Computational Physics
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Lecture – 28
Diff. Coupled Equation Non Linear Equation Part 01

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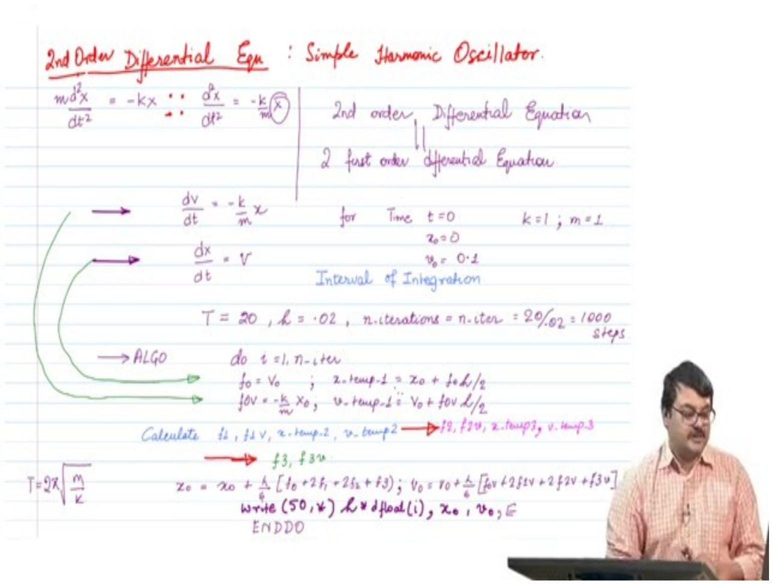

Welcome back. So, in the last class, we discussed how to solve first order differential equations using the Euler, Improved Euler, modified Euler and the Runge Kutta method. And we saw that the Runge Kutta method was better and more accurate by quite some bit. So, basically what we are going to do is focus on discussing say 2nd order differential equation today. And in particular we shall discuss, take the example of simple harmonic oscillator. As I will show you in just 1 or 2 steps that 2nd order differential equation solving it is pretty simple, once you know how to solve the first order differential equation.

Basically the second order differential equation we will be writing it as 2 first order differential equations and solving them in parallel ok. So, let us focus and get into the details. So, suppose that you are asked to solve m d 2 x d t 2 equal to minus k x which is the equation of motion of our simple harmonic oscillator a spring if you like. And of course, this can be solved analytically; but the reason we shall take this example to learn the system and then of course, go over to more complex systems. It is because again that this is analytically tractable, whatever your solution, it can be compared with the exact results and seen whether you are getting correct results. Once you have developed the method you can of course, substitute this minus k x by more complex potentials right.

Now, m d 2 x d t 2 there is a second and there is a double derivative of x with respect to t, that is why it is a 2nd order differential equation and m is mass and that is equal to minus k x; k being the spring constant right. And this equation can be written this m you can write it like this and then you basically this k by m is a constant and that decides the time period of oscillation right and this is your 2nd order differential equation. Now this can also be written as d x d 2 x d t 2; but you know that d x d t is nothing, but velocity V right, that is how you relate it.

But if you just look at it as a 2nd order differential equation and not the velocity V, just a new variable V, right we have. Because here, we our focus is, in general to learn how to handle 2nd order and higher order differential equations. So, just imagine that d x d t equal to V and you can give some physical meaning to V or you can just say, it is some new variable; the first order derivative you call it a new variable V. And then d 2 x d t 2 which is the equation of interest the 2nd order differential equation of interest then you can write that as d v d t equal to minus k by m x. So, this is the first. So, these two equations are two first order differential equations right and from what you learned in last class you can solve each of them in tandem.

And so, basically you will have v as a function of t. So, how does v the first derivative evolve as a function of time, moreover you will have x as a function of time. So, when we were solving this 2nd order differential equation, your aim was when you solve it to get x as a function of time, x as a function of t; if you do not want to ascribe physical meaning to the quantities x and t. So, suppose x is a general variable, right. So, what have you done? By just redefining variables a 2nd order differential equation has been written as 2 first order differential equations. And even if you had a 3rd order differential equation or a 4th order differential equation by a similar redefinition, you can convert a 4th order differential equation to 4 first order differential equation, right. If you had a 4th order then you will say d v d t equal to such and such and then you can define even higher order derivatives in terms of new variables and then you can solve it.

