Computational Physics

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

Lecture – 29
Diff. Coupled Equation Non Linear Equation
Part 02

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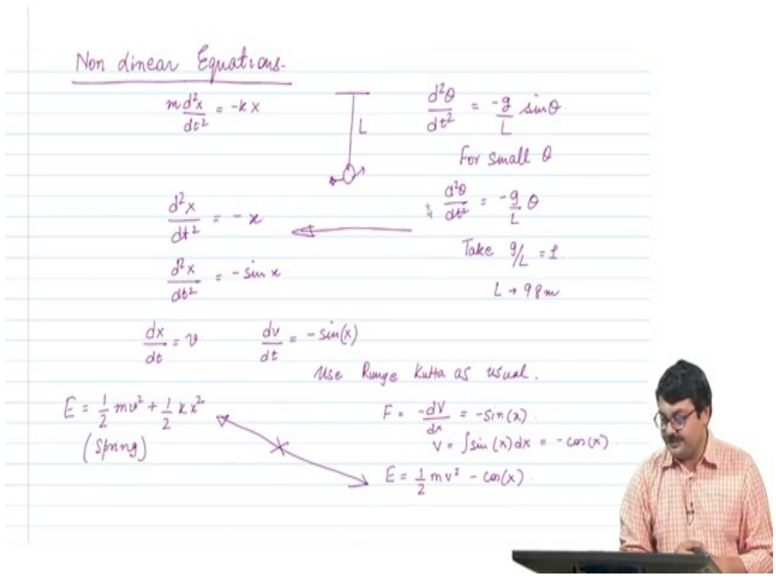

So, the complicated problem that I have in mind is again system which is very familiar to you which is basically the pendulum right. Basically you take a blob of mass suspended by a thread it is fixed here and do not suspended by a thread, but by a suppose a rod, you will soon know why I am saying that and basically the thing oscillates like this right and what you do. So, basically the equation for such a pendulum is d 2 theta dt 2 equal to minus g, g being the oscillation due to gravity 9.8 meters per second.

L being the length of the beam and d 2 theta dt 2 equal to minus g by L sin theta right you can just look up your classical mechanics book and you will get the derivation of this. What do you do? We often say oh for small theta sin theta equal to theta and we write down the equation as minus d 2 theta dt 2 equal to minus g by L theta which is nothing, but again the equation of a spring right. So, basically there is a 1, 1 to 1 mapping with this, this is for small oscillations it goes periodic oscillations or of course, you have neglected friction. The friction due to a and you can put that in also since now you know how to solve equations 1 plus y square that the n square that was a non-linear equation right anyway.

So, for this you have which is just equivalent to this put g by L equal to 1. So, we have nothing except this equation similar to this equation where k by m was equal to 1 and we have done the solution, but this, but the small oscillation case one can do easily analytically there is no problem right, but what would happen if you actually kept sin theta you did not have. So, if you had large oscillations then you cannot work with this equation right, then you have to work with this full equation because you cannot take the approximation of sin theta equal to theta.

Suppose the pendulum was like this right you give it a large kick. So, that the theta will be large, then you cannot find its motion by the simple harmonic or the sin theta equal to theta approximation which will convert it to the equation of a spring and now you can analytically you do it. So, we want now to solve for the full equation sin theta as you would know can be written as x minus x cube by 3 factorial and so on so forth, it is a highly non-linear function.

So, basically what are you doing? You are solving a second order differential equation non-linear right with all the complexity. What will you do? Well, the equation instead of this now becomes this right d d 2 x dt 2 equal to minus d 2 d 2 x dt 2 equal to minus sin x I have just written for in terms of x change the variable from theta, because in general we are learning how to solve non-linear differential equation right. And now, this is the operating equation and just like we wrote down a second order differential equation.

We broke it down into 2 first order differential equations. So, now, these are the 2 so, the first derivative you define by some new variable v right, where in this case you can give a physical meaning dx dt equal to v the velocity, but in general you might not need to or might not want to and dv dt equal to minus sin x right. And, now basically what changes is nothing, but the value of f 1 f 0 v and then f 1 v where we were previously using minus x now it is minus sin x. But, suppose you give the same initial condition as before then you can easily solve this you get the solution of this these two equations x as a function of t, and v is a function of t for the same initial conditions say right.

Now, here I want to say something, now you know even before trying to look at the entire solution you know that for small x sin x equal to x. So, even if you solve this equation in full glory and suppose was v equal to v the initial velocity right was some small number 0.1 or

0.01 right that is a small velocity. Then of course, though you are solving a different differential equation, but since sin x equal to x for small x and basically the system will deviate away from it is equilibrium position the pendulum will deviate away from it is equilibrium position by a rather small quantity.

So, you know that the solution will be very similar to what you would get if you had used d 2 x dt 2 equal to minus x and in fact, first of all since sin sin x is a unknown problem to you right a solution we can not exactly envisage, you should plot, you should do the solution with a very small perturbing term v equal to 0.01 or even smaller and see whether you are getting the same solution that you would have got when you had solved the previous equation right.

Now, once you have done that and you are assured that your Runge Kutta scheme is working perfectly even with having changed just one term f 0 v n f 1 v n f 2 v this has to be the new those are the only things you have to replace. You can start playing around so that you give a higher kick. So, basically you have a pendulum you are giving it a higher initial velocity. Of course, you are free to also give x 0 to some finite value 0.3 or whatever as well as v 0 those are your choices the here the initial conditions are your choices right.

