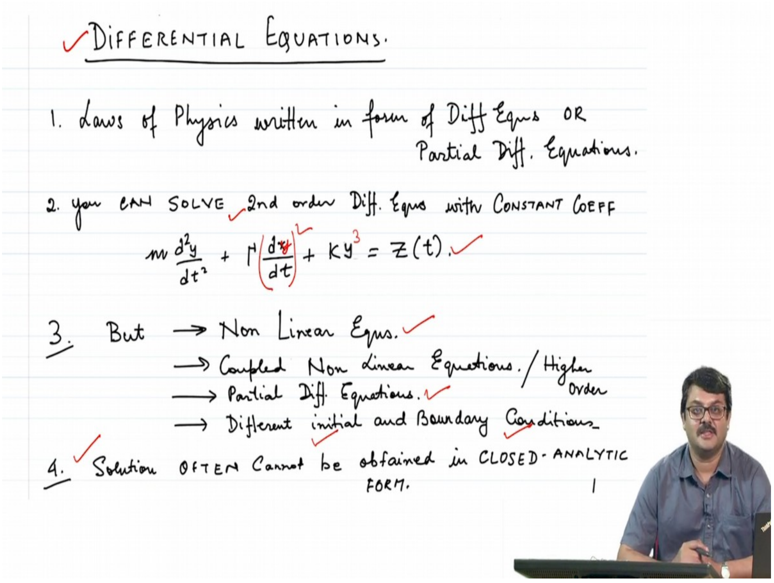
Computational Physics
Dr. Apratim Chatterji
Dr. Prasenjit Ghosh
Department of Physics
Indian Institute of Science Education and Research, Pune

Lecture - 26
Differential Eqns
Euler and Runge Kutta
Part 01

(Refer Slide Time: 00:17)



So, welcome to the next module of this course, where we shall be discussing Differential Equations for the next few 4 or 5 classes, ok. Now, as you would know that the laws of physics are written often in terms of differential equations and partial differential equations. Examples are Newton's laws, Maxwell's equations of electromagnetic theory, the diffusion equation and the heat equation and so on and so forth.

And typically, the equations are written in partial differential equations or differential equations and you give the initial conditions or the boundary conditions as the case may be. And then to understand what the phenomena is happening you solve for the differential equations to get a value of the field at different points in x the position or time, right. I mean, suppose you are starting with the partial with the Maxwell's equations for electromagnetism, then you basically specify that the electric field is such and such at the boundaries of the dielectrics and then you solve for the electric field given the boundary conditions for the space within the dielectric, right.

So, in this module, we shall be focusing on solutions of different kind of, differential equations we shall also do some simple partial differential equations with boundary conditions. Now, what you would have already learnt in your mathematical physics course is basically solve second order differential equations, maybe with constant coefficients and even with maybe a forcing term, right.

And with constant coefficients where m, gamma, kappa, are constants with certain numerical values and as you see that this is a second order differential equation because you have double derivatives here, right. And this is what you would see if you had some particle moving in a viscous medium and in the presence of a spring force and with some forcing. So, these are the things which you would have already looked at or analyzed, solved in your mathematical physics course.

But often in nature when you study different phenomena you come across non-linear equations, where you have a power suppose this for something like this. So, this becomes now a non-linear equation. You do not have a linear equation in dy dt. So, you often come across non-linear equation and suppose you have something like this. So, this is again because you have x cube and not a linear term in x, is a non-linear equation both here and here.

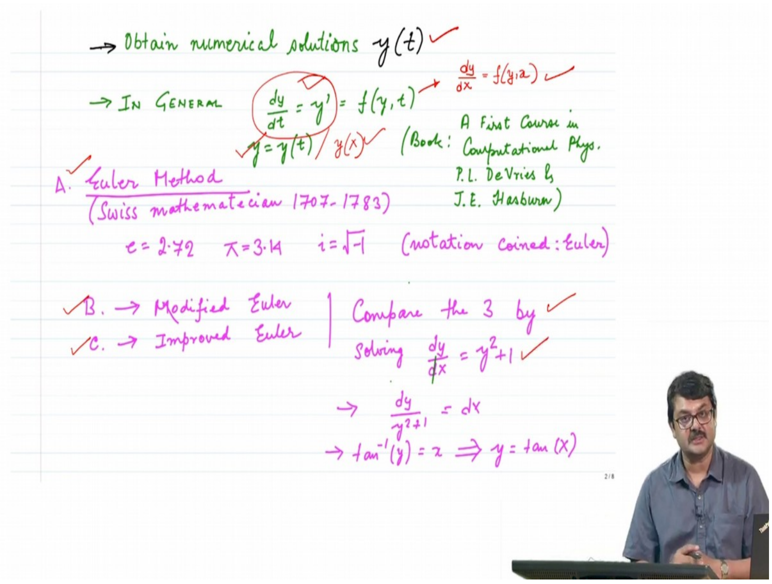
You can have coupled non-linear differential equations, so they are basically different equations for different fields and each is evolving depending on the other, so one example of a coupled partial differential equation would be suppose curl of b equal to minus del e del t, all right. And you would have a similar equation for e. So, b f x e and e f x b and so on so forth.