So, what I shall do is basically discuss the aogorithm, this is just our one small step more complicated than the previous equation. Previously you were solving just one equation, now we are going to solve two equations, 2 first order equations in tandem. Now since you have a 2nd order differential equation as you would be knowing from your mathematical physics course to, that you would need two initial conditions to solve it, right; at the moment we are discussing differential equation where the initial condition is given.

So, you need, you shall need an initial condition for x. So, suppose at time t equal to 0 that is the beginning of the interval, at time t equal to 0 x equal to 0 and v 0 equal to 0.1 ok. So, if you want to give physical meaning to it, just say it is that there is a spring, at time t equal to 0 it is sitting at the origin; so there is no compression or extension of the spring if you like, that is the x equal to 0 and then you it has an initial velocity of 0.1 right. And for simplicity you can choose k equal to 1, m equal to 1 of course, you can choose different values of k and m as well and that will basically change the amplitude of the oscillation, it will change the time period of the oscillation given the initial conditions, right.

Moreover since you are solving the differential equation numerically, you have to give the interval of integration. You are going to integrate say, you are going to look at the motion or look at the solution to the differential equation from time t equal to 0 to say time t equal to 20 just as an example. What else do you need to be able to solve it, what is your integration constant, what is not the integration constant; but what is the interval of integration what is the value of h. So, we are going to calculate x at different time points and what is the difference between these two different time points and here you can just say h equal to 0.02 and then you have to do your Runge Kutta iterations.

Suppose you use Runge Kutta to solve the differential equation, you are free to use Euler also; but the, an Euler you will have more errors as you know and we will discuss that and see the examples later. But suppose what is more typical is Runge Kutta is the method of choice, right; and then you have to iterate to calculate x and v at different time intervals if your t equal to 20 and h equal to 0.02. Then the number of iterations which I shall typically refer as n iter; n for number, iter for iterations will be 20 by 0.02 equal to 1000 interative steps.

So, what would the algorithm be, it can be very different from what it was last time. Here the initial condition initial values are given, for the two differential equations as x equal to 0 or v equal to and v 0 equal to 0.1, those are the initial conditions. So, the ALGO will be basically do i equal to 1 to niter number of iterations and at the end there is the n do loop, right. And what do we have to do? We have to and for a first order differential equation, if you are using Runge Kutta, you had to calculate f 0, right. And f 0 in our case from this equation, use this equation and we know f 0 equal to v 0, right ; that is what d x d t equal to v. So, that is what it is.

So, in this case f 0 equal to v 0, then you take small predictor step, you try to evolve the system. But of course, store that in a temporary variable because you want to calculate the slope of Runge Kutta at different points and then average it over, as we if you remember. So, x temp 1 is x 0 right you have the value of x 0 here and the temporary value of x 1 when it is when the position is moved ahead for a time h by 2 is nothing by, but x 0 plus f 0 h by 2 you have calculated f 0 here from this equation.

But now, you have another first order differential equation and that has to be solved in tandem. So, rather than just f 0, you shall also have f 0 v corresponding to this equation, right. So you have f 0 v which is nothing but, minus k by m x 0 right; x 0 happens to be 0, but it could also be any finite value, right; it is basically x at time t equal to 0 and then you evolve v for time h by 2. So, v temp 1 equal to v 0 plus f 0 v into h by 2 having got that, you can calculate f 1 which is basically the values of f 0 and f 0 v using this value and this value. So, you can calculate f 1 and f 1 v, with that you can calculate x temp 2, right.

