Computational Physics
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Lecture - 31
Differential Equation with Specified Boundary Conditions Part 01

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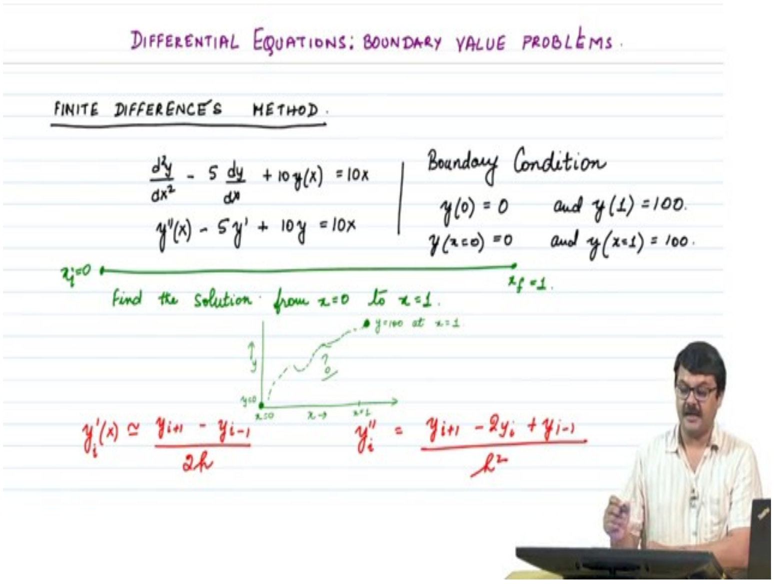

Hello everybody. So, today we will be discussing about differential equations, but boundary value problems. How is it different from what we did in the last class. So, what we did during Runge-Kutta or Euler was we had first order and then we learnt about second order differential equations, where we gave the 2 initial conditions.

The value of say x at time t equal to 0 and d x d t or velocity at time t equal to 0 and then what we did is basically calculate the values of x at subsequent times. So, at time t equal to 0, time t equal to 0 plus h time t equal to 0 plus 2 h and so, on. So, we basically had the value of the position say and velocity now just let us talk about d x d t or the first derivative of the function at different instances in time right.

And we basically integrated the equations from time t equal to 0 to time t equal to whatever we want and we also looked at many coupled differential equations, basically various particles were moving with each other with respect to each other and the forces depended on the separation between the 2 neighboring particles in the y direction.

However, the problems we are going to discuss today are different. We are not going to tell or give the initial conditions at time t equal to 0 where, but we are going to give the boundary conditions which means at one end of the interval and the other end of the interval.

So, let us be more specific. Let us suppose that we have a differential equation d 2 y d x 2 minus 5 d y x plus 10 y y of x equal to 10 x right and we have to solve this differential equation, this equation can also be written as y double dash x but where the double dash basically stands for d 2 y d x 2 and y dash stands for d y d x and so, on so, forth and the boundary conditions are y at x equal to 0. So, so y at x equal to 0 equal to 0 and y at x equal to 1 equal to 100 which can also be written as y 1 equal to 100 right.

So, here you have two conditions, but now they are given at the 2 ends of the interval, and you have to find the value by solving this differential equation you have to find y as a function of x for the intermediate points right. So, this is a simple toy problem, but the way we are going to solve it is the so called finite difference method and in the finite difference method the things that we learned are particularly useful to solve partial differential equations which will be the topic of the next class.

So, but first let us figure out how we do finite difference methods and solve this particular differential equation for these boundary conditions right and we have to solve this get the solution from x equal to 0 to x equal to 1. So, just to look at it graphically so, you have to solve y as a function of x by solving this differential equation.

You know the boundary conditions that is at x equal to 0, you know that the value of y that the value of y is 0 you know that at x equal to 1 right the value of y is 100. So, this point and this point you know the value of y and by solving this differential equation you have to essentially figure out what is the value of y at the intermediate points.

