Numerical Methods and Simulation
Techniques For Scientists And Engineers
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Lecture 23
MD Simulations: Verlet Algorithm

We will continue with our MD simulation and discussion and in particular we shall learn that how to use a particular algorithm namely the Verlet algorithm in order to calculate the position of the particles or generate a trajectory of the particles at all times that is T and then T plus some small increment. And then again some increment and so on so that we can entirely simulate the trajectory from some T is equal to 0 to some T equal to capital T which is the full course of motion.

The one that is most popular among this and it is a drift free higher-order algorithm. It is in fact it is the second-order algorithm generator we will see that.

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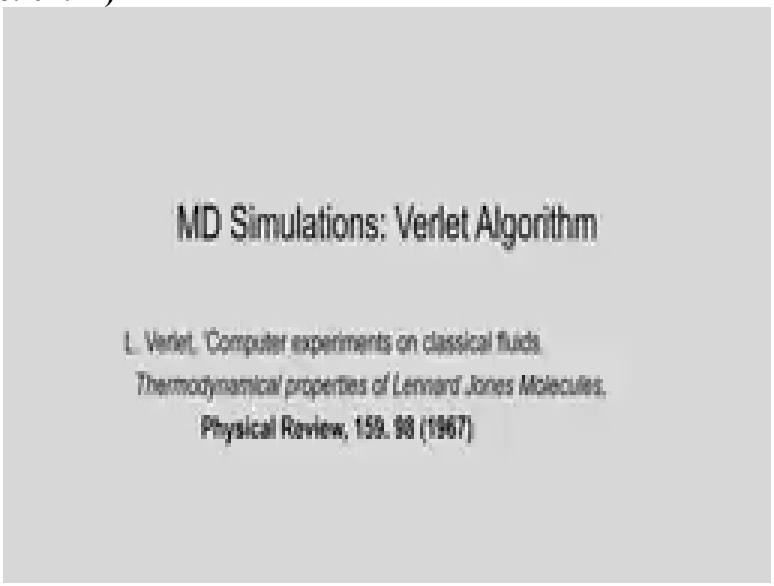

It is due to Verlet which appear in the first thing appeared in this paper by varlet in 1900 and 67 in physical review. The title of the paper was computer experiments on classical fluids thermo dynamical properties of Lennard Jones molecules and its volume 159 page 98 and it is in 1967. And in this paper he discusses the method and applications to Molecular dynamics simulations.

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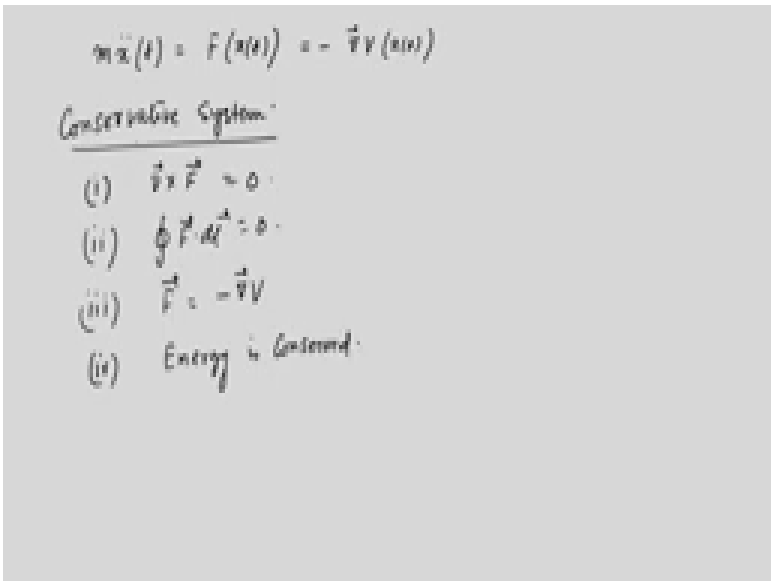

So just to remind ourselves that we are going to discuss these equation of motion once again repeating what I said in the last discussion that there is no binding on us to use Newton's equation equation of motion instead Lagrange's or Hamilton's equation of motion could be used but this is most common and familiar to everybody that is why I am using this. And so this is something that we need to solve.

And this is implicit one doesn't have to say but still I am mentioning it for the sake of completeness that we are talking about a conservative system. And if you have read statistical mechanics and classical mechanics in your undergraduate syllabus, it means that the force that we are talking about here, so we are writing it in one dimension. So maybe that will sort of remove this force the vector on the force but in any case this is we know that if it is a force actually which is a vector.

And so this means that the curl of the force taken is to be zero okay. And this also means they are of course related by what is called as a Stokes theorem is that the F dot dl should be equal to zero and it is also the same statement is that the force can be written as a negative gradient of a scalar potential. And the scalar potential in our case is dependent only on the positions of the particle.

And we have talked about at least two or three kinds of potential one being the Lennard-Jones the others are say most potential or the Coulomb potential and so on. So these are all equivalent statements and we are really talking about such systems where the energy is conserved. And

this is the last thing that energy is conserved okay. So armed with this we will have to solve for the X as a function of T.