But after checking that only you should do that and now you can have a look at the solution of how this pendulum moves actually x as a function of t and v as a function of t in it is full glory, moreover you have access to the energy right energy should be conserved. There is a one small detail to be careful about previously you were using the expression of energy equal to half mv square plus half kx square half kx square is the potential energy when the force is minus kx. However, now the force has changed to minus sin x right and so, the expression for the potential energy is not half kx square anymore, but minus cos x.

So, the total energy of the system will be half mv square minus cos x that is the integration and that is the thing which is conserved and you should of course, even for large amplitudes this should always hold and you should check that out right. So, I will leave it to you for you to check the solution x versus t and v versus t for small kicks small values of v 0 the initial velocity.

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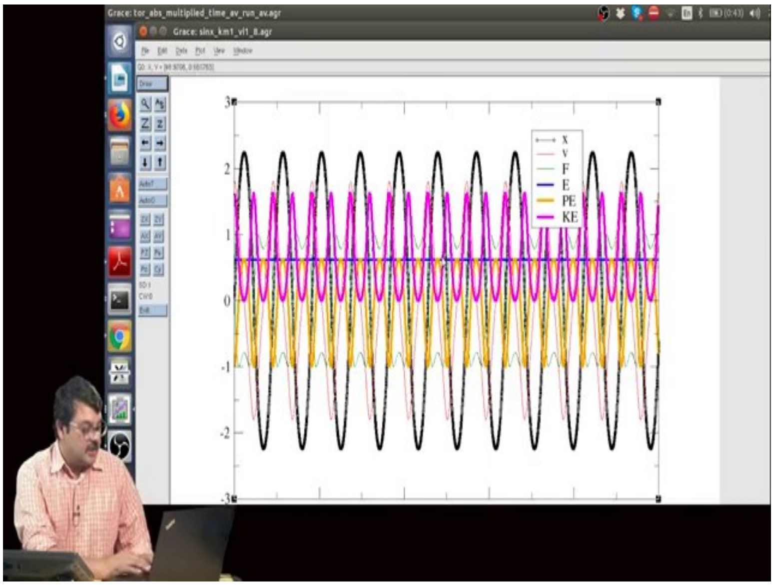

So, here what I am going to show you is the Runge Kutta solution where I plot x v and then energy and the potential energy and the kinetic energy as a function of time where I have given the initial kick v 0 to be 1.8 right, x 0 remains 0 at t equal to 0 and what you see is x of course, oscillates there is this black curve, the red curve is the velocity.

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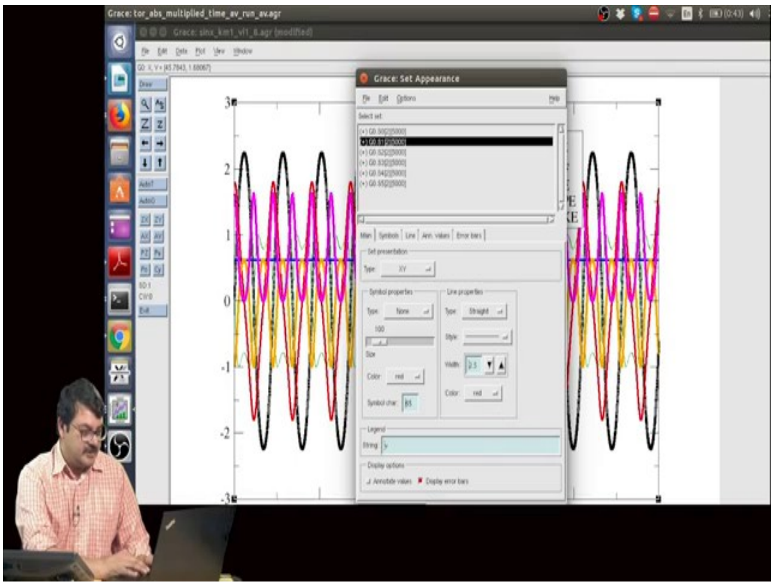

So, that you can see clearly let me.

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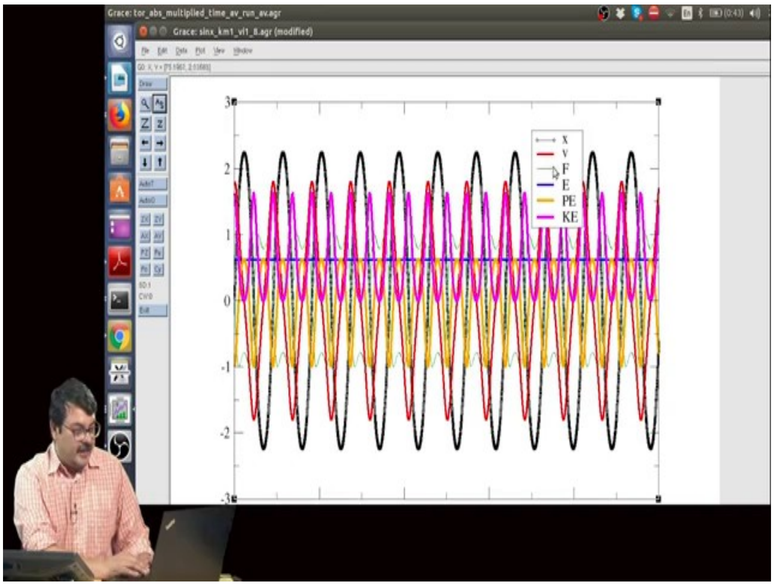

So, that also is, but it is not a sin curve anymore right previously x versus t and v versus t where sin and cos functions, but it is not.