And of course, we have already been discussing partial differential equations, heat equation, Maxwell's equation, they are partial differential equations, and you can have cases with either initial conditions given or boundary conditions given, right. So, you have all these complications and more often they are not the solution cannot be obtained, the solution to the differential equation or the partial differential equation cannot be obtained in closed analytic forms, right.

Now, you I have a, we often have a series solution, infinite sum that is even tractable, tangible, but in general you might not have the option to even solve it in a series solution, but we want to know the solution. So, nature is complex, nature has a coupled non-linear differential or partial differential equations and one does need to solve for those to find out the solution.

So, what we will do in this course is first look at first order simple differential equation learn, what are the techniques to solve it compare across different techniques and then basically increase the complexity, make it a non-linear differential equation, have two coupled differential equations maybe and then keep on increasing the complexity, where we have many coupled differential equations.

(Refer Slide Time: 05:13)



I shall basically be of course, teaching you standard simple textbook stuff. But as and when need be in the future whenever you need to solve differential equations numerically you can scale up the complexity, you at least you shall have some exposure to the basics of solving different kind of differential equations.

At the end, we shall also spend be one and a half classes discussing some simple partial differential equations where boundary conditions are given. Initially, we shall be mainly discussing differential equations where the initial condition is given and our aim is to basically obtain numerical solutions as the solution as y of x.

In general, if you have a first order differential equation, you can write your differential equation like this dy dt equal to y dash, so I mean you can denote dy dt to be y dash. So, the dash denotes the derivative and that in general will be a function of y or t. So, if y is not there it is simpler, you can maybe even solve it analytically, but in general the function the dy dt can will be a function of both y and t. Or I mean you can also write instead of dy dt because t is reminiscent of time, but you can also a similar equation you can write dy dx equal to f y x whether you write this or this, so equivalent.

And what our aim is if you cannot solve it analytically, you need the solution to the differential equation y of t or y of x, right. And the first methods that we shall use and of course, we should need improvements of it is called the so called Euler method. Euler was a Swiss mathematician, who lived from 1707 and to 1783, and he had many contributions to give in mathematics and the method that we should use is also basically Taylor expansion, right.

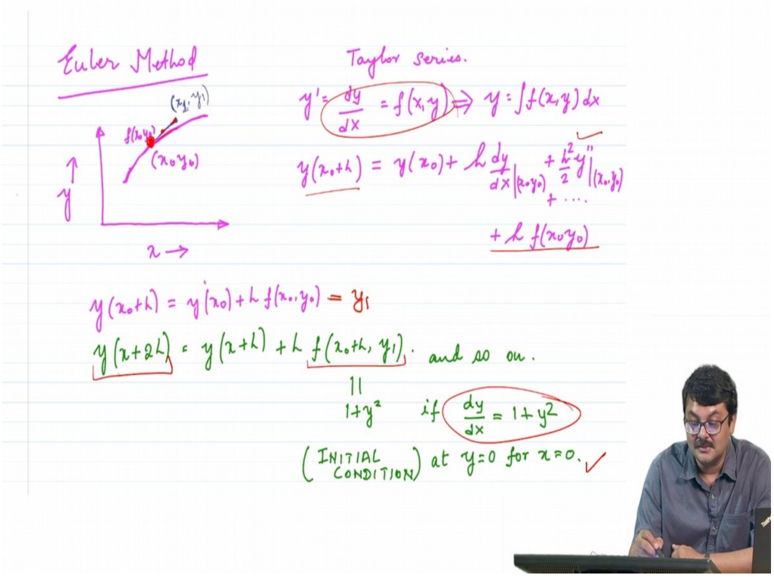
And Euler we are not here to discuss all the contributions of Euler, but just to give an example that much of the notation that we use today in physics or in maths like e its 2.72 or pi which is 3.14 or i the imaginary number i which is square root of minus 1, all these notations where coined by Euler. Just that is a side story.