And so in order to solve this numerically this equation numerically, Verlet suggested that we develop an algorithm for getting these positions at times T, T plus delta T plus 2 Delta and so on where Delta is a small increment of time very important to understand that Delta actually holds the key to a successful numeric computation in terms of getting the total energy conserved and also the numerical stability of the equation, the kind of solutions that we are looking for. So let us just talk about the varlet algorithm or the Verlet method okay.

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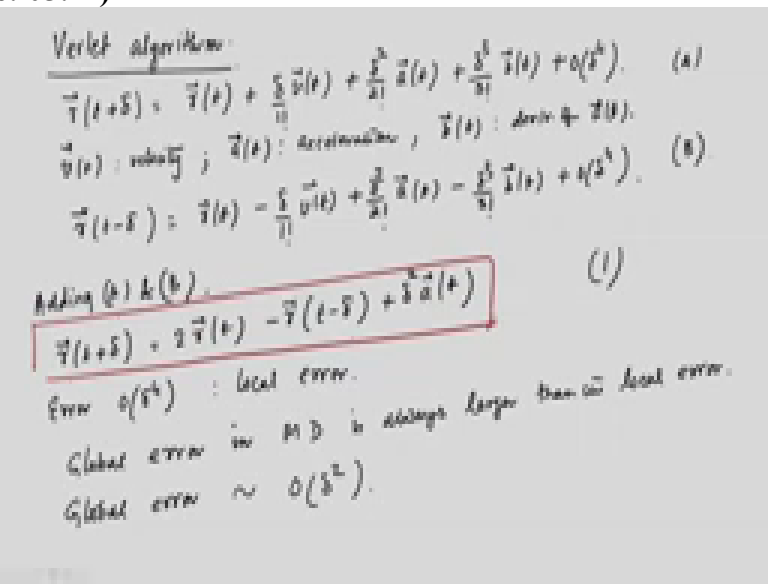

So this tells you that I am writing it in terms of vector R but it can be easily you know sort of simplified to one dimension by just writing the vector R - scalar X. So this at T plus delta is obtained from a Taylor expansion about the time t whatever is the initial time and this Delta is a small increment of time. Now I will take a dr dt which is the first derivative that is nothing but equal to V evaluated at this time T whichever time that we are talking about the initial time.

And a plus delta square by 2 factorial a t and plus a delta cube by 3 factorial. So if you want you can put a 1 factorial here and this I am writing it as b of t something that we are not too familiar with in dynamics which is the derivative of the acceleration so a is acceleration V is velocity and b is the derivative of acceleration which we are calling it as b. And we would neglect from order Delta 4 onwards and we will see that this is actually accurate up to Delta to the power 4.

So let us just write down all these notations. So V of T is the velocity a of T being the acceleration and B of t is derivative of acceleration okay. Now, this is of course the Taylor expansion of these quantity r T plus Delta about r equal to T and one can do a little bit of rearrangement of this. And one can write this as r of t plus Delta equal to twice of r t minus r.
Let us write down the other time term as well.

So this will have to write our t minus delta as well pardon me for this mistake. I have skipped one so again the r at t minus delta can also be written down which is is r of t and a minus Delta by 1 factorial V of t plus Delta square by 2 factorial a of t minus delta cube by 3 factorial b of t and plus order Delta to the power 4. Now adding let us call this as 1 and this is 2, or let us call this as just four.

Let us call this as A and B because this is not the equation that we are looking for. So adding A and B one can write with a little bit of rearrangement of terms. So this is like r T plus Delta equal to 2r t minus r t minus Delta plus delta square a of t. So you see that when you add the odd terms cancel, the odd terms in Delta they cancel and one lands up with only the even terms in Delta and since we have omitted terms from Delta 4 onwards.

So we got a delta square term and so on. So this is so error is of the order of Delta to the power four and this is called as a local error. One important problem with the Mont molecular dynamics simu simulation is the following: that the global error in MD is always larger than the local error. So this is a local error because we are just talking about one time step.

So if you evolve the system in one time step going from you know r of t to r of t plus Delta, one actually picks up error which is of the order of Delta to the power four whatever is your delta delta is up to you to choose a value, of the increment of time that you want the system, to you know between two successive times, this is the time interval that I want. so it is completely up to you and this error is of the order of Delta four but when you actually do a simulation over several deltas.

And we actually evolved the system from say t equal to zero to t equal to some capital T where capital T has a very large number of deltas that is capital T equal to say n delta where n is a very large number. And then these errors ideally we want them to either remain same or they even we I, I mean could be more ambitious and one there to reduce.

However what happens in this particular case is that the error does not reduce in fact it grows; that the global error is of the order of Delta Square which is larger than a delta to the power 4 because Delta is small okay. And let me show you that how this thing arrives, one is arrived at this global error.