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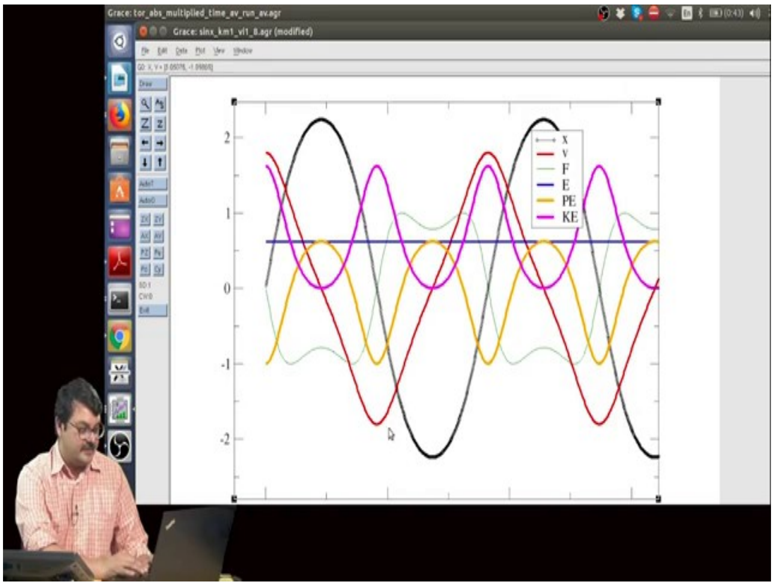

If you look carefully if you blow up or you can see that you can see easily see some deviations right this is a relatively straight line and similarly you can fit to it and check right. And that the blue curve is the energy which is conserved as it should be thankfully else you should be worried.

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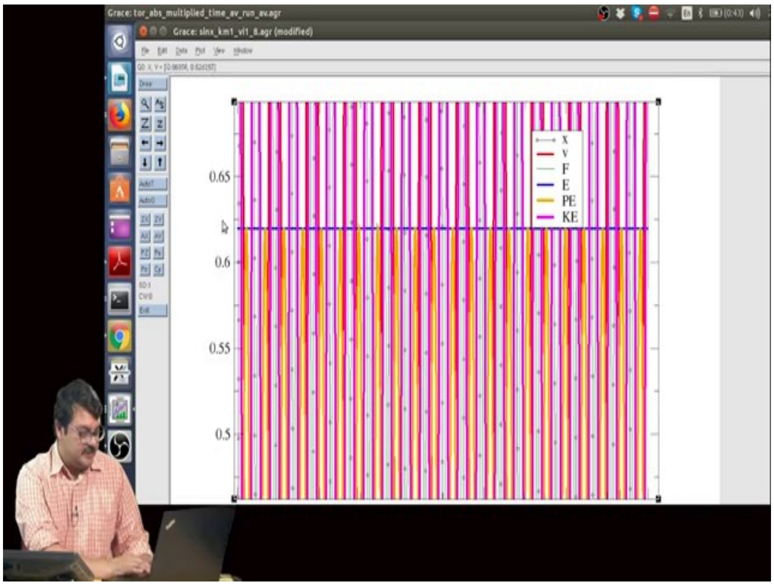

So, this blue curve is the energy it is completely conserved with the right expression for the potential energy and I have plotted the potential energy in the kinetic energy as well and then you can plot it and analyze it and convince yourself about it.

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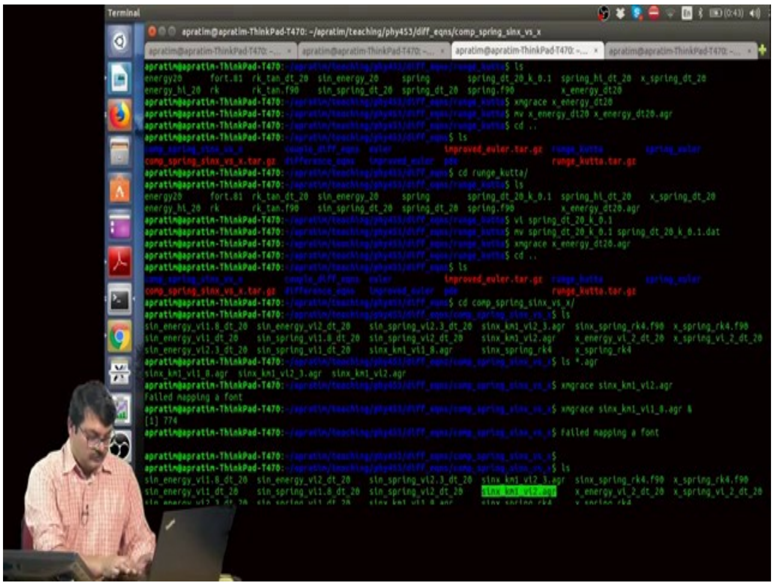

But then what you could do is also give.

