

Computational Physics
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Lecture – 46
Molecular Dynamics Introduction Part 01

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Molecular Dynamics Simulations (Classical)

- Integrating Newtons Equation for a large no. of interacting particles
- Physics of the problem decided by interaction potential.
- $m \frac{d^2 \mathbf{r}}{dt^2} = -\nabla V(\mathbf{r})$.
- $\mathbf{r}_i(t)$ and $\mathbf{v}_i(t)$ or $\mathbf{p}_i(t)$: i - particle index.
- Time evolution of a system of particles
- Once EQUILIBRIUM is reached → take Statistical time average.

However one can also study Time evolution of a NON-EQUILIBRIUM System

So, welcome to the last module of this course where we will be discussing Molecular Dynamics Simulations and in this part we will be talking about classical molecular dynamics. There can also be quantum molecular dynamics. So, in classical molecular dynamics simulations we are doing nothing more than integrating Newton's equations of motions for a large number of interacting particles.

So, basically there are particles they are moving around in space and you are following the position coordinates and the velocity coordinates of the particles. The physics of the problem is decided, I mean what you want to study, the physics of the problem is decided by the interaction potential. So, depending upon what physics you are studying you choose different expressions of the interaction potential.

So, if you are doing Newton's equation of motion it is nothing but solving $m \frac{d^2 \mathbf{r}}{dt^2} = -\nabla V$; V being the interaction potential. You choose different potentials depending upon the physics of the problem and on solving this second order

differential equation you essentially get positions and velocities of positions or momenta as a function of time. Here i is the particle index, of course you are not looking at just one particle, but you have a bunch of particles interacting with each other right.

So, in molecular dynamics simulations you are essentially looking at the time evolution of a system of particles and if you are doing statistical physics then once equilibrium is reached you can take the statistical time average. So, here you are basically taking time averaged molecular dynamics simulations in Monte Carlo simulations the ising model which we discussed.

Previously you are taking the n symbol average the system works going from one microstate to the other different copies of the n symbol. Here also the system is going if the system is in equilibrium the system is going from one microstate to the other, but as a function of time. So, when you take a statistical average you are essentially taking a time average of the system.

However, in molecular dynamics one can also study the time evolution of a non equilibrium system. Suppose your initial coordinates the positions and the velocities of the system of particles they are not in equilibrium, they are in some special initial condition. Then you can also study how the system is moving towards equilibrium, especially since you have access to positions and velocities of all the particles and you are doing a classical simulation, just integrating Newton's equation of motion right.

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N particles.
 V Volume.
 T fixed temperature. \rightarrow Constant Pressure Simulations (N, P, T).

Equipartion Theorem (in equilibrium)

$$\left\langle \frac{1}{2} m v_i^2 \right\rangle = \frac{1}{2} k_B T.$$

$$\left\langle \frac{3N}{2} m v^2 \right\rangle = \frac{3}{2} N k_B T.$$

Simulation box with PBC.
(periodic boundary condition).

$$\text{Hamiltonian} = \sum_{i=1}^{3N} \frac{p_i^2}{2m} + V_{ij}(r_i, r_j)$$

Quadratic term in Hamiltonian.

In general $V(r) = V_{ijk}(r_i, r_j, r_k, \theta)$.

So, what would be the picture what you will have is a simulation box with PBC, PBC being periodic boundary condition. So, here you have a box blue colored right and within that you have many particles which are basically moving around in space. So, I have labeled 1 2 3 and here you have i and you could $i + 1$ in general you could have N particles in a box of volume V . You can take a cubic box you can also take a spherical box and so on so forth.

But here we have periodic boundary condition remember you can also have a box with walls. So, you can have also a confined system and you see how the particles are moving around due to interaction with each other. As well as when they reach the wall they could collide with the wall and come back into the system right. So, basically you are trying to model nature with the appropriate potential.