Now, I would request you to remember, when you learnt about differential differentiation and integration in class 12 and what you learnt in class 11 or 12 was suppose you had a curve like this right then at each point what you could do is basically calculate when you change x in this direction suppose how much would be the change in y and then you would say d y by d x; sorry, the change in y with respect to x and that you would calculate as d y d x and then you will take d x the limit tends to 0 right; and similarly at each point in space you could also calculate the second derivative d 2 y d x 2 by taking the suitable derivative of d y d x.

Here you have the opposite problem where you have expression you have d 2 y d x 2 d y d x at different points in space and you have to solve the differential equation to get y as a function of x. What we were going to use is basically write these double derivatives and single derivatives as difference equations right.

So, here you are saying that you are basically writing the difference in a neighboring value of y . So, when you are calculating the y at a particular point say i here at this point at a particular value of x. So, you are trying to calculate the derivative you are writing the expression for d y d x by discretizing space .

And then that I shall write down the derivative as the value of y at a neighboring point say i plus 1 and at another neighboring point the change in the value of y by the interval 2 h which would be equivalent to d x to d x right. And similarly you have this expression for the double derivative and this can all be derived using Taylor expansions, I am not going to go into that I am rather saying that if you accept these and you can derive those how to basically solve the differential equation in a hands on manner. So, that is what my focus is.

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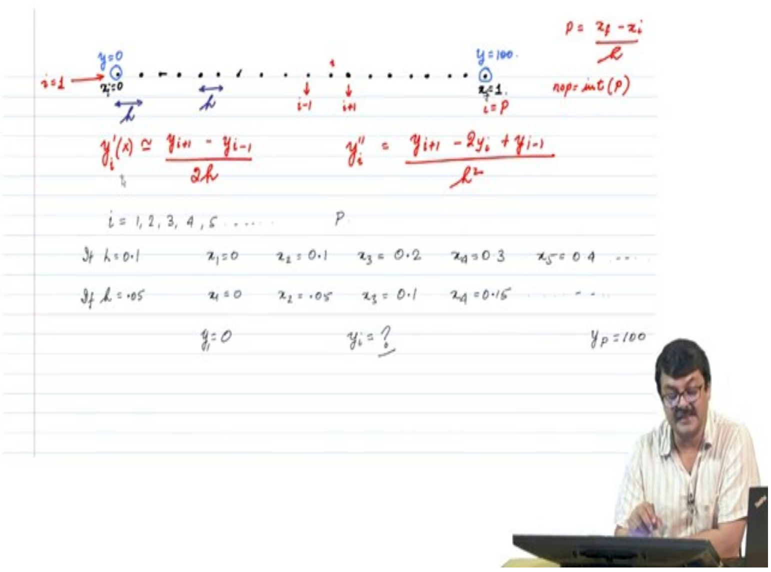

we have to find the value of y as a function of a over this interval right. From x equal to 0 equal to x equal to 1 and we have to solve it on the computer we cannot work with d x or the interval going to 0, where we need a finite value of the interval say h. So, d x tendsto 0 but h always have a; has a finite value, what we do is discretize this space.

So, suppose this is x equal to 0 right at this point and this is x equal to 1 and we divide this entire range between x equal to 0 and x equal to 1 into discrete points. So, suppose this is x equal to 0 and this is the value of x is at a distance h from this point and so, each of these intervals are called h. So, h can be supposed 0.05 as an example. So, then. So, at this point x would be 0 at this point x would be 0.05 at this point it would be x equal to 0.1 and so on so forth.

Now, we can call each of these points at which we are defining these values of x to be i. So, this is i equal to 1, this is i equal to 2, i equal to 3, i equal to 4 and so, on so, forth and it goes up till i equal to p right. So, what is the value of p; well, p would be except the final value in our case it is 1 minus x i the initial value in this case x i equal to 0 divided by the interval. So, it depends upon how finely you do you divide this entire range from x equal to 0 to x equal to 1 and how finally, you want to divide it? You can choose h equal to 0.05 in that case you shall divide this entire interval into 20 points.