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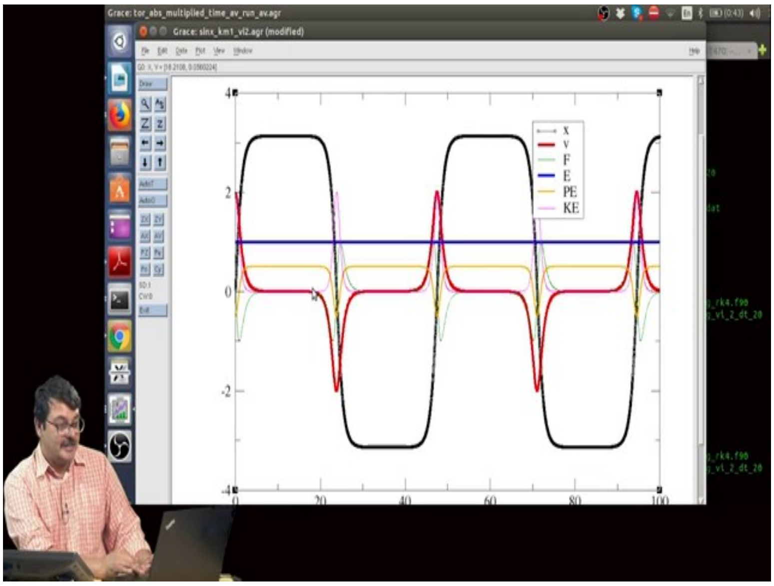

But then you could also give the initial velocity v 0 to be 1.9 and maybe 1.99 all right and give it 2 and exactly 2 and then you will see that x is basically see the range of time over which I have integrated is 100. So, that is a pretty long time you were having many oscillations if you remember in at even 24 and time t equal to 20 because the period of oscillation was 6.28. But here I am integrating up till 100, but x is increasing, but remaining flat for a very long time and then coming down again that is an oscillation, but is it is nowhere close.

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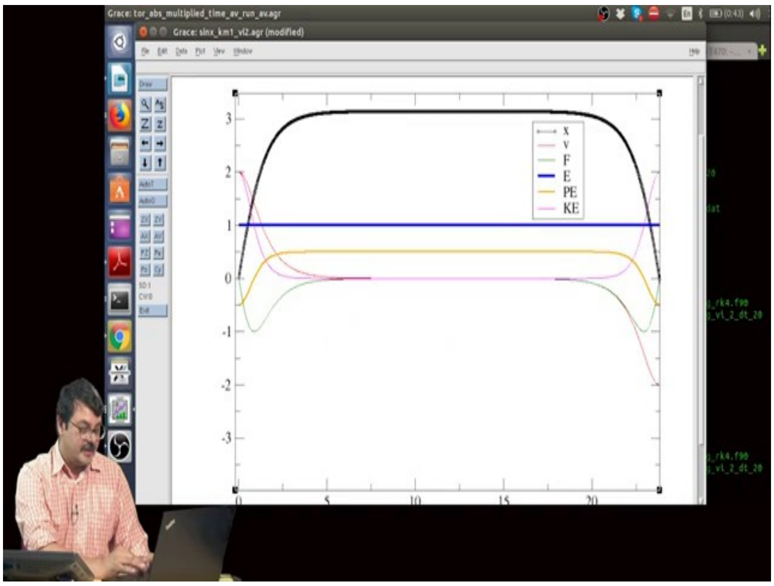

So, if you plotted it over a range of say 20 right, you would see that the position starts from 0 go increases because you have given a finite kick, but then it remains flat means there is hardly any change in x, can you physically visualize this. This is basically this case suppose this was a pendulum and you gave it exactly the kinetic energy. So, that it would overcome the kinetic energy is just enough and it will overcome a potential energy and if you give it to the right velocity at this point all the kinetic energy has been converted to potential energy if it has been exactly equal it would come here and stay as an equilibrium position.

But here it s velocity will be very low right and if you give your initial velocity for k and m equal to 1 if you give h to b 2 or 1.99 then it has just enough kinetic energy to overcome all the potential energy, but here it starts to move very slowly till it decides to return back right and that is exactly what you see. So, it is basically x as increased or theta has increased if you like 3 to 3.14 pi and then it remains at that angle for an extremely long time compared to previous time previous case when you were doing simulations where the d 2 x dt 2 equal to minus kx, this you will see only for sin x and then it again decides to go back.

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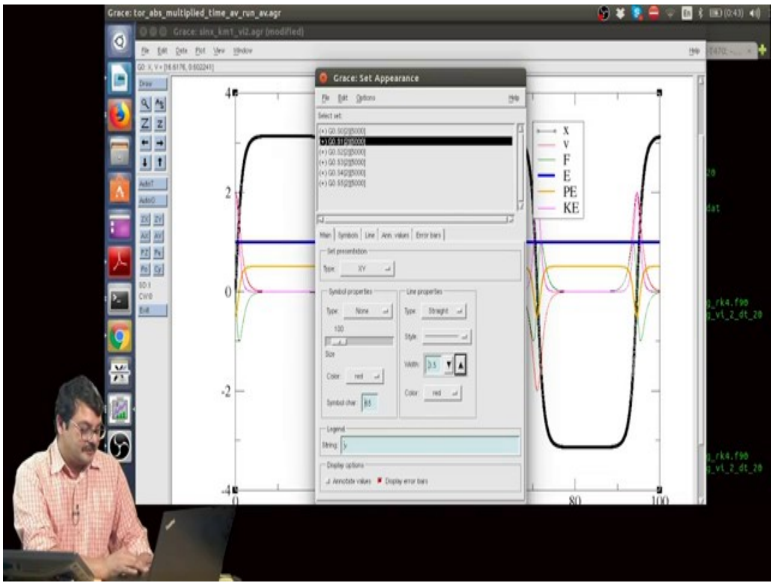

And, correspondingly the velocity you would see and this is this red curve and you should check it out for yourself, remains nearly 0 for a very long time right and then it goes to the other side velocity becomes negative right and so on so forth. So, check this out and I will also show you what happens then you give a kick v 0 at the initial time t equal to 0 is say 2.3.