And so you have N particles in volume of box V and you could also basically fixed are you looking you will typically be looking in the system at a fixed temperature. You can also change temperature there is no from if you want to look at a system at different temperatures, then you also can change the temperature. How do you decide how do you measure the temperature, it is by equipartion theorem which holds in equilibrium. Where $\frac{1}{2} m v_i^2$ for a particle equal to $\frac{1}{2} k_B T$. So, this is for every degree of freedom right.

So, this would be like $\frac{1}{2} m v_x^2$, in the $\frac{1}{2} m v_x^2$ expectation value average value equal to $\frac{1}{2} k_B T$ and that is what the equilibrium equipartion theorem says. In general if you have N particles and if you are in 3D and you have $3N$ degrees of freedom. So, then $\frac{3N}{2} m v^2$ over all the particles basically calculating the total kinetic energy of all the particles, an expectation value of that will be equal to $\frac{3}{2} N k_B T$. Here the Hamiltonian is of the form $\sum_{i=1}^{3N} \frac{p_i^2}{2m}$.

So, basically my half I mean $\frac{p_i^2}{2m}$ is also nothing but $\frac{1}{2} m v^2$. So, you have $\frac{1}{2} m v_x^2 + \frac{1}{2} m v_y^2 + \frac{1}{2} m v_z^2$ it is every degree of freedom. So, basically if i was the particle index then i would run from 1 to N . However, this i corresponds here to the degree of freedom. So, in 3 dimensional space you have v the x is 1 degree of freedom, y is another degree of freedoms, z is another degree of freedom and if you have N particles i runs from 1 to $3N$ and this is the potential term.

Now, for equipartition theorem you might know that only terms which are quadratic in the Hamiltonian like P_i^2 by $2m$ is quadratic in the Hamiltonian. So, only if you have terms in the Hamiltonian where it appears as a whole square P_i . So, P_i being the momentum whole square kinetic energy only then does the equipartition theorem hold. So, you cannot say that half of potential energy average potential energy is related to half $k_B T$, I mean per degree of freedom right.

So, here we have considered a potential which is basically dependent upon the position of two particles. But in general you can have potential which is a three body interaction, four body interaction it can depend. If it is a three body interaction it will depend upon r_i r_j r_k these are basically the position index of three different particles it could also depend upon θ , you could have a θ dependent potential you could have a θ where θ is essentially the angle.

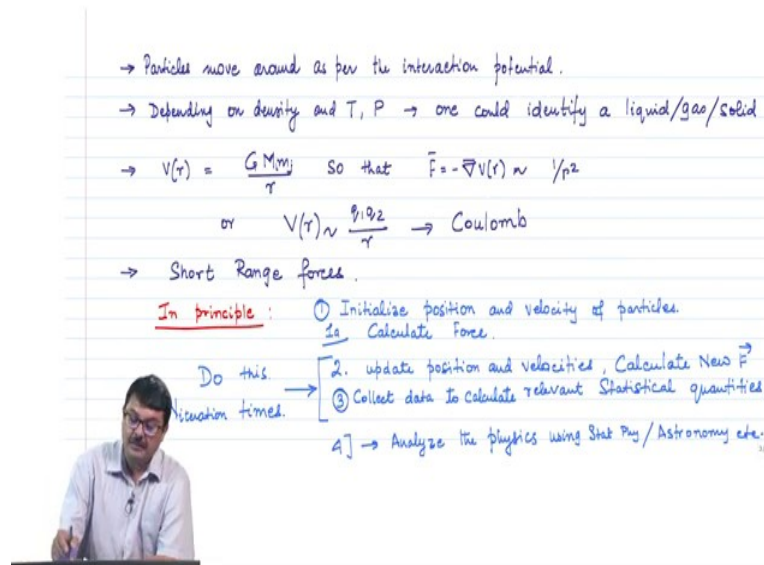
So, between vectors or suppose that this is a particle this is a particle and this is a particle and suppose they are connected like this. So, this is i say this is j and suppose this is k and then basically r_i minus r_j . So, you will basically have this vector and then you will have another vector like this. So, if you have a three body interaction you potential will depend upon all the relative values of r_i and r_j and also on θ it could I mean.