So, p equal to x f minus x i the x; f for final, i for initial by h, h being 0.05 and then you will get p equal to 20 and you can take the integer and then you get the number of points. But if you take suppose h equal to bigger 0.1 right then you will have 10 points between x i equal to 0 and x f equal to 1 I will run from 1 to 10 right.

Now, at each of these points. So, you have discretized space along the x direction now you have to find the value of y at each of these points if you like you can say we have to find the value of y for i equal to 1 what is the value of y at i equal to 2 and so, on so, forth and at each i point i you have a certain different value of x, x if h equal to point 0 5 then x 1 will be 0, x 2 will be 0.05, x 3 will be essentially 0.01.

So, you have to calculate at each of these i points the value of y and basically plot y as a function of x which is a solution right. Now in the differential equation where you have double derivative and a single derivative you can write down y dash is the single derivatives and as y equal to i plus 1, if i is any particular point then the value of y.

So, if this is suppose i here then what is the value of y at i plus 1? What is the value of y at i minus 1 and of course, you do not know that that is what you are after I have to find out right ah, but if you knew its neighboring values, then you could find out or write down an expression for y dash the single derivative and similarly y double dash double derivative can be written down as this.

So, y at i plus 1 minus 2 y i and y at i minus 1 right. So, you have basically discrete expressions for the derivatives at this using the values of y at discrete points in space that is why you called it a difference equation, and not a differential equation.

Because now as you are writing it in discrete values of y and at discrete points in space not continuously we have discretized this space into a certain point.

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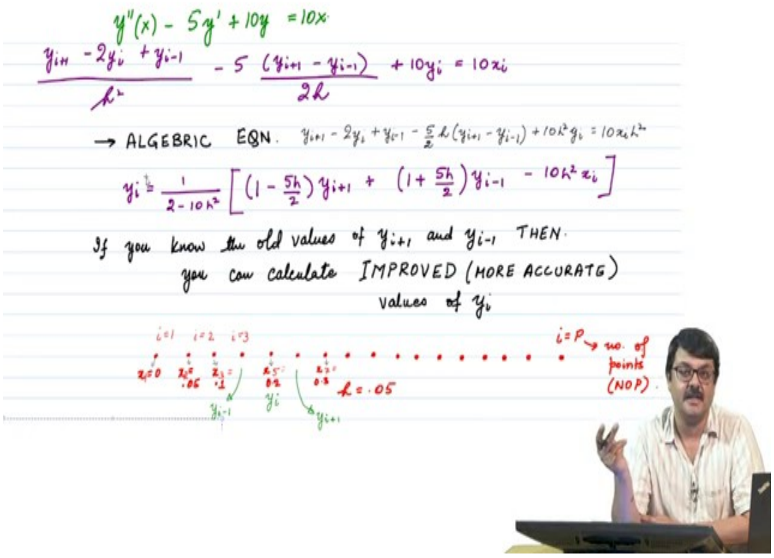

Now if you have these expressions for y dash and y double dash right then what you can do is, substitute these expressions these difference equation expressions in your original differential equation. So, basically here instead of y dash I have written the expression for the difference equation y i plus 1 minus 2 y i y i minus 1 where i runs from i say 1 to 20 if h equal to 0 point 0.05.

It could run from i could run from 1 to 100, if h was 0.01 right so, on so, forth and here I have written the expression for y dash right and this is plus 10 y. So, basically at each point you can write down y:i and you have to solve for y i of course, into 10 x i whatever the value of x is at each point at for i equal to 1 to y equal to p right.

So, what you have done consequently is basically converted this differential equation into an algebraic equation. So, if you multiply h square over this entire equation what you get is, y i plus 1 minus 2 y i y i minus 1 into 5 by 2 into h because there is a denominator there is h and you are multiplying by h square right similarly you will get a expression of h square here and 10 x i h square right because we are multiplying the entire equation by h square.

And now you can rearrange the terms and you can write y i as 1 minus 2 minus 10 h square plus 1 minus 5 h by 2, y i plus 1 plus 1 plus 5 h by 2 h is this distance between grid point d x if you like to y i minus 1 minus 10 h square x i what is the message? If somehow you knew the value of y i plus 1 and i minus 1. So, if you somehow knew it or even if you guessed it suppose you try out with the trial solution you do not know what the solution of the differential equation is, but you could have a trial solution. Especially since you have an idea of the limits, you know that at x equal to 0, y equal to 0 and at x equal to 1, y equal to 100.