And we shall solve a differential equation, simple first order differential equation by the Euler method. See that it is not a great method the deviations, and then we shall go to the so called modified Euler and the improved Euler and we see we shall see that solution to the differential equations becomes much better.

So, we shall compare the 3 methods by solving dy dx equal to y square plus 1. It is a non-linear equation of course. Now, this particular differential equation can be solved analytically which is basically you divide by y square plus 1 can be written as dx, and if you integrate both sides you will get tan inverse y equal to x or the solution is y equal to tan x.

So, we chose this example intentionally though we know that it can be solved analytically, so that we can compare our numerical solution to the differential equation with the exact analytical one. So, basically we can compare and have an understanding of what is going wrong, where it is going wrong and once you have standardized the methods of course, you can apply it to an unknown problem which cannot be solved analytically, right. So, this is just for comparison, this is just for learning that we are choosing this differential equation to learn to solve. And after that we shall keep on increasing the complexity of problems as we develop better and better methods, ok.

(Refer Slide Time: 09:47)



So, what does the Euler method say? So, here we essentially are using Taylor series and y dash the single derivative which is dy dx is in general f x y, right. So, y equal to integral of f x y dx and if you can do that integral analytically, well and good, but often we cannot. And in our case, f x y is of course y square plus 1 divide x equal to y square plus 1, so in our case the case we shall be discussing is this quantity is 1 plus y square.

And in general, in the Taylor series if you know the value of y at a certain point say x 0, right, so then y x plus h at a slight distance away from x 0 x 0 equal to; so, at some x which is x 0 plus h, h is small, you can write this as the value of y at x 0 plus h, h is the small increment it is this one dy dx calculated at x 0 y 0, all right. In general, x 0 y 0 f x y and this dy dx for our case at x 0 y 0 is nothing but h into f x 0 y 0, right. This is the definition, this is the differential equation we are starting out to solve anyway, right. Plus h square by 2 y double dash double derivative calculated at x 0 y 0 plus higher order terms, right.

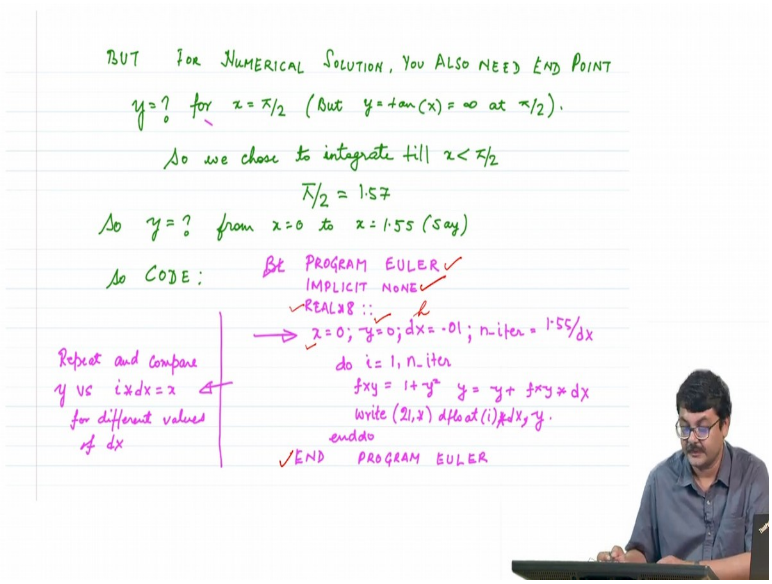
So, that is all that is there to the Taylor expansion and in the Euler method what we do is neglect the terms of h square and higher order terms. And then what you have is if you are neglecting the higher order term and if h is small enough then one can write this equation to be y x 0 plus h equal to y x 0 calculated at x 0 plus h into f x 0 y 0, and we have neglected the higher order terms, right. So, that will be the value of y at a point slightly away from the value of x 0.

Now, suppose you specify as an initial condition, you know what is the value of y at x 0 as an initial condition, then you can calculate what is the value of y at x plus h, right where this is nothing but dy dx and this is the differential equation you are starting out to solve. Now, if you know that then you know the value of y at x 0 plus h call it y 1, right and then you can calculate basically the value of f at x 0 plus h and at y 1, right. So, it is like x 1 and y 1.