And, then what do you expect you expect the pendulum to go round and round and do you get that solution let us check.

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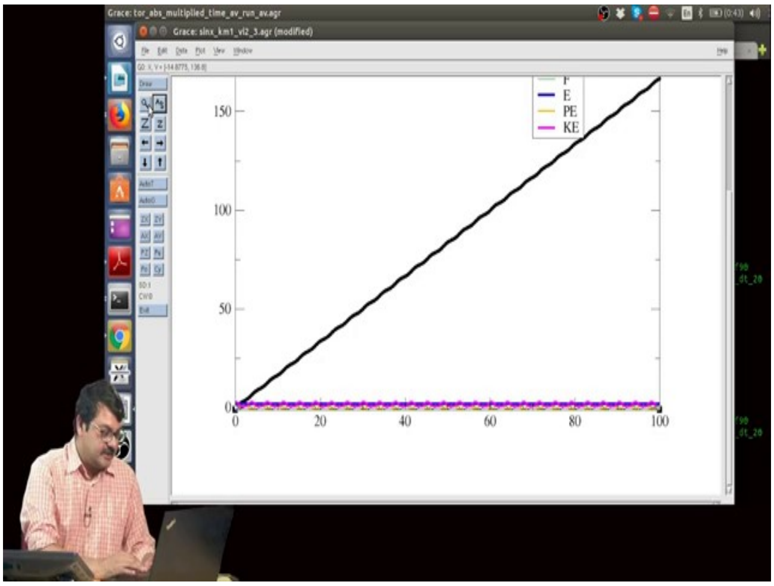

So, x I have integrated to hundred what you see is x is constantly increasing and what; that means, or if f axis theta it is basically covering and then going like this continuously so, theta x keeps on increasing right. On the other hand as the pendulum goes from here to here it is potential energy would increase, here the kinetic energy would this position would be the maximum, those will keep on going in oscillations increasing and decreasing, that is exactly what you see here.

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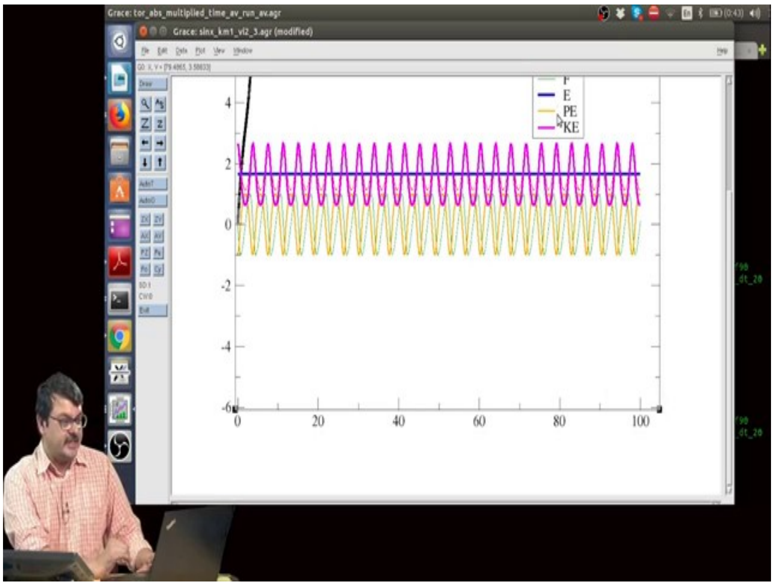

Where this orange line is the potential energy, the magenta line is the kinetic energy and total energy is conserved as before even over larger integration scale of integration time t equal to 100 right.

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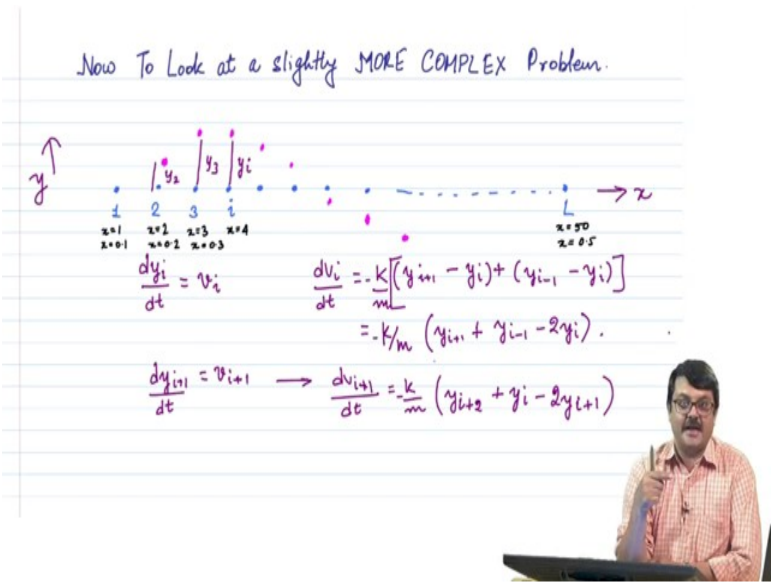

So, now to look at a slightly more complex problem, till now what have you been looking at is so, there is one particle and it has it had a spring interaction so, you were updating it is position and velocity and later what you did. I mean instead of the spring you instead of the spring for which the force term is minus kx you basically substituted it by minus sin x right.