So, let us suppose the solution will be something close to a straight line it is a trial solution and then you say that let me see whether you can I solve iteratively can I move closer to the actual solution iteratively in by some method and finally, arrive at the correct solution of the differential equation. So; so, that is the aim and with suppose a trial solution you knew the value of y i plus 1 and y i minus 1 right then you could calculate an improved value improved or more accurate value of y i by solving this so, called difference equation right.

So, that is what our aim is. So, basically what we are trying that at different points grid points along the entire range, you have x at different points 0.05, 0.1, 0.02 at each point you have a guess for the value of y i and y i minus 1 and y i plus 1 over the entire range you have there you have a initial guess solution right and using that guessed solution you basically calculate improved value of y i over the entire range.

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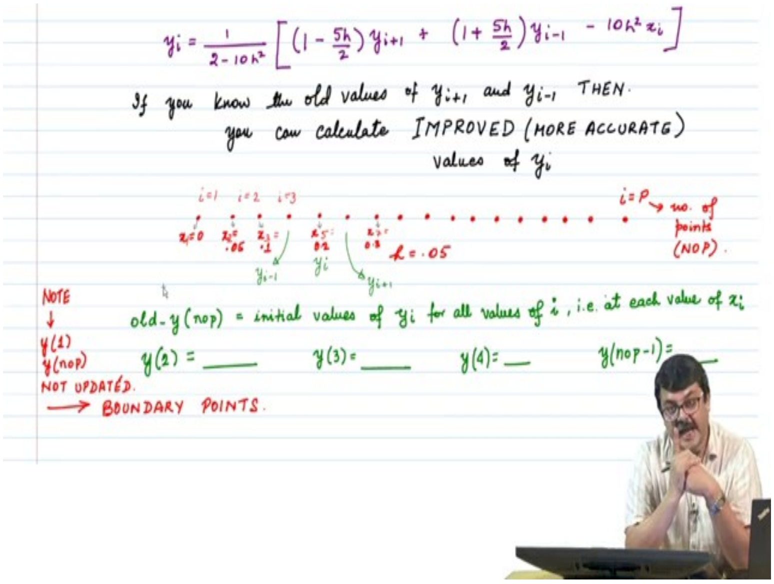

So, you have a guess you get an improved calculation of y i over the entire range and you keep on doing it iteratively right.

So, there would be if NOP number of points p and the integer value of is nop if there were nop grid points you can in your old or initial guess of the value of y at each of these grid points, you could store in an array called old y right, you just suppose it stores the initial value of y for all values of i that is at each value of x i right. And using this formula here this formula right you can basically at each point at each grid point calculate a better and improved value of y 2 and then y 3; sorry, and y 4 and y and y nop minus 1 right.

And then what you do is basically store these improved values of y 2, y 3, y 4 so on and so forth into old y, you save them and use that to have better estimates of y 2, y 3, y 4 y 5 over the entire range you keep on doing this iteratively and your solution will relax or converge towards the correct solution.

Now, for that what you need is that you need a reasonable guess of your initial guess of the solution. If their solution is very far away the initial guess is very far away then this by doing this process iteratively you are not going to converge to the actual solution right. So, you need some estimate you similar to using some analytical methods that this should be the solution yes I cannot solve it exactly but this could be the nature of the solution you can have a guess from the boundary conditions as well and then basically the system if you have a reasonable guess not too far away then basically you will iteratively move converge or relax to the accurate and correct solution.

Note when I said that you can update the values of y for each of the grid points, I started from y equal to 2 and stopped at y equal to nop minus 1 right NOP is basically the number of points which I refer to as NOP you can also say p basically if you take the integer of p you get NOP.

So, those 2 the boundary points the boundary points I did not update, because the boundary points are fixed they do not change right. When I do the iterations the boundary points the where this solution and the boundary points are given and they do not change. So, you do not update that but any point between the range between the boundary are is iteratively corrected for and you slowly relax to the correct solution.