So, you basically if f x y, so suppose this is a graph this is y and x and f x y this quantity, this function is suppose this curve like this, right. You know, you have been given the initial condition, the value of f x 0 y 0 at this point, right at this point. And then, if you know this point then you are calculating the value of y x 0 plus h x 0 plus h using the slope dy dxs using the value of x 0 y 0 at this point and if you know the value of y 1; y 1 is this. Then putting this and x plus h you can again calculate this quantity and thereby calculate this quantity. Having known this you can again calculate the value of y at x plus 3 h and so on so forth, right. And that is all that we are going to do.

In our case, just to remind you f x 0 plus h is 1 plus y square because this is the differential equation we are solving and the initial condition we shall be solving is y equal to 0 for x equal to 0, because we know the solution, right we are basically learning to do it. So, for tan x equal to 0 we know that y is equal to 0 and that is the initial condition I have chosen, right.

(Refer Slide Time: 15:01)



But if you are calculating the numerical solution you not only need since you are calculating in numerically, you not only need the initial condition, but you need to tell the range over which you want to calculate the solution because you are going to calculate it y plus h, y plus 2 h, y plus sorry y at x 0, y at x 0 plus h, y at x 0 plus 2 h, so on so forth and y at x 0 plus n h, when n is the number of iterations, n is some large number, right.

So, basically, since you do not have an analytic form you have to specify the initial condition and calculate the solution for a certain range of x, right. So, you not only need the initial point you also need the end point, in this case we know the solution is y equal to tan x and we know that at x equal to pi by 2 tan x goes to infinity, the computer cannot handle infinities.

So, here having the hindsight we shall choose to integrate the function divided x equal to 1 plus y square from x equal to 0 to x equal to some value slightly less than pi by 2, because exactly at pi by 2 it is going to go to infinity pi by 2 is approximately 1.57. And say, we are going to calculate what are the values of y, is a solution of this differential equation from x equal to 0 to x equal to 1.55 say. I mean you can even do it 1.56, but there basically f x y well the solution will sharply increase and so, you have to take smaller and smaller values of dx; dx is nothing but h the point which is basically moves you away from x 0, x 0 plus h, x 0 plus 2 h and so on so forth.

So, for an Euler since you just have a simple first order differential equation and you have the first term in the Taylor series the code when you write it should be should look something like this. Of course, I am not writing everything, but suppose you call the program Euler and you have your end program Euler always do implicit none that is a good practice, so that all the variables you have to define by hand. And you can basically define all the variables REAL star 8, and INT, whatever variables you shall be using.

Now, say that x equal to 0 that is the initial condition, at that value y equal to 0, dx or h you got a 0.01 say and we shall see if you change the value of gx how good or how bad the integration becomes. And the number of iterations n iter, n underscore iter stands for number of iterations is basically the range over which we are going to integrate, suppose 1.55 by dx, so, many times iterations we have to do, right; x plus h, x plus 2 h, x plus 3 h, x plus n iter h, right.

And so, the Euler scheme is rather simple. The loop shall, the code shall look something like this do equal to 1 comma n iter number of times, you know you are going to change x 0. You are basically calculating the f x y at these different values of x 0, right. And f x y in this case is 1 plus y square.

So, the new value, so basically you have value of f x 0 at this point where x equal to 0 and y equal to 0, so f x y in our case is 1 plus 0 y square is 1, right. And you are trying to calculate the value of y at a slightly farther distance away, at a slightly from this point from this point, right, you are going to calculate what is the value of y when you are displacing from this point. So, this new value of y is nothing, but y which is the value y at x 0 y 0; so in this case it is. For the initial iteration it is value will be 0 plus f x y, right whatever 1 plus y square, y square 0 into d x.