And similarly v temp 2 then and that is also over a interval of just h by 2. Using that this position and this value of v you can calculate f 2 v, f 2 and f 2 v; using that you can calculate x temp 3 and v temp 3 those are again temporary values of the variables, right. Using which we again calculate, f 3 and f 3 v; this was discussed in great detail in the last class, if you have any confusion please refer to the end of the last class. And once you have f 0, f 1, f 2 and f 3 and similarly f 0 v, f 1 v, f 2 v and f 3 v, then we can do the actual update of the position or the variable x; and similar which is nothing but x 0 the previous value x 0 plus h by 6 f 0 plus 2 f 1 plus 2 f 2 plus f 3.

And similarly the new value of v 0 this is not now the this is not this v 0 is not anymore, the initial velocity; I just updating the new the new value of the velocity after time h using Runge Kutta is nothing, but the previous value of v 0 plus h by 6 and this formula, right very similar to this. So, what have you obtained? You have obtained both the updated position and the updated velocity at time t equal to 0 plus h, right. Now using these values of x 0 and v 0 which are calculated at time t 0 plus h, you can do exactly the same thing and calculate the position and velocity at time t equal to 0 plus 2 h and so on so forth, up till the end of the interval.

After you have done this step one iteration, you can basically write down the time of integration h into d float i; i shall run from 1 to 1000 and write down the position and velocity at each of these times. And once you have written this, once the program has finished running, you can use these quantities and plot them to plot x versus t and v versus t, right. And you know how it is going to be it is going to be basically sin and cos curves, because you know the solution to this differential equation; it is a periodic motion, it is a spring after all.

Moreover what can you calculate and use it as a test to validate whether your simulation is working correctly or not? You know for a spring there are some conserved quantity and in this case it is the energy, right. So, while you are solving the differential equation you are also taking the help of physics, the background knowledge of physics to devise tests, to assure yourself whether you have done your calculation correctly or not, right. And for the simple harmonic motion, you know that there are there is a constant of motion called the energy, half m v square kinetic energy, plus half k x square the kinetic energy sorry the potential energy, right. And so, we can just plot the total energy as a function of time if you like, write the energy here and plot energy is a function of time; and if you are doing your simulations correctly it should be conserved, right

So, now let us see that. So, this is the algorithm for Runge Kutta and of course, you can do the same thing using the Euler method and the modified Euler method and the improved Euler method and so on so forth. So, what we will discuss in a practical example, I shall show you what is the kind of solution that you get. If you use the Euler method; and how would there is creep in and then do the same show you the data for Runge Kutta. And what you should do is basically implement it on your own, so that you assure, that you are able to solve a simple at least 2nd order differential equation with full confidence. And once you have done that of course, we shall go to slightly more complex problems, you will make this x, suppose a non-linear function; but let us first look at the solution to this differential equations ok.

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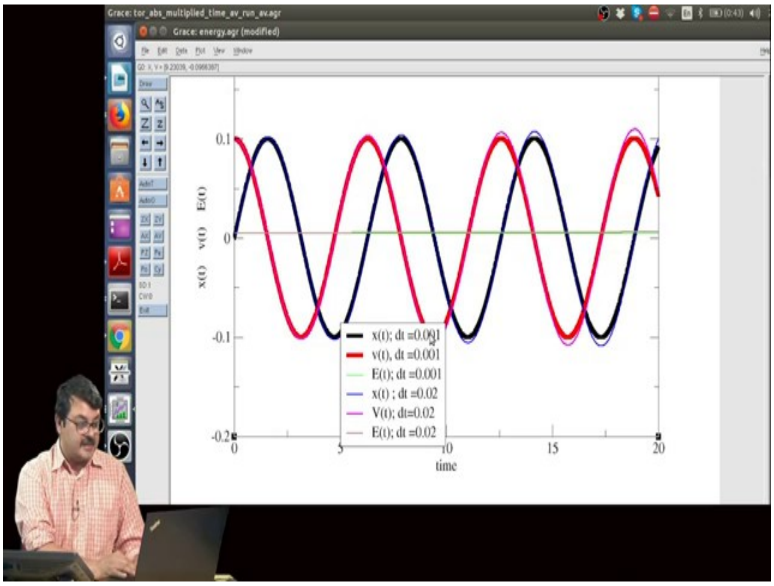

So, what I have plotted here is x as a function of time, velocity as a function of time and energy as a function of time. So, this is what is there on the x axis and the legend explains what these different colored graphs are, and on the x axis you have basically time. So, y has all these quantities, right. And this has been solved using a simple Euler method, with velocity equal to initial velocity equal to 0.1, I just as discussed in the notes, right.