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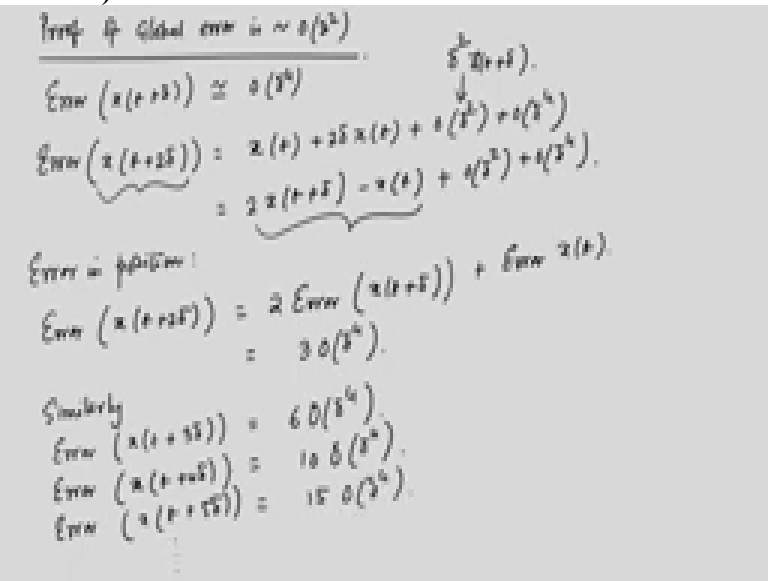

And so we present a derivation is simple derivation for that. So we will prove this that so proof of global error is of the order of Delta square okay. So local error as we have just learnt x t plus Delta is of the order of Delta to the power four let us just write equal to Delta to the so error x t plus 2 Delta equal to x of t plus 2 Delta x of t plus order Delta square plus order Delta to the power 4. This Delta square of course involves acceleration but we do not we are not writing it explicitly because you know the so this this term is like Delta square 80 and so on or 80 plus Delta.

So this would be this term but we do not need it that is why we are not writing it here. So this is that term but anyway we are neglecting terms from here onwards. So this thing can be written in a slightly tricky way or rather with a bit of a manipulation. We can write it as twice of x t plus Delta minus x of t. And then again this term let me write it as order Delta Square order Delta to the power 4.

So you see that the error in positions so this error for this quantity actually goes as error for you know this thing this is the error in acceleration which is a derived quantity which we are not considering here. So the error in position would be simply equal to so error x t plus 2 Delta is 2

error x t plus Delta ahm and error x of t ahm and each one of them is actually of the order of Delta to the power 4.

So I am writing it plus sign because these errors are always additive, so this is 3 order of Delta to the power 4. So this is the error at this t plus 2 delta level and similarly if one looks at error at x t plus 3 Delta, so this is 6 order Delta forum. So this is just by induction. So this O is of the order of okay. This O is of the order of and similarly error for x t plus 4 Delta, it is equal to 10 order of Delta 4.

So this is just by a similar you know manipulation here error x t plus 5 delta it is equal to 15 order delta to the power 4 and so on okay. So there will be a number of them for delta 5 delta 6 delta 7 delta and all that. And these all these numbers would get added up now you see that what you are adding up is actually terms such as as you go.

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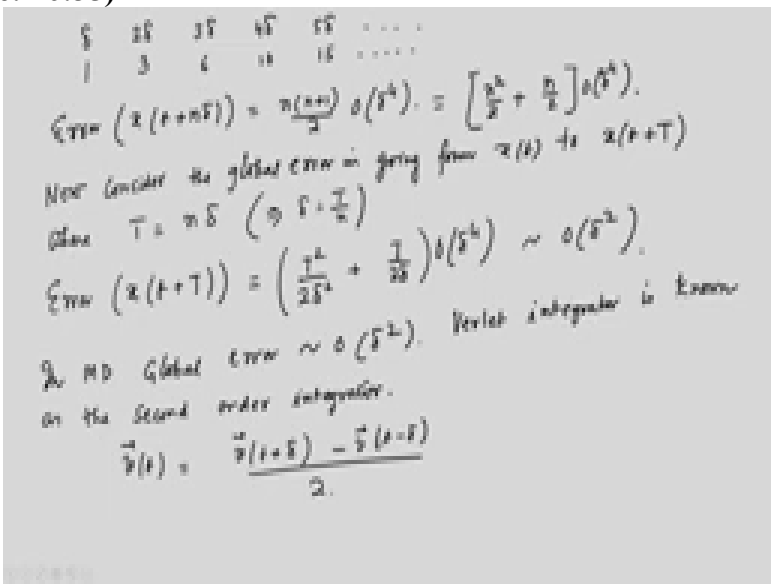

So Delta comes with a term 1 to Delta comes with a term 3, 3 Delta comes with 6, 4 Delta comes with 10, 5 Delta comes with 15. So if you follow it like this then, you get a by induction what one gets is that for the error x t + n Delta ok, this is n into n plus 1 by 2 order Delta to the power 4 ok. Now you see for n equal to the 0 at step that is the first one, so or rather for the first step one gets, 1 into 1 plus 1 to 2 divided by 2 will cancel. So we will get a 1.

For 2 Delta n equal to 2 put n equal to 2 so 2 into 2 plus 3 which is 6 divided by 2 is 3 and for n equal to 3 it is 3 into 4 by 2 so it is 12 divided by 2 is 6 and similarly it goes on ok. So this is the by induction. So this can be written as n square over 2 plus n over 2 and there is an order

Delta to the power 4 alright. So now consider the global error in going from x t to x of t plus capital T where capital T is to say the final time where capital T is nothing but n Delta or rather this also gives Delta equal to T over n.

So this tells you that the error the global error rather which is picked up from all the errors. So this is capital T plus small t plus capital T. This is equal to T Square over 2 Delta square plus at T over 2 Delta and this is order delta to, multiplied by order delta to the power 4. So there is a delta square and there is a delta. So the leading one leading is of the order of delta square okay. So the global error is actually large as compared to the local error.