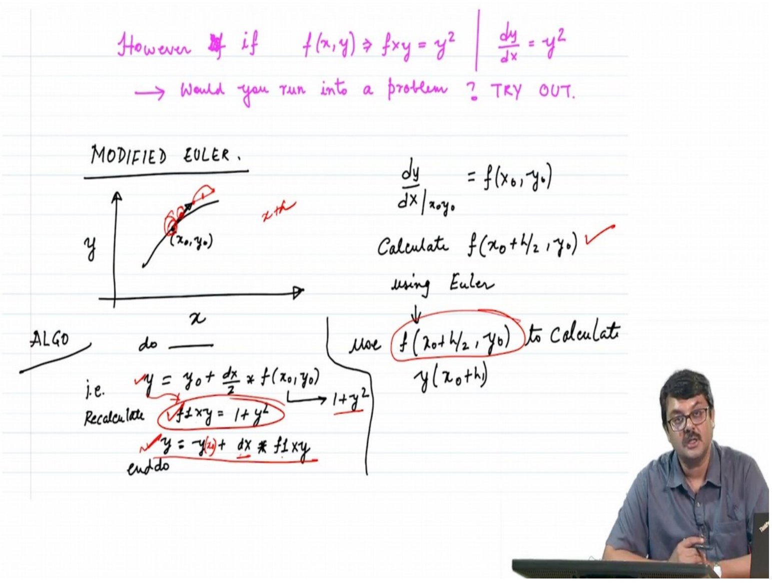
Now, you have a new value of y, right and with that new value of y you are going to again calculate f x y to calculate the new value of y. So, the loop looks like this do I equal to 1 to n iter, you calculate the value of f x y, update the value of y, write it down in a file, suppose you call that file where you want to write it down 21, d float i, you just write the number of iterations into dx. So, you are changing x on the x axis and the value of y and you keep on doing this in a loop. So, basically repeat this in a loop and i into dx is nothing, but x and keep on doing this every time the value of f x y will change as the value of y will change, and you keep on doing this from x equal to 0 to x equal to 1.55, right and then compare, and then compare with the analytical solution and see how good or bad the integration is, right.

Now, this I am already telling you and we shall see it we shall see it in the code what the result of the integration is. Euler, you are just keeping the first term in the Taylor expansion and it does not work very well. Why? Because you are just using this value of f x y to guess the value of y at a slightly far away point from the original point, right. And this slope, and this function could is basically changing like this.

But here you have to take a finite value of the h or the dx and so, you are not calculating this correctly, it will be absolutely accurate only when dx goes to 0; dx goes to 0 to even go move a slight away point you need infinite iterations not very useful, right, you want to have the you want to have a nature of y as the function of x some finite time, not with infinite not with the infinite loop.

So, here the value of f x y is changing, but you are using the value of f x y at this point to guess what is the value of y at the next point and that is of course, not very good. So, what is the correction? What is the better correction that one could do? One says, let me use Euler method not to calculate the value at y equal to y at x plus h, but let me calculate using Euler what is the value of f x y at x plus h by 2 or dx by 2 here. So, use the slope here to guess what the value of y 1 is and that is nothing but the so called modified Euler, right. And in the modified Euler what you do is basically dy dx equal to f, so dy dx at x 0 y 0 is nothing but f x 0 y 0. Calculate using Euler method f at x 0 plus h by 2, right.

(Refer Slide Time: 23:03)



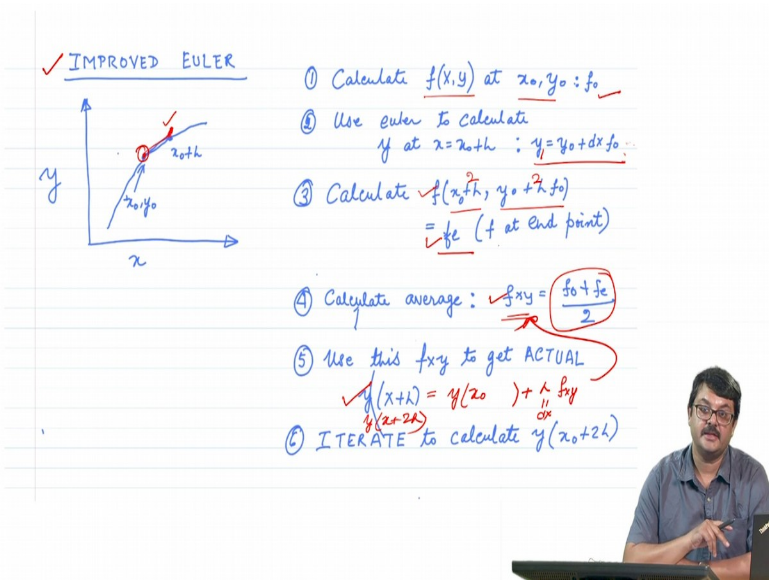
Now, you have a new value of y 1 not at x 0 plus h, but x 0 plus h by 2. With this value of, so with this value of y 1 recalculate f x 0 plus h by 2 and this new value of y 1 that you get. So, what you do is basically use this new value of f that you have calculated at x 0 plus h by 2 and thereby the new value of y 1 that you have to really calculate the value of y at x plus h.