So, it is still a one particle problem, now instead of a one particle problem look let us look at a n particle problem, what would be the physical picture in mind vibrations of a string we have all studied in class about the vibration of a string and what happens suppose there is a straight string like this right.

And then suppose you pluck it and then the entire spring vibrates and you have studied about normal modes to analyze the problem. Now, suppose you wanted to know the position of each of the points on this spring right and you wanted to know it exactly of course, there is a toy problem to learn about coupled differential equations, but suppose you wanted to do that to do it computationally what you would do is discretize the positions of the particles on the string.

So, now suppose basically what you have is, this is the string like this along the x direction and you have various particles fixed at discrete points along the x direction. So, this particle number 1, particle number 2, particle number 3, particle number i say which is on the left hand there would be essentially i minus 1 and i plus 1 and there is L particles L could be 50 suppose right. And they are fixed at positions x equal to 1, x equal to 2, x equal to 3, x equal to 4, there is nothing only about these positions because the x position is not changing, you could as well put them as x equal to 0.1, x equal to 0.2, x equal to 0.3, it is thus just this x direction different points along the string.

But what makes these particles move is the displacement in the y direction which is so, this is your string you have plucked it suppose and now it will start vibrating. So, along the y direction the position of each of these particles will go up. So, suppose to x at a certain instant in time suppose particle number 2 has been displaced to this magenta color this position, particle 1 has still not moved, particle number 3 has moved here and particle number i has moved here and so on so forth right.

So, then what would be the equations of motion well, it will be basically I am writing a second order differential equation Newton’s equation into 2 first order differential equations hence just as before dy i for the ith particle dt equal to v i the velocity of the particle i and the force equation is this dv i dt dv i dt is the acceleration m into dv by dt equal to force equal to minus. So, k by m right and the distance in the y direction so, if this is y 3. So, y 3 minus y 2 that is the force acting on y 3 essentially and whatever and it is other neighbor.

So, this might so, because of there is a spring here minus kx types right. So, y 3 will feel a force in this direction in the minus y direction due to y 2 whereas, if this particle is at higher up in the position y 3 will feel a force in this direction the positive y direction due to this particle right. So, that there is how it works and that is exactly what I have written that basically the force dv i dt will be y i plus 1 minus y i. So, y i plus 1 minus y i and y i minus 1 minus y i so, because there are 2 neighboring particles to the ith particle so, the difference in position and the values of y i plus 1 and y i it could be negative also right I mean. So, in some case it could be negative or positive and that will take care of the direction of the force.

We just have to write down the equation properly discretize it and the direction of the force will automatically be taken care of right and this can be written of course, simplified into minus k by m y i plus 1, y i minus 1 and minus 2 y i. So, I m just written the equation and this is for the ith particle. Similarly you will have a equation for the i plus 1th particle which in turn. So, this equation depends only upon the value of vi plus 1 the velocity of the particle, but here for this the i plus 1th particle the velocity of the ith i plus 1th particle depends upon the position of not only i plus 1 but also upon i plus 2 and I and I just like here the velocity of the ith particle depended upon the position of the ith particle as well as i plus 1th particle and i minus 1th particle right.

So, what so, this is the point is that the equation of motion of the ith particle depends upon the position of the i place 1th particle and y i minus 1th particle. Similarly the velocity of the next particle depends upon it is neighbors so, this is essentially a strongly coupled equation right it is a coupled equation and that is why in your classical mechanics normal modes analysis class you did a normal mode analysis to make it a uncoupled equation. But suppose you want to do it in real space and you want to solve this equation. So, you are essentially solving right if there are 50 particles you will have essentially a differential equation for vi equal to 1 to 50 right.

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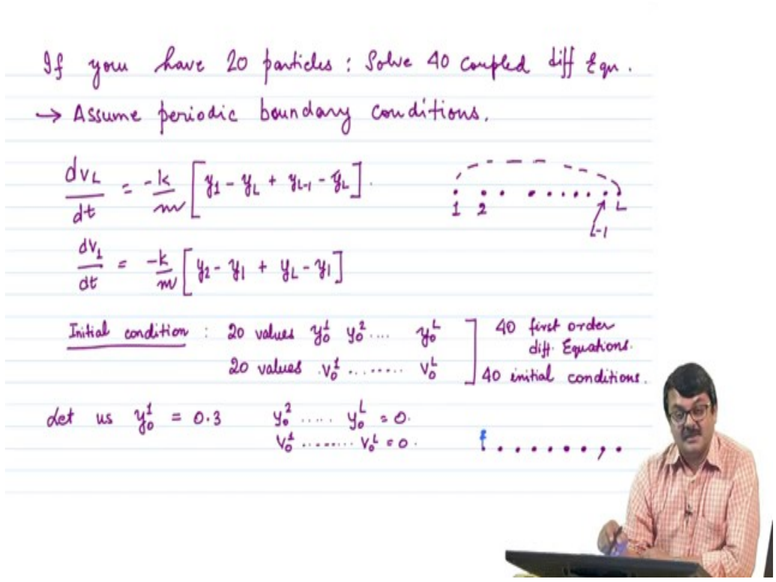

So, essentially you will have 100 differential equations. So, if you have 20 particles, you will have 40 coupled differential equation because v 1 depends upon the position of the second particle. The velocity of the second particle depends upon the position of the first particle and the third particle and each and the position it is itself is governed by a differential equation right position itself is governed by a differential equation. So, this is a coupled differential equation.