So they pick up errors at every stage and if you add them up it becomes of the order of delta square. And so this basically this in MD, the global error is of the order of delta square, this what i have said also and that is why the verlet integrator is known as the second-order integrator okay. Now there is a bit of a problem with this version of this varlet algorithm that we are talking about.

What is important is that we are not getting the velocities which may also be needed for a reason that we want to calculate the energy and the kinetic energy crucially needs the information about the velocity. And here we are not getting the velocity but we are only getting the the positions. And of course the velocities can be determined using this divided difference formula which is v t plus Delta minus v t minus Delta and so on divided by 2.

But we still have to get this v t plus Delta and v t minus Delta these will correspond to positions x t plus Delta and x t minus Delta and so on ok. So it is important to get these velocities. Let me just go back once and call this equation as equation 1 and maybe box it because we are going to need this equation for several of our and discussion. So this is the position evolution of the particles and this has to be now combined with the velocity.

And there are several algorithms and we are going to talk about to three of them but mostly going to use the velocity verlet method ok.

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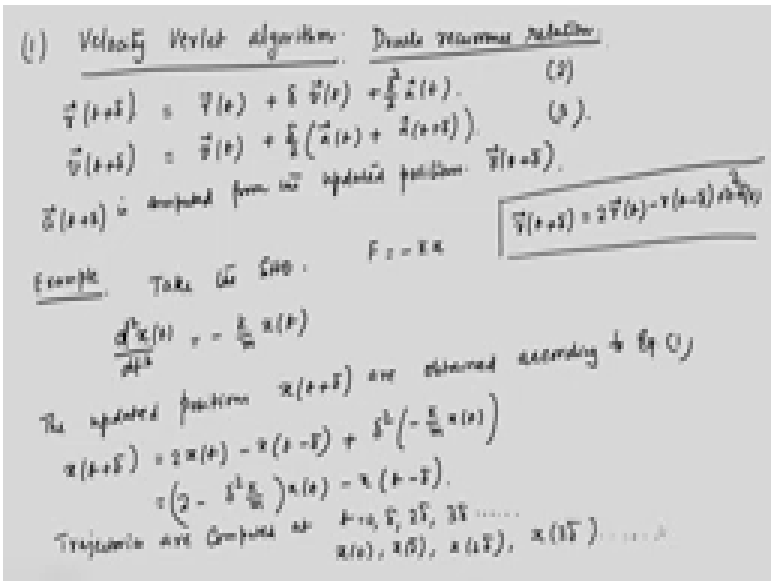

So it is important that we also know the velocity along with the positions of the particle at x, x at t, v at t also needs to be unknown. So to overcome this difficulty a number of algorithms have been mentioned or proposed and let us see some of them. So we will start with the important one for us which is the velocity verlet algorithm okay which is a recurrence relation of a combined x and t.

So here the r t plus Delta so this is a double recurrence relation okay so it is for both. So double is for both position and velocity so r t plus Delta this is written as r t plus Delta v t plus Delta square by 2 plus a t okay. So this is for the position and for the velocity it is v at t and Delta by 2 a t plus a t plus Delta and so on. So let us call them as equation 2 and equation 3 where the a t plus Delta is computed from the updated positions r t plus delta okay.

So this is important. This is called as a velocity world let algorithm. So let us take an example. So take the simple harmonic oscillator and the equation of motion is given by d2 x dt 2, x is a function of t. It is equal to minus k by m x of t. Just to remind you that this k is equal to the force constant. So it is a Hooke's law pretty much that is written which says that F is equal to minus k x so as the force this is the restoring force.

So once when a spring or you know an elastic object is displaced or stretched from his natural position x equal to zero by a distance x, the restoring force that acts on the system is proportional to the displacement. So as you displace the part more a part of that elastic body more so there'll be a larger restoring force. And so this goes as f going to x and because it is restoring there is a negative sign there and it depends on the material.

So if you have an elastic material of one kind as compared to an elastic material of another kind you will have a different k value associated with it which is called as an elastic constant or a spring constant or a force constant. All these names go with it almost synonymously and this is the equation of motion that one gets. So the updated positions x t plus Delta are obtained according to equation 1.

So let me remind you of equation 1 here which is r t plus Delta equal to 2 r t minus r t minus Delta and plus Delta square a of t. So that is the that is equation 1 and we will sort of if written it earlier but now written it here just for you to follow better and this is same as now as we are doing it in one dimension. So it is a x t plus Delta it is equal to twice of x t minus x t minus Delta.

Those are the first two terms. Now for the last term it is easy because your acceleration is nothing but minus k by m x. So we will write that down instead of the acceleration here. So it is a minus k by m x of t. Now you see that you can combine it with this and write it as 2 minus Delta square k over m and x of t and minus x of t minus Delta. So the trajectories are computed at t equal to 0 t equal to Delta 2 Delta 3 Delta and so on.

And so which are termed as x at 0, x at Delta, x at 2 Delta, x at 3 Delta and so on. So this is the way the trajectories are generated in successive times. As I told that Delta is a small increment of time and this increment of time is so the positions are calculated at each of these increment values. And this is how things proceed and the velocities of course can be obtained by the finite difference or the divided difference method.