Now, this black curve is the Euler method, with d t the integration constant or h if you like is 0.001, right and what do you see? So, if it is position, position was 0 at time t equal to 0, position is 0 here; and this is black curve, where did the blue one go. And you see that basically the position increases and then decreases and increases in an oscillatory motion ok, hardly surprising. And what does the velocity do? The velocity is the red curve and in case you cannot see it, I will just make it thicker; velocity was 0.1 at time t equal to 0 it is 0.1 and as thus basically the position changes, it goes away from the equilibrium position the velocity slowly become 0 and then they and then it becomes negative and so on so forth.

So, these are the two position and velocity as a function of time, there are of course, out of phase with each other and you can see if you that the period of oscillation when k was equal to 1 and m equals equal to 1. So, that k by m is 1 essentially that the time period is 2 pi, right. So, you can just check for yourself that this position is 6 point approximately, equal to 6.28 as it is expected. Now I have done this integration with 0.001, here I have also plotted the energy in this green line and we will discuss energy in further detail.

Now, just for comparison, I have also done the Euler integration with h or d t equal to 0.02 which is much higher, right. And what do you see? Of course, the initial part of x versus t and V versus t are exactly same as what was obtained, when x when the d t was 0.001. But at longer times say here, you see that the x with d t equal to 0.02 is this blue curve and you see deviations ok; you see deviations from what was plotted when d t was 0.001.

Similarly, when h equal to 0.02, the velocity it again shows deviations. Which one is correct? Well at least you know that; you know the velocity should be, I mean the peak of the velocity should be constant, the energy should be constant, the total energy should be constant.

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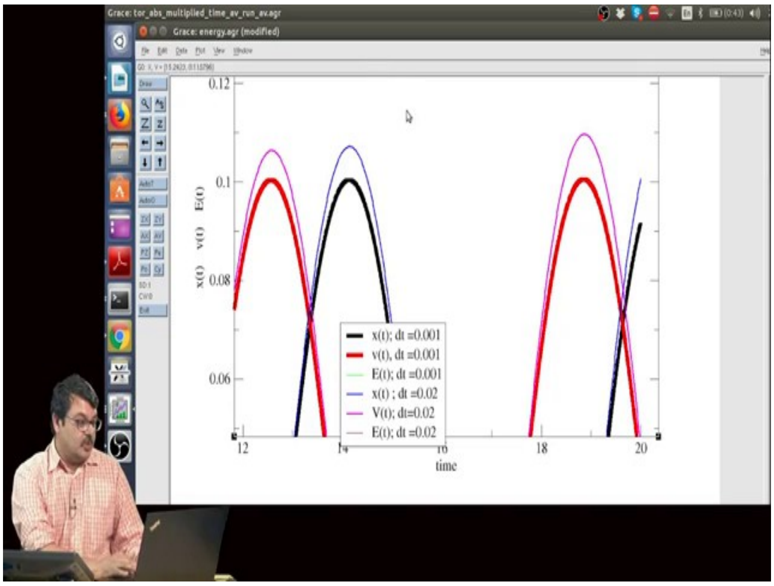

And you will see that when you had used up h equal to 0.001 or d t equal to 0.001, the peak of the velocity always remained 0.1 oscillatory motion; kinetic energy to potential energy, potential energy to kinetic energy.