So, what you are doing is basically from here you are moving a small step here half by h by 2, calculating f x y at the value here and use this value this mid value of f x y to move to calculate the value of the new y starting from here. So, what you do is y equal to y 0 plus dx by 2 or h by 2 into f x 0 y 0 which in your case is 1 plus y square, right. Now, with this value of y calculated at dx by 2, you calculate your new f 1 say x y, right, use this value to calculate this.

And your final, your actual updated value of y at x plus h is y equal to y at x 0 plus dx, now you have that entire interval dx into f 1 x y. So, you are basically using the value of f x y calculated here. Previously you were using the value of f x y calculated at this point. Now, you are doing half a step calculating the value of f 1 x y at this point using this value to update and get your new value of y. Keep on doing this.

Now, you have the value of y is suppose here and use this to again take a half step calculate, so take a half step here calculate the new value of f 1 x y, right using this and then from here move to here, which is again this step and keep on doing this. And this is the so called modified Euler.

(Refer Slide Time: 26:27)



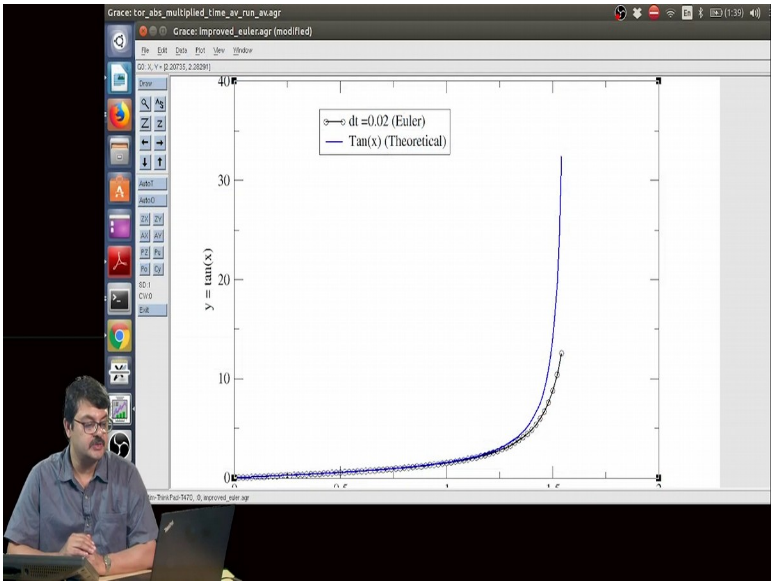
Even better than that is the so called improved Euler. So, what do you do here? You use Euler integration step to calculate f x y at this point then do (Refer Time: 26:41) x plus h Euler method and move suppose here, right. Now, calculate f x y also at this value and take an average. So, calculate, so what does improved Euler entail? Calculate f x y at x 0 y 0, suppose call that f 0 which is basically here. Then use Euler to calculate y at x plus h, y equal to y 0 into dx into f 0 that is your standard Euler method, right.

Now, we have moved, we have your new value y 1, right at y 0 plus dx into f 0. Now, using y 1 recalculate f at y 1 and x 0 plus h, right. So, it is x 0 plus h and y 0 at h f 0 which you have done Euler. Let us call that fe; fe is at the end point, where end point of the step which you have done using Euler. Calculate the average. This is the average slope, is this is this f x y here, and f x y here, and the average of the f x y at this point and at this point, and using this average f x y which is f 0 plus fe by 2 use this to calculate the actual y at x plus h.

So, here you have taken a dummy step, you have updated your y 1 by an Euler step, right, but using this y 1 you basically calculate fe and thereby f x y which is an average of f x y here and here, and using this value of f x y you actually calculate y x plus h which is equal to y at x 0 plus h or dx, I am stretching between these two into f x y which is nothing, but this quantity.

Keep on doing this and this is the one which you want to plot. This is the one which is your actual integrated y at x plus h. And similarly you can repeat this. From here, you again take an Euler step, thereby you can calculate f x y at basically 2h, right and then again calculate the average, and then you can calculate y at x plus 2h and so on so forth, right. Keep on iterating that and you will get y as a function of x and you can compare the 3 cases. That is exactly what we shall do now.