And so, if you do the same thing with the velocity Verlet, so this is just the position formula which is equation 1 and doing the same thing with the velocity verlet.

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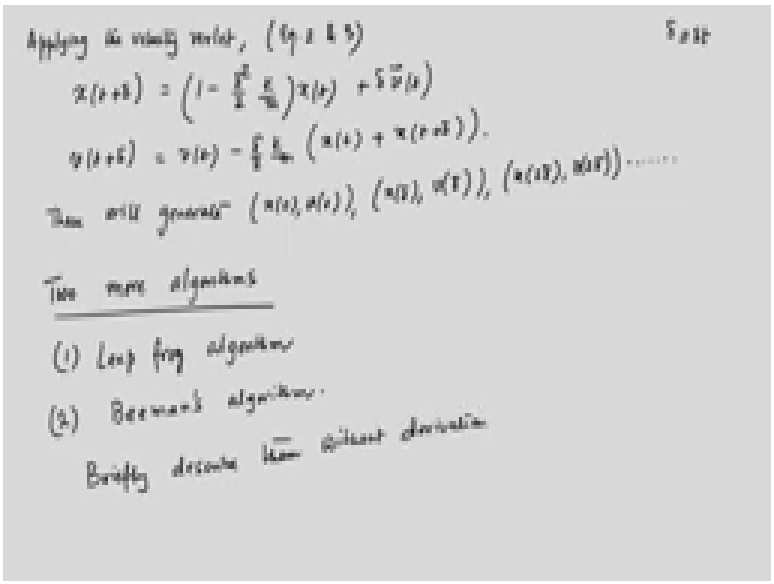

So these are applying equations two and three. These are right here which you can see that r t plus Delta equal to r t plus Delta v t and Delta square by 2 and a t where v t plus Delta equal to v t and then Delta by 2. And a t and a t plus Delta. So these are the acceleration computed at those values. So let us use them and can we can write this as one minus Delta square by 2 k by m. We have already shown the acceleration is this. So we combine it here and then there is a delta v t just be a little careful.

This is not Delta v is not this Delta x v. So Delta is a small increment in time if you are feeling uncomfortable you can write Delta to be equal to delta t which means that it is a small increment of time. Now the velocity expression is written as v of t and a minus delta by 2 k over m x of t plus x of t plus Delta. So these are the two recurrence relations that we have to compute for you know.

So these will generate pairs of x 0 v 0 x Delta v Delta x 2 Delta v 2 Delta and so on ok. So now it is worthwhile that we talk about a couple of more algorithms and show that why they are you know why were let is probably most commonly used. Somehow those algorithms are also popular and people have used it and so they are known as so two more algorithms one is called as a leapfrog algorithm and the second one is called as a Beeman's algorithm okay. So we briefly described them without derivation. So let us talk about the Leapfrog algorithm.

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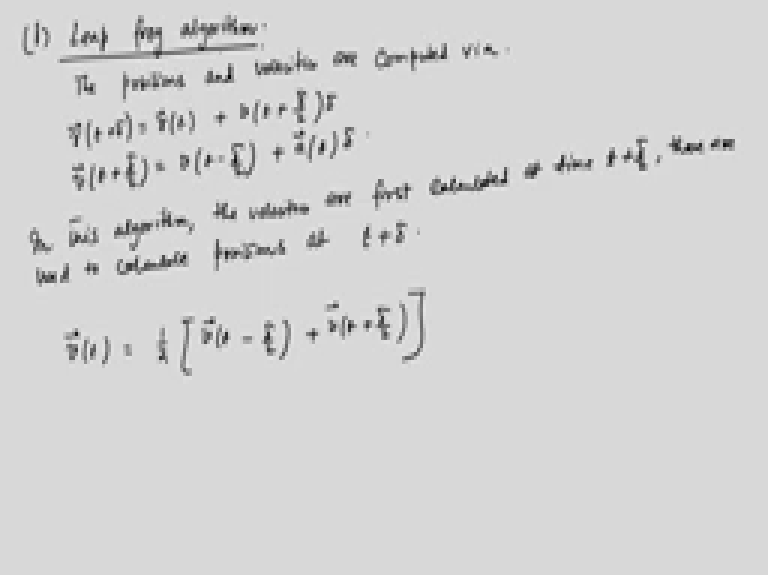

So let us see what this is the positions and the velocities are computed via by this. There is a position generator and the velocity generator is given by this. So in this algorithm, the velocities are first calculated at time t equal to or at time t + delta by 2. And these are used to calculate used to calculate positions at t + delta. So you see that they are not calculated at the same time. So the velocity is calculated at this time t + delta by 2.

At a later time the position is calculated at t + delta. Now again the velocity will be calculated at t + 3 Delta by 2. And then one will go and calculate the positions at t + 2 delta. So they will leap frogging they are actually leaping the velocity is a leaping over the position. And then the position is taking over in the next round. And then the velocity is taking over in the next round and so on.

So they are not calculated together. However, one can actually approximate to calculate the velocity from this expressions which is v t - Delta by 2 + v t + Delta by 2. And so this is the velocity. So if one calculates the r at p then one can also get the velocity as t. But these only an approximate expression and really one is leaping ahead of the other. Of course it has some advantages that it is a fast algorithm.