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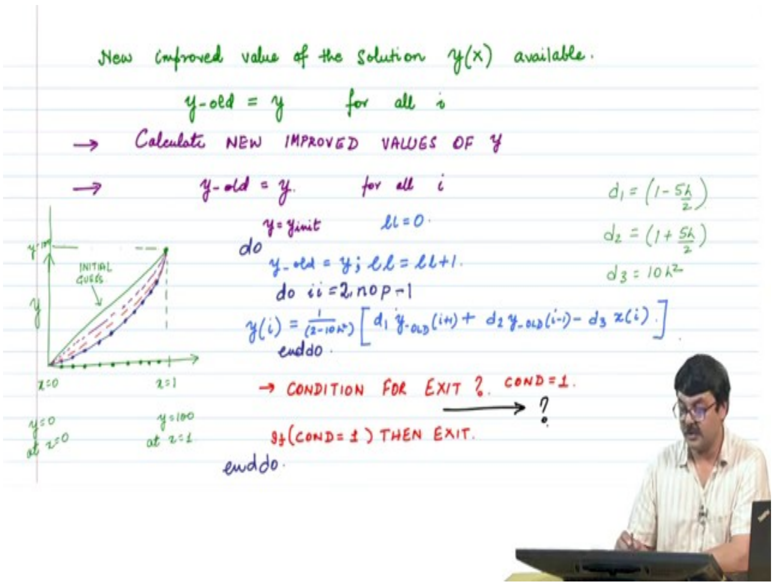

So, that is basically what the plan is, that is how you solve a differential equation where the boundary conditions are given. So, you use the boundary conditions write down d 2 y d x 2, d 3 y d x 2 if you had higher order terms there are formulas given in books, you can look up the derivation, basically Taylor series expansion.

And if you have the expressions given, then you substitute them into the differential equation convert it into an algebraic equation as we did here right. Then write y i in terms of the values of y of its neighbors and then you solve it you have an initial guess where you have y i defined at each of these grid points and then iteratively you say that if this condition is to be satisfied the value the improved value of y i should be such and such as per this equation I mean if you have a different differential equation of course, this expression will be different right.

This is derived from this from this differential or rather difference equation right and then you solve it for each value of y and use this to get improved estimates of y i and so, on so, forth. So, basically what I have written here in this slide is what I already said that, every time you calculate the improve values of y using the old values of y and then you save the values of y into y-old for all i and then again calculate the new y.

So, how should the code look like? how should the code look like? It should be basically .... So, there should be a do loop, but look this is an open ended do loop because you do not know how many times you have to iterate to reach the improved and the so, called correct value right. You will not ever reach the exact value you will never reach that because after all you are discretizing space there will be some rounding of errors but you can reach reasonably close to the actual solution of the differential equation, but in how many iterations that is unknown.

So, here what I have given is an open ended do loop. So, do end do here right and say i before that you have some guess for each value of y i, the value of y at each of the grid points and suppose y-old stores that, the basically the y-old is an array and it is of length p of course.

So, I have first saved the value of ye old for the purpose of the do loop right. So, suppose you stored the value of y i need the initial values in this array y right I had been mistake. So, I added this statement and basically y-old you. So, the value of y is stored in y-old first and then you update the value of y here right. So, is this same formula do i i equal to 1 to number of points rather it should be 2 to number of point minus 1 right.

Because you do not have to you do not have to basically update their boundary points, the end points and for all i in this range basically you update the value of y using the same formula that i wrote where for d 1. So, d 1 is nothing but this quantity, the same as this quantity you do not need to calculate this quantity every time hence you can calculate d 1 some dummy variable right at the beginning of the code so, that you save basically computational resources.

So, d 1 into y-old the older value whatever was saved i plus 1 then d 2, d 2 is nothing, but 1 plus 5 h by 2 the same as expression here h of course, is the difference between grid points d x. So, d 2 into y-old the older value of y at i minus 1 minus d 3 being this do x i right.

