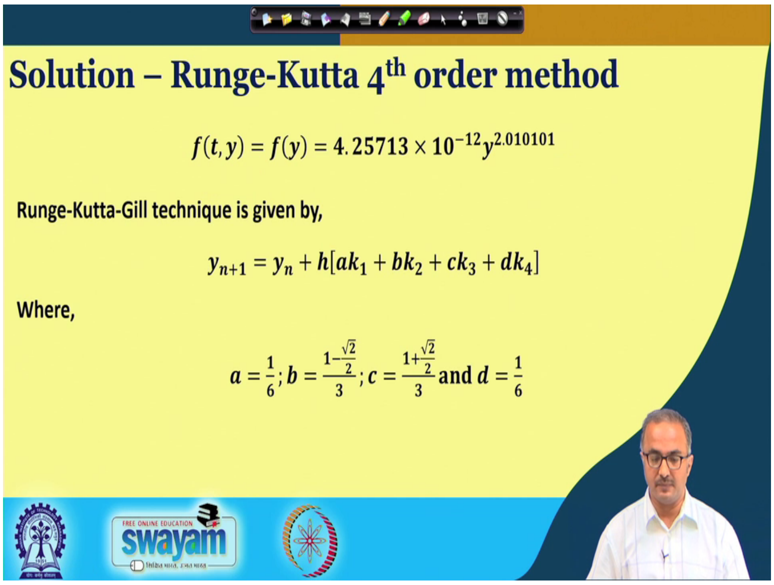

Now, here is that here this is the particular expression this is the heart of the expression which has to be used for this Runge Kutta method, this is the particular expression. And here you will find that all these values of a k 1, b k 2, ck 3, d k 4, all these things are obtained from some expressions given by this Runge Kutta Gill. So, these are the particular expressions for a b c d.

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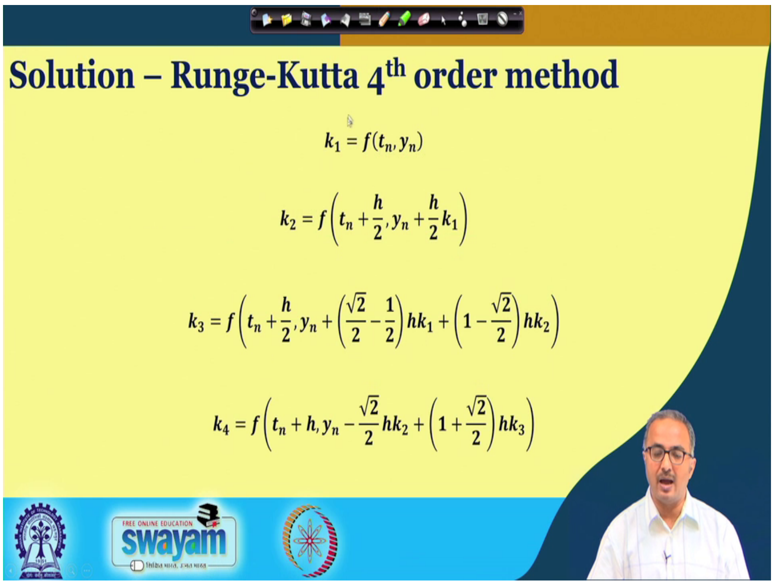

Similarly, you have these expressions for k 1, k 2, k 3, k 4, generally these expressions and not to be remembered, they will be given to you simply have to refer to these equations and if evaluating the values of a b c d k 1 k 2 k 3 k 4 ok. So, there is nothing to grab in this for this particular method.

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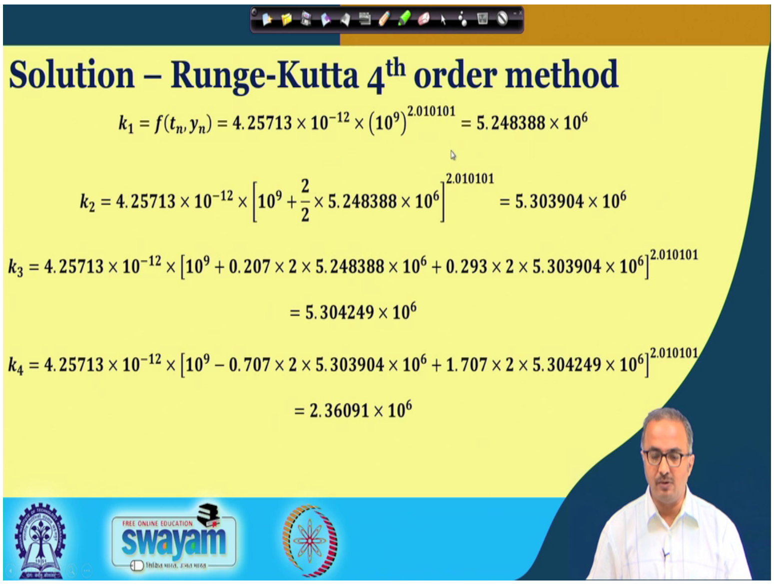