And one gets a lot of data generated within a shorter span of time but they are not pairwise they are not calculated at the same time. Let us look at the second one called the Beeman's algorithm okay.

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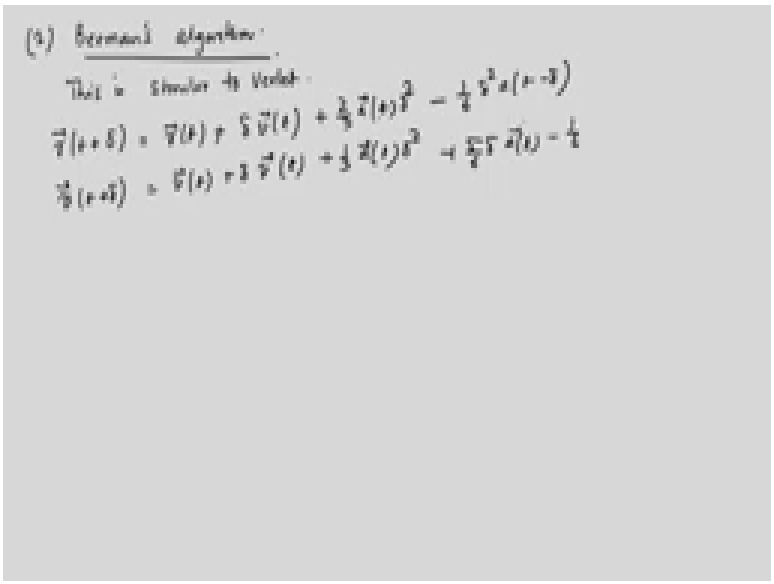

So, this is similar to Verlet. And so this is written a slightly more complicated expressions equal to r t + Delta v t + 2/3rd a t Delta square minus 1/6 th Delta square a t - Delta and v t + Delta it is equal to v t + Delta v t + 1/3 rd a t Delta square + 5/6 th Delta a t and - 1/6 th Delta a t 0 Delta and so on. So the advantage of this algorithm is that it provides a more accurate expression for the position and the velocities.

However, the disadvantage is that as you see that there are more complex expressions to be coded or rather they are more difficult than the Verlet algorithm. In any case, there are probably more algorithms for generating the x at t + Delta and v at t + Delta. But we shall be mostly using the Verlet integrator or the Verlet generator. So let us look at the Verlet method.

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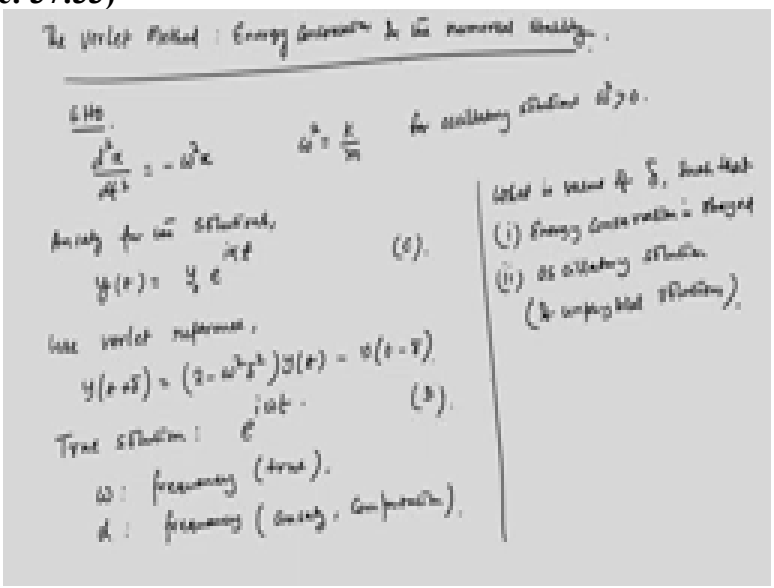

And in particular talk about the energy conservation and the numerical stability. So let us take again a specific example. Let us take the example of simple harmonic oscillator which is now written as d 2 x dt 2 equal to minus Omega square x where we write Omega square equal to k over m and for oscillatory solutions, we really want to retain the negative sign. So Omega square it should really be positive.

And these things are of course positive because k is your force constant and m is your mass both are positive definite quantities. And we can write down and answers for the solutions namely y at y equal to some amplitude y 0 exponential i alpha t. So this is the answers of this form. So for the discrete evolution of so use varlet reference so y at t plus Delta, it is equal to 2 minus Omega square Delta square y at t minus y t minus Delta.

So this will give a handle of how far the solution y that is proposed as an answers is going to be closed to the actual true solution because we know the true solution is of the form exponential i Omega t. See one thing are to be noted with a bit of a care that is omega is actually the frequency, the actual frequency, true frequency. And alpha is the frequency for from the answers or from computation okay.

So they have to have a relationship amongst each other. Or they should be related in such a way that we should not miss the oscillatory solution and get a solution which is you know dying solution or some hyperbolic solutions and so on okay. So this is important that there has to be a relation and one has to really find out the relation. And this is also needed so we really need this for what is the value of Delta such that a. energy conservation is obeyed b. or rather two one gets an oscillatory solution which means and No ah unphysical States or unphysical solutions.