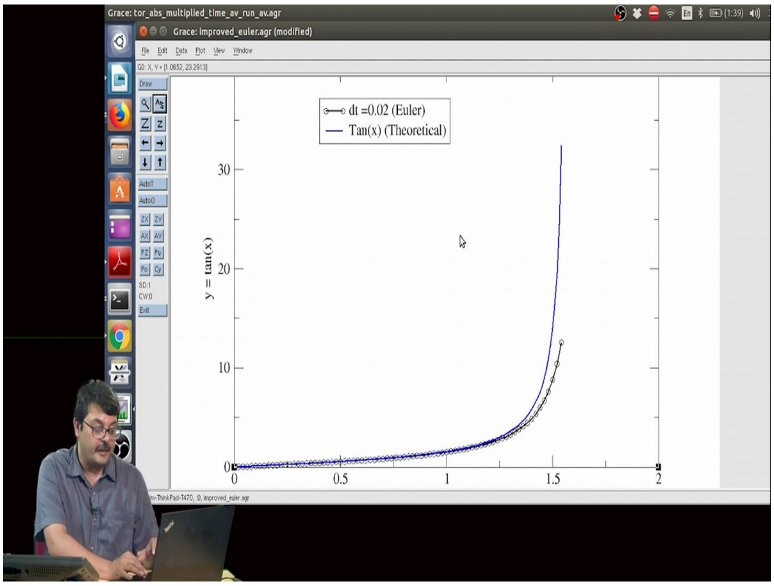
(Refer Slide Time: 29:49)



Now, switching to the computer what I have done is basically already integrated this function dy dx equal to 1 plus y square using the Euler scheme, the modified Euler's scheme and the improved Euler scheme and we shall compare what is the quality of the integration with the theoretical function.

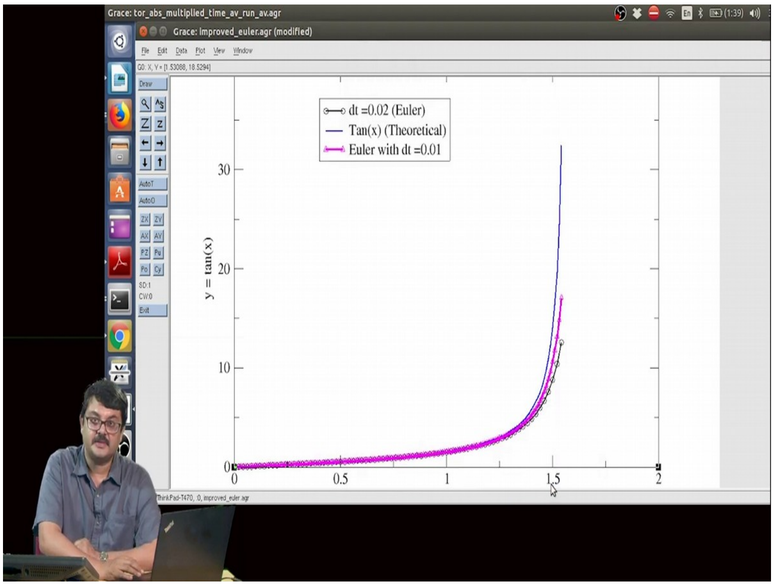
So, here in this blue line we I denote the theoretical tan of x and it of course, goes to infinity as you go towards 1.57, right which is pi by 2. And using the Euler scheme and if you have dx of say 0.02, then basically at these points when x is small there is a very good match with the theoretical curve, right.

(Refer Slide Time: 30:47)



But as you go to larger values of x and in particular when the slope becomes higher one sees a distinct deviation from, so, this is this black curve is the Euler scheme, right and there is a distinct deviation from the theoretical curve. So, you see that the integration here, the solution to the differential equation here at this point for x closer to 1.5 is pretty bad, it does not match, right.

(Refer Slide Time: 31:33)



But what happens if we basically look, what happens if we basically did the integration with the smaller value of this integration this value of h? Right. So, here I have integrated using the Euler scheme, but with dx of 0.01 and you see that well at smaller at smaller values of x of course, this is a very good match this there will be an even better match. But as x approaches 1.5 where the function the solution to the differential equation is sharply increasing while it has improved from the previous case this black curve, but this magenta color curve is closer to the blue curve which is the analytical this is theoretical solution, but it is still not good enough. So, you do not you, have not really even with a relatively small value of h. Yes, it has improved, but not good enough.