But when you are using a higher value of h, you are getting an error, the initial this peak of the velocity is growing higher. So, these; obviously, the integration is not being performed in a good enough way, though it is difficult to see; but at longer time so, an initial times, they fall on top of each other. But at longer times just 3 or 4 oscillations and you see deviations and the integration is not being done accurately for higher values of h. But that is not surprising, as we discussed in the last class that in Euler method, the error right the local error; the local the error at each integration step goes as x square and over the entire interval it goes h, it increases the linearly with h and that is exactly what you are seeing, so hardly surprising.

What about the value of energy?

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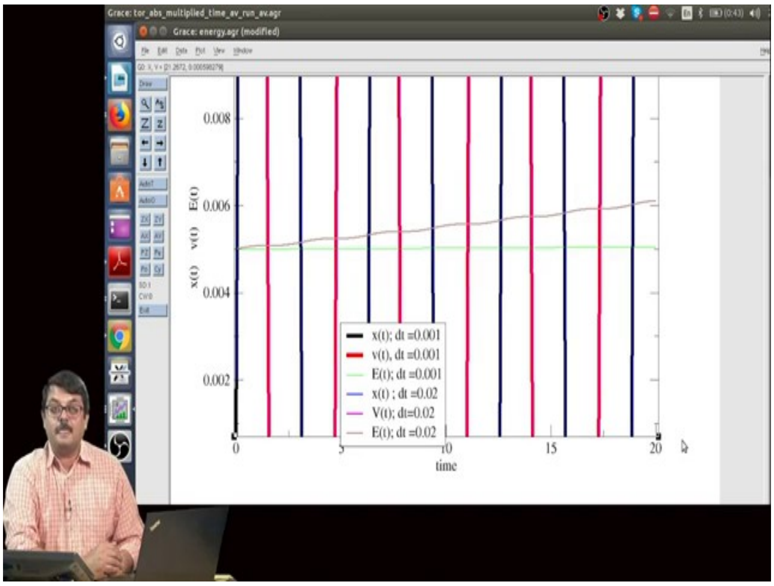

So, here I am just blowing up the value of energy, right. And you know what should be the value of energy, at time t equal to 0 there were was the position was 0 and it had initial velocity. So, the kinet[ic]- and. So, the total energy was essentially kinetic energy half m v square; v being 0.1, 0.1 square 0.01 and half of that is 0.005; and that is exactly what you see at time t equal to 0, right. Now energies should remain constant as position and velocity exchange in their amplitude kinetic energy to potential energy and you can see that energy with time d t equal to 0.001 remains nearly constant; well nearly constant even this has shifted a bit right, here you can see the ideal it should be exactly here 0.005.

On the other hand d t equal to 0.02, there is a clear and distinct increase in the energy consistent with what you saw that x was gradually increasing out of the peak position of x was gradually increasing. So, of course, again, I am emphasizing that Euler is not a great method it works; but you have to use very small integration intervals right, the value of h has to be 0. Now if you did the same, now suppose we did exactly the same calculation with Runge Kutta right with h equal to 0.02 it is a much higher interval, you have to take only 1000 iteration.

On the other hand if you had 0.001 to run for time equal to 20, right; the number of iterations you would need is 20 pi 0.001 that 20000. So, 20000 iterations when you have d t equal to 0.001 for a time range of 20; on the other hand just 1000 iterations when you have d t equal to 0.02 and let us see how the Runge Kutta does.

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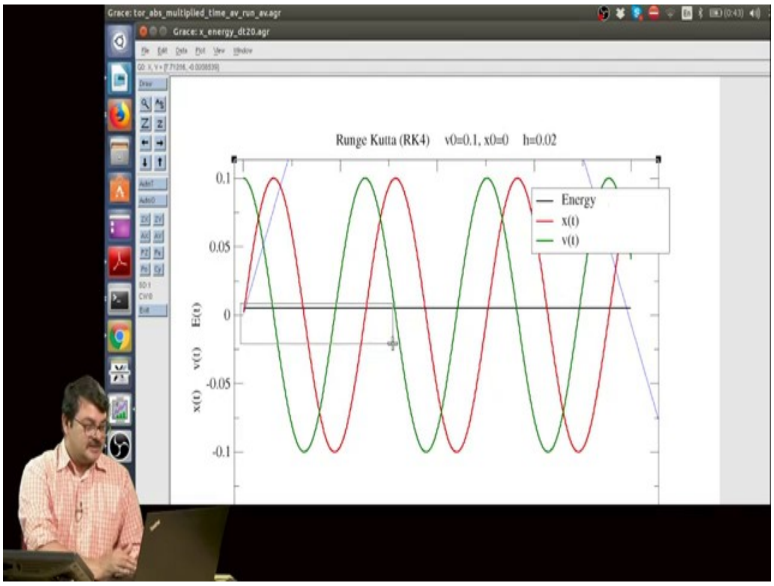