So let us see what is meant by that and what has got to do with this value of alpha. So this you know the Alpha should be actually capturing the fastest oscillations in the problem. At least that is what has to be ensured that. And let us see how we ensure that that so we should not get a non-oscillatory solution. So to say so if we so this is answers. So let us call this as equation C and this is the true solution is d. So plug in the ansatz into a equation of motion.

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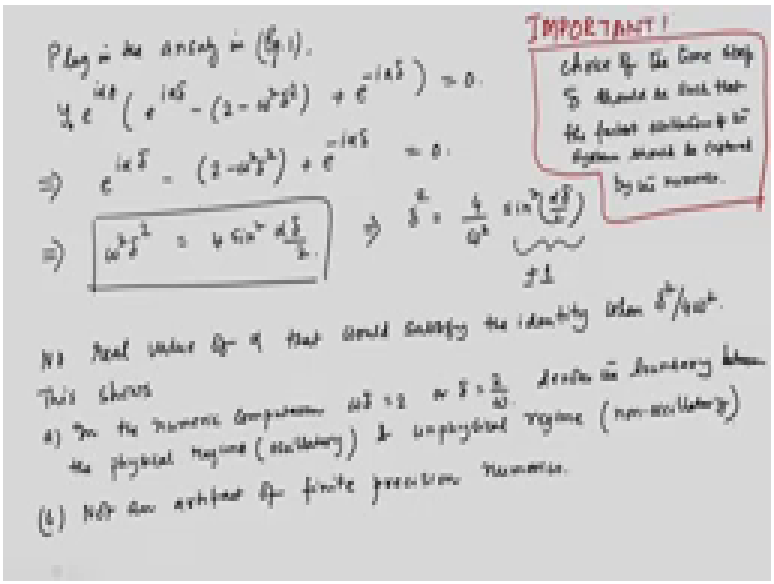

So plug plug in the ansatz into equation 1 if you remember what equation 1 is which involves that x t + Delta in terms of x t - Delta and the acceleration. So it is a y0 do it carefully exponential i alpha t it is i Alpha Delta - 2 -s Omega square Delta square plus exponential - i Alpha Delta. This is equal to 0. So this is the and the position generator from the varlet scheme.

And so this gives that exponential i Alpha Delta minus 2 minus Omega square Delta square + exponential - i alpha Delta that has to be equal to 0 and hence the Omega square Delta square is 4 sine square alpha Delta by 2. So, very important thing here is that see if I rewrite this as Delta square equal to 4 Delta square equal to 4 over Omega square sine square alpha Delta by 2, now you see that this can take maximum value which is 1, so it is the extreme values are plus minus.

But that will be violated if your Delta Square for it becomes greater than 4 over Omega square. So if that ratio, so if I bring this here and if this ratio becomes Delta squared becomes greater than 4 by Omega square, then, there will be no real value of alpha that would satisfy this identity ok. So important statement, no real identity above when Delta square is greater than four Omega square.

So, this of course, shows that two things. One is that in the numeric computation, Omega Delta equal to two or Delta equal to two over Omega denotes the boundary between the physical regime which is oscillatory and unphysical regime which is non-oscillatory. So this tells that what should be my smallest time scale that I should choose, in order to get a numerically stable solution.

And also very importantly the average energy to be constant, ah so which is a requirement for a conservative system, okay. So we cannot just choose anything so what is important is this that to understand that this is not an artifact of the numerical precision finite precision numeric. So very important statement is that let us make here that choice of the time step delta, should be such that the fastest oscillations of the system, should be captured by the numeric.

I have written it a small font but I hope you will be able to see it. Let me circle this very important statement, or rather box it okay. So this is very important mostly in cases where one has a sinusoidal driving say for example or a periodic driving of a system and say there are transitions going on between various states of a system, various states means various energy levels of the system.

And so there is a natural frequency of oscillation or there is a natural frequency of these transitions and along with it basically because there is a periodic driving. So there is also this period or rather the frequency of the driving force that is also kind of coming to play. So one has a fast motion and one has a slow motion. In fact in the MD simulation that Delta should be such that the fastest motions or rather the fast of these two motions, faster of these two motions should be captured in the simulation.

Otherwise it will lead to unphysical solutions and will not give rise to something that we want to you know sort of display.

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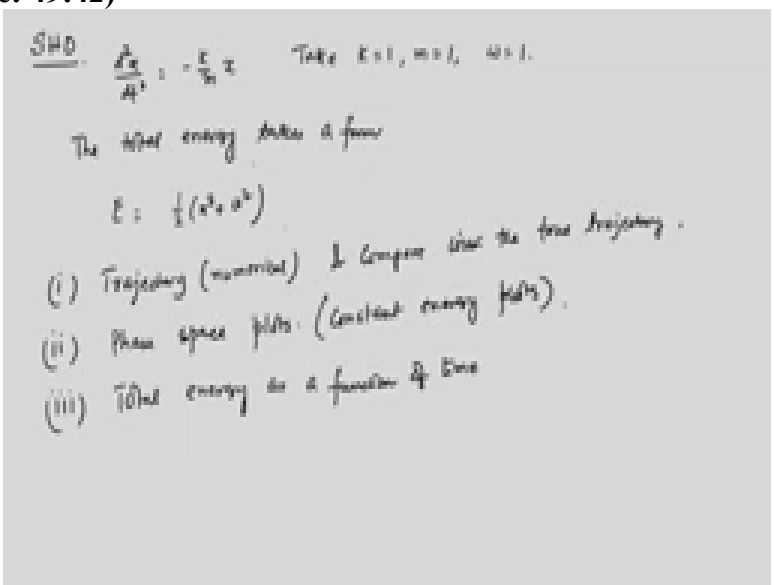

So let us look at a situation again at the SHO and so just write down the equation of motion. So take k equal to 1 m equal to 1 and so on which makes of course your Omega equal to 1. So in these units the total energy takes a form that this is a potential energy 1/2 m Omega square X square all are equal to 1. So coefficient is 1 and 1/2 MV square it because m equal to 1 so it is 1/2 V squared and so on.