So, essentially you have to solve a set of equations right second order converted to first order double the number of first order differential equations and if you have 20 particles you have 40 coupled differential equations, 20 for the velocity coordinate of each particle and 20 for the position coordinate of each particle right. Moreover to simplify the problem what you could do is assume periodic boundary conditions of course, you can do it with fixed boundary conditions also, but let us assume periodic boundary conditions that will make the things like a little simpler.

Because, now the first particle will not only feel the force from it is neighbor, but the first particle will feel the force from the L th particle right. So, each particle will have 2 neighbors essentially if you did not have periodic boundary condition then the first particle and the last particle would interact with only 1 neighbor right. Whereas, of course, 2 3 4 5 6 they have all 2 neighbors, 1 neighbor on the left and 1 neighbor on the right, but the first particle and the last particle would not have neighbors if you did not have periodic boundary conditions.

So, by assuming periodic boundary conditions I am actually simplifying the problem that the first particle has a neighbor in 2 or the other left neighbor is then L. Similarly the L th particle the last particle along the line would have the left neighbor as L minus 1 whereas, the whereas, the right hand neighbor would be the first particle right. So, then basically there are corresponding differential equations would be something like this dv L dt for the L th particle would be minus k by m and y 1 minus y L right because it is a right hand neighbor is y 1 plus y L minus 1 minus y L right this is the left neighbor.

And similarly the differential equation for the first particle will be slightly different minus k by 1 y 2 minus y 1 plus y L minus y 1 and for the other particles of course, it is much simpler right. So, I mean I have already written it moreover what do we need we need the initial conditions, but now you have if you have 20 particles you have 40 equations. So, you need 20 different initial conditions 20 different values y 1 0 y 0 2 y is 0 l and so on so forth for the initial positions of each of these particles and similarly the 20 initial velocities of each of these particles right.

So, that is not surprising you have 40 first order differential equations you have 40 initial conditions now suppose let us simplify and say that only the first particle has been displaced by say 0.3. So, x remains the same, but the first particle has been displaced that is the initial conditions say has been displaced by 0.3 the position of all the particles along a line is 0 similarly the velocity of each of these particles is 0. So, basically along a line along a line only the first particle is displaced, but this is going to pull the particles on it is left and right.

So, it will feel a force so, the second particle will start moving the second, if the second particle starts moving the third particle will feel a force and will it will start moving and similarly you will finally, have something like the vibrations of a string all right. So, that is what we are trying to model though our focus is basically solving 40 different coupled differential equations.

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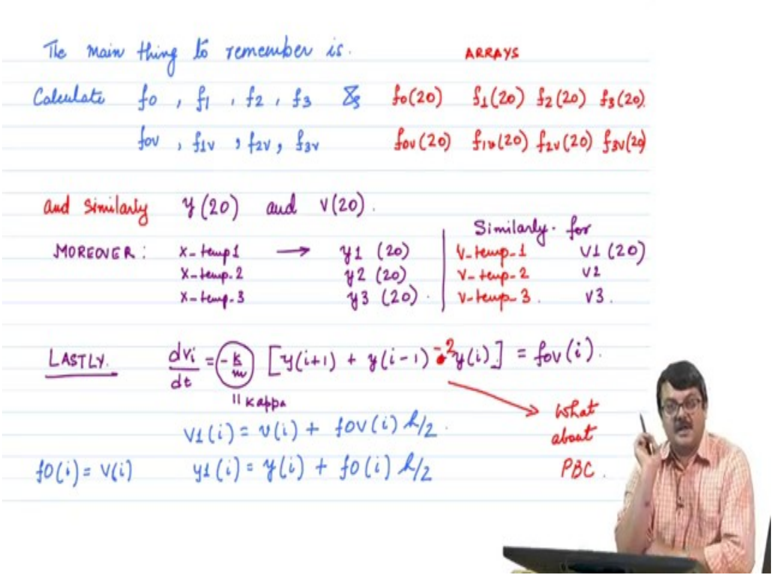

But now previously when you are solving 2 different initial equations using the Runge Kutta method you were calculating f 0, f 1, f 2 and f 3 and similarly f 0 v and f 1 v and f 2 v and f 3 v. Now, you have 20 particles so, that so f 0 v will be now be an array because you have to calculate f 0 for each of the 20 particles. So, f 0 will go into f 0 an array of length 20, f 1 will again be an array of length 20 f 2 will be an array of length 20 and so on so forth. And similarly for f 1 v because for each particle you have to update both the position and velocity those are 2 differential equations right. Now there will be one f 0 v and f 1 v and f 2 v and f 3 v what each of these 20 particles.