And now it becomes a simple to you, you can see that here that this k one depends on the initial values of y and t then depending on the then once you find k 1 the k 2, we have dependent on the step size and the k 1 value, then k 3 is a function of the step size the k 1 value and k 2 value, k 4 is the function of again step size, the k 2 value and the k 3 value; that means, you have to go in this particular order, you cannot take any trapezoid way of finding the k 1 k 2 k 3, if we could because there is a particular direction of the dependency of these four parameters that you have to take care of.

And here we have shown you this that here you can check the values of k 1, then the k 2, then the k 3 and the k 4 these have been obtained from the earlier formulae.

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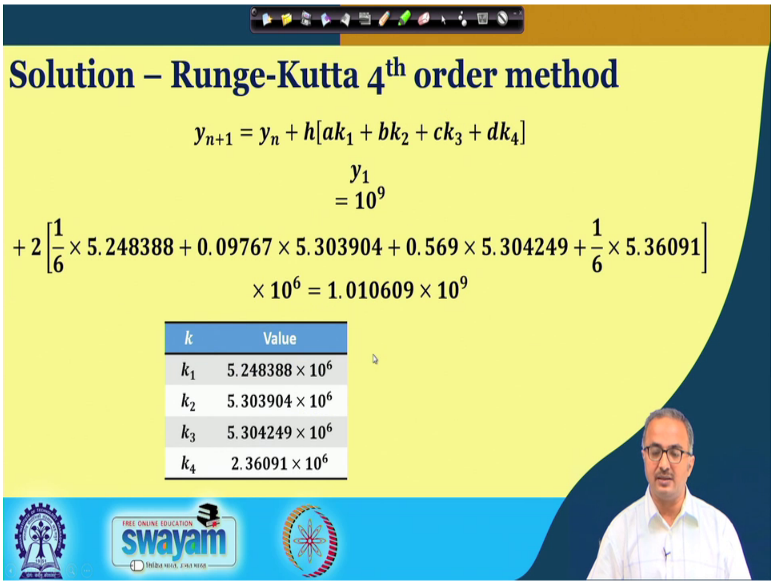

And using those and the values of the a 1, a b c d, we can find that the value of this particular this y for the next time steps ok.

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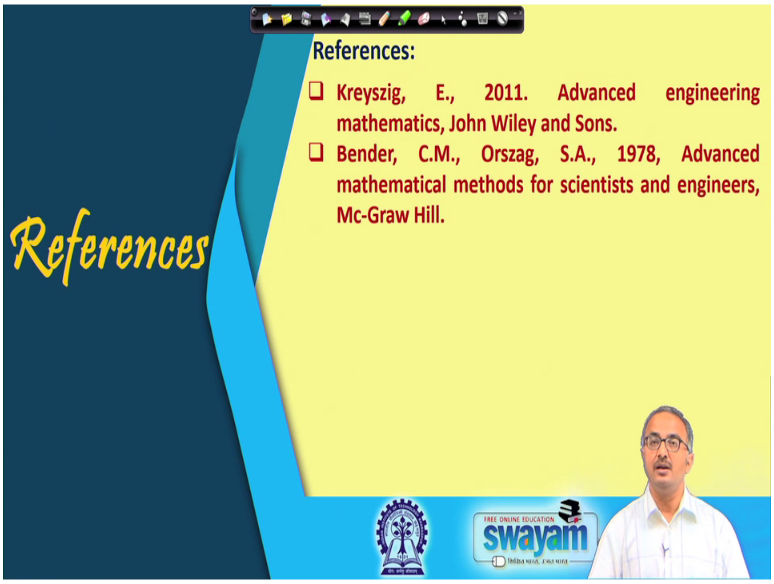

So, here are the references in way in which you can find more details about the methods I taught you today.

Thank you.