So let us show three things in fact this is from a book will show you the results from a book. So this is will show three things: one is the trajectory the numerical trajectory and compared with the true trajectory, two is the phase space that is the space of position and velocity so phase space plots so it is a constant energy rather the constant energy plots and third is total energy or as a function of t as a function of time okay.

And we show this and understand that as Delta is increased beyond a certain value one gets poorer and poorer select I mean solutions and beyond a certain value of Delta one gets very unphysical solutions. So let us use this is the solution.

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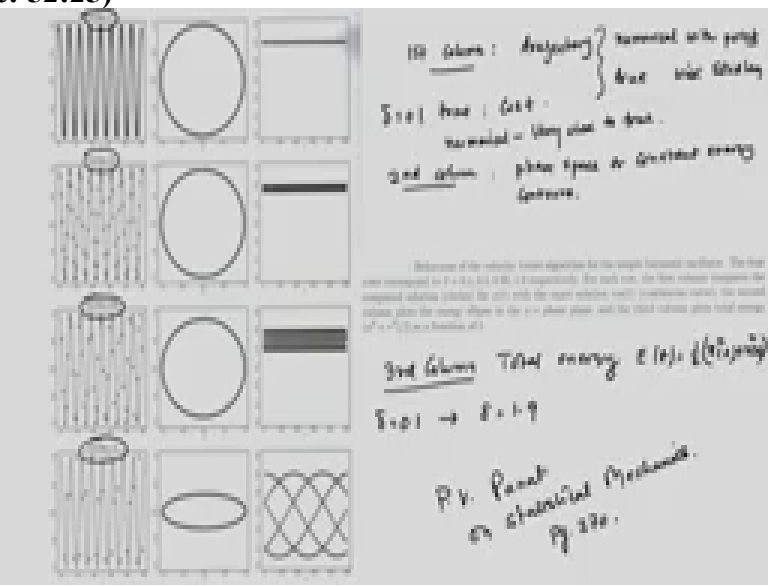

So you see that this is the trajectory part. So this is the trajectory. The first column, the trajectory with points the numerical ones are with points and true trajectory, true with solid lines okay. So this is from a book by P V Panet on statistical mechanics okay. So you will find this on page 370 alright. So let us see this that you see the solution is pretty much following for t equal to a time step equal to 0.1 a true trajectory is cos of t.

And numerical one is very close very close goes to true so you see that they are all falling 1 these circles are falling on the straight lines or the rather the bold lines continuous lines. And this the second column actually correspond to the, what we said is the basically the phase space or the constant energy contours okay. So it is exactly a circle it is and then as you increase this Delta to 0.5, so this is the initial one is Delta equal to point one.

We pretty much get you know the same trajectory here with these because we have increased delta to 0.5 the frequency of the point so the number of points have gone down but they are still showing us fairly good cosine t behavior and the phase space is also a circle. Now the last column the third column is basically the total energy E as a function of t which is half x squared and plus v square all right.

So this is showing just a sharp line at half at a value half which is these two are there as a function of time and time goes from zero to some 500 time steps and they are still at that value 0.5. At this larger time steps it the even though the phase looks phase based trajectory looks circular these things the energy actually have broadened. And one if one increases the time step to about 0.1 or rather one that is 0.95 one gets much lesser points and they can still probably be approximated as some cosine t lines because most of these are falling in this cosine t.

However the phase space trajectory is becoming of the constant energy contour is becoming a little elliptic. Not only that the total energy is spreading rather it is deviating the, from the value half and it is spreading over says if from 0.4 to 0.5 and so on. And then, ah for a larger time step 1.9 which is very large, one gets a phase based strategy free to be a flat ellipse. And not only that you see that the energy is undergoing a lot of fluctuation and the energy is not you know as a function of time the energy is changing quite a bit.

It is not a value so it is from 0.1 to 0.5, it is having a variation and it is having some kind of a sinusoidal variation there. So that tells that as you know of going from Delta equal to 0.1 to Delta equal to 1.9 one has actually the solutions have sufficiently deteriorated and beyond that that is beyond rather greater for Delta to be greater than 1.9, there is no solution that is oscillatory and hence cannot be an acceptable solution or a numerically stable solution.

So we reject we have to reject all these solutions. So in this we clearly show that how Delta plays an important role or the time step that you choose plays an important role in deciding on

the varlet trajectory that we have studied in this section or in this discussion. So it is it is important for us to understand that Delta should catch or capture the fastest oscillations going on in the system. And if it doesn't then of course we get solutions which could be unphysical and may be something that we cannot trust on it.