So, basically what you have is so, either so, if you have 20 particles each of these becomes an array of length 20. Similarly previously you are updating the position and velocity of one particle when you are doing looking at m d 2 x dt 2 equal to minus k x which you solved previously, but now we have 20 particles. So, your position array is of length 20 and your velocity array is of length 20 and you have to initialize them the initial velocities and keep updating the values of y and v by the Runge Kutta method because you are solving the differential equation.

So, that you get y as a function of t and v as a function of t right that is what you are doing in the difference it is by solving the differential equation. Moreover the quantities like x temp 1 x temp 2 the temporary positions right where you were calculating the we are essentially calculating the value of f 0 and f 1 and f 2 that itself will go into an array and similarly the temporary v temp 1 because you have another set of differential equations that those will also become arrays.

So, when you are writing down the algo in the equation in the code you will essentially have d vi dt equal to minus k by m you replace it by some constant kappa we will fix it to 1 y i plus 1 plus y i minus 1 because these are all now positions are being written in an array.

And this is an error and this will be basically y i plus 1 plus y i minus 1 minus 2 y i right because the y coordinate is being written in arrays right and this is essentially equal to f 0 v. Now once you have calculated f 0 v for each of the particles you can just update and calculate this temporary this temporary corresponding to temporary position sorry not the position the velocity which is just consider it to be a differential equation the temporary value of v at h by 2 which is updated by as v as per this equation right.

The initial velocity plus f 0 v which you have already calculated here into h by 2 and similarly, if f 0 for the position variable is just v i, then basically the position variable temporary 1 so, it has can be updated as y i plus f 0 i to h by 2 and of course, you have to calculate then the value of y 2 and similarly v 2 and y 3 and v 3. And finally, you will correspondingly calculate f 0 all these quantities for each of the particles and then update the actual position. Those are those temporary calculating the values of f zeroes are different points within the interval and then you average over and then calculate the final update the values of a y and v right.

The solution of the differential equation, this is all very good, but remember for the first particle and the last particle when i is equal to 1 or equal to l, you have to correctly choose the neighbors you have to implement the periodic boundary conditions. So, that is something to be remembered I will show the code in the next class how it is to be done ok.

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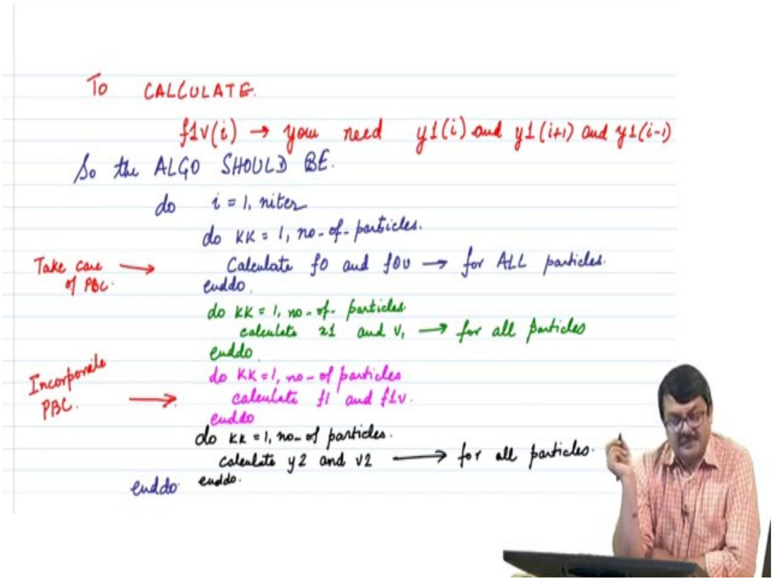

So, that is basically it, but there are still some buts you have to be careful remember to calculate f 1 v f 1 v right, you need the updated values of y 1 i say f 1 v i you need the updated values of f 1 y 1 i as well as y 1 i plus 1 as well as y i minus 1 right so, you need all these. So, the algo should be so, do i equal to 1 to niter this is the number of iterations then this will essentially change h 2 h 3 h.

So, basically the positions are these different time intervals this is that loop and suppose do KK equal to 1 to number of particles then you first calculate f 0 and f 0 v for all the particles and there is a small loop here right. Once I have calculated f 0 and f 0 v then you calculate x 1 this temporary x 1 and v 1 for all the particles in this loop where you will be basically using these quantities to calculate this having done that you shall be using these quantities to calculate f 1 v and f 0 v.

So, there has to be a loop over all the particles here and a separate loop of particles over all the particles here. So, you calculate f 1 v and f 1 for all the particles using this you calculate y 2 and v 2 for all the particles and there is a loop over all the particles here using this you calculate basically f 2 and f 2 v and so on so forth right. In this step and in this step wherever you are calculating f 1 v and f 1 f 0 v and f 0 you have to remember to incorporate the periodic boundary condition right.

So, one has to be a bit careful you do not do though you can do you do not calculate f 0, f 1, f 2, f 3 for a particle and then calculate it for the second particle, for each particle you have to calculate this entire array this entire array right because you are going to use that to calculate this for all the particles. So, you do not calculate f 0, f 1, f 2, f 3 for one particle then you calculate f 0, f 1, f 2, f 3 for another particle and so on so forth. So, this is a very place where people make mistakes. So, I that is why I am explaining this in great and gory detail and basically that is all that I have to say in this class.

In the next class we will actually implement it see how a f 1 how this y and v vary as a function of time ok.

Thank you.