So, at the end of this do loop you have a new value of y stored, that is stored in y-old again and repeat this and you keep on doing this iteratively and this. So, with every iteration you will have improved values of y i which means that suppose that if your guess for the initial condition was the straight line, the straight line joining x equal to 0, y equal to 0 at x equal to 0 and y equal to 100 at x equal to 1 suppose your initial guess was the straight line, with each iteration you will have this line as an improvement and then this line and so, on so, forth and then finally, your final solution would be this.

Right that so, there is a blue line which where you have the value of y at each of these discrete points the question is when. So, how many times will you iterate when will you go out of the loop? Here you see as I told before that I have not given a any particular number of iterations, because number of iterations number of times you have to iterate is typically unknown.

So, to get out of this loop when you have the final solution, you shall need a condition of how to exit this loop right and suppose you define a variable called COND COND for condition and COND equal to 1 suppose you set it equal to 1 when a certain criteria or condition is satisfied and depending upon the value of y and if COND equal to 1 then you say , exit this loop and that is your final converged value of your yi .

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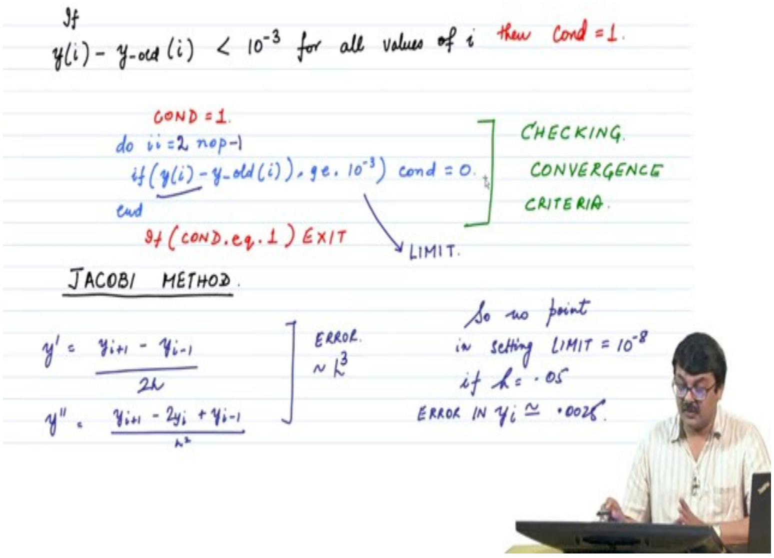

So, let us suppose your condition. So, the condition when COND will become equal to 1 when you will exit the loop, you can set that to if y i that is the new values the updated values of y i in this particular iteration minus y-old the previous value of if this difference is less than some limits say 10 to the power minus 3 for all the values of i then you set COND equal to 1 and then if COND equal to 1 then exit but you have to check that for each value of i for each of these grid points then grid points between the boundaries that this the difference between the older y i and the newer y I is less than a certain limit. So, how do you implement it?

Now, suppose you. So, basically it is here that this code will go in here you are constantly updating, but after every update you check whether the condition for convergence to the final value has been reached or not and if the condition for convergence has been reached you exit.

So, basically here you are checking whether you have reached convergence or not. So, at this part what you do is to check and how do you check you say do i i equal to again there should be 2 to nop minus 1 between the between the boundary points. If y i; if y i minus y-old the older value is greater than if this condition is not satisfied if it is greater than your limit right 10 to the power minus 3, then you say COND equal to 0 and if COND if becomes 0 then you do not exist the loop.

So, we have set COND equal to 1 the condition equal to 1 before the loop in the loop if any of this points for any i, if COND if the condition is not satisfied you change the value of COND to 0 and it remains there right there is no condition which is given that it will become again equal to 1 between this loop right.

And if COND equal to 1 then exists then exit but if COND becomes 0 if any of this condition a for any i is satisfied then you do not exit it what do you do? You go back here you set y-old equal to y update y i again check if any or for any i if the difference between the new value and the older value is less than the criteria that you have set the convergence limit that you have set and you keep on doing it.