So, here what I have done is plotted basically x versus time, v versus time and energy versus time exactly as previously, no difference a with v 0 equal to 0.1 and x 0 equal to 0 and h equal to 0.02.

The x axis is labeled time, right. Whenever you show graphs, please do label axis ok. You cannot have a graph where the axis's are not labeled; so you do not the viewer does not even know, what is being plotted, right. And energy is plotted in the black, in the black line x versus t and v versus t in red and green lines, respectively. What do you see? Well you can see that, especially if you blow up the energy with even this larger value of h, h is equal to 0.02 over the range the energy is perfectly within the range that we are looking at compared to Euler constant, right.

So, it is much more accurate, hardly surprising because Runge Kutta is supposed to be much more accurate than the Euler scheme, right. At each step, integration step you are making a error of h 4 and the global error in the entire range will be h cube, right. So, you will see that it is not exactly constant only at 0.02 to the power 3; so basically 10 to the power minus 6. So, if you blow up this energy data to 10 to the power minus 6, then you will be seeing that well the energy is not perfectly conserved because i the error in the energy will be only at that scale, right.

But within the scale that we are looking at, it is perfectly conserved, you can go to smaller and smaller values and you see it is perfectly conserved.

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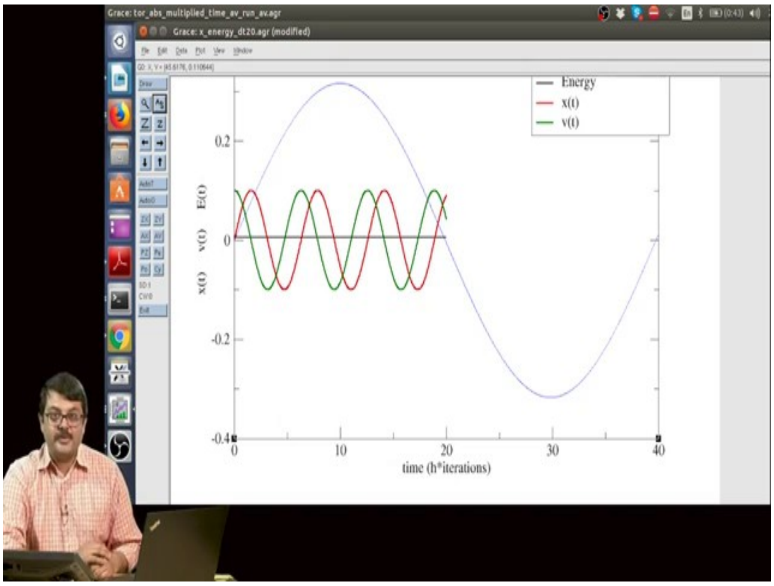

What happens if we change Kappa say, suppose you changed Kappa equal to 0.1; what do you expect, you already expect, you know that the spring constant that time, the time period of oscillation is going to change. This blue line is just been tried out with kappa equal to 0.1 and you can see that, basically the time of oscillation will be significantly more, right. So, that is all that we have done.

So, what is the message? The basic message is the Runge Kutta is working pretty well, we have demonstrated it, we are solving a 2nd order differential equation; you can fit your sin omega t with where you can calculate omega, cos omega t and see that it will matches and that you are getting a good result with your Runge Kutta, ok. So, having got you have to implement this and after that having got confidence in this, let us look at a slightly more complicated problem.