So, it depends as I told you the form of the potential depends upon the physics of the problem right and you could have also have torsion terms, if need be I mean angle dependent potentials as I said. So, in this course we will be basically looking at a canonical and symbol, where we are fixing N V and T . So, number of particles fixed or volume fixed and temperature fix, but you could also look at constant pressure simulation.

So, when you go fix a pressure, so then you would basically look at N P T simulation, number of particle fixed pressure fixed which means volume can fluctuate. And the instantaneous volume can fluctuate, of course we will have an average volume and affects the temperature. Of course, these each of these coordinates can also be changed, but then you are changing this is not the system not the interaction.

But you are taking the system at a higher temperature or a higher pressure or if you are changing v keeping n constant then you are changing the density of the system and so on so forth right.

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→ Particles move around as per the interaction potential.

→ Depending on density and T, P → one could identify a liquid/gas/solid

→ $V(r) = \frac{GMm}{r}$ so that $\vec{F} = -\nabla V(r) \sim 1/r^2$

or $V(r) \sim \frac{q_1 q_2}{r} \rightarrow$ Coulomb

→ Short Range forces.

In principle :

1. Initialise position and velocity of particles.
2. Calculate Force.

Do this → [

2. update position and velocities, Calculate New \vec{F}
3. Collect data to calculate relevant Statistical quantities.

Simulation times.]

A] → Analyze the physics using Stat Phys / Astronomy etc.

So, we will be considering N V T, but we can also do N P T simulations molecular dynamic simulations. As I told you particles move around as per the interaction potential, the potential determines whether there is an attraction between them then particles will come close together. And depending upon the density number of particles by volume temperature pressure one could identify whether the set of interacting particles is a liquid a gas a solid, there could be many other phases depends upon.

Again I mean there could be the pneumatic phase they could be a complex crystalline phase and so on so forth. So, as I told you the molecular dynamics simulation the physics of the problem is decided by the potential, you could even using molecular dynamics simulations look at how Neptune is going around the sun. But if you are looking at Neptune then we are basically looking at is the Newton's gravitational law GMm by r square.

And of course, Neptune or whatever planet or whatever you are interested to look at it would be affected by not only the sun, but by the earth Jupiter Saturn and so on and so forth Pluto asteroid belt and so on so forth. So, if you were looking at gravitational potential you would have the 1 by r square, if you are looking at a charge system you would be looking at the coulomb interaction this is 1 by r.

So, gravitational potential coulomb interactions these are typically long range interactions, they really act as 1 by r and this 1 by r fall off can be felt over very large

distances right. But in principle you can do molecular dynamics simulation with that, but calculation of long range forces is slightly more complicated. You have to calculate part of the force in Fourier space and some in real space and so on so forth.

So, we will be mainly concerned with short range forces. The calculation method will remain the same if you have interactions like this, calculation of force becomes slightly more complicated. But rest of the algorithm remains the same if you are doing a molecular dynamics simulations with short range forces it is slightly simpler than dealing with long range forces. For this since you are just learning the principle of molecular dynamics and we will calculate some quantities.

We will take the simpler problem of a problem with short range forces. Having said this what does actually molecular dynamics simulations entail going to a slightly more details and what I have been discussing up till now. Basically will have N particles so you initialize the position of and velocity of N particles right. Now if you have a potential then if you know the position of the particles you can calculate the force acting on each particle.

Once you know the force and you already have the velocity because, you have initialized it you can update the position and velocities of the particles. So, you have the new positions and the new velocities of the particles Newton's law that is for Newton's law tells you and once you have the new positions you can calculate the new force right. So, you have access to the new force, moreover you should collect data to calculate your relevant statistical quantities rights, because the particles are going to move.

Basically, if you are looking at the statistical averages you could be identifying phase it could be identifying the dynamics and that is all that is there in molecular dynamics simulations. Just three steps initialized position calculate force, update position and velocities calculate new force with that to update the position and velocities and with that calculate new force and do this any trace in time.

So, then you basically get a trajectory of all the particles in space. At the end of your simulations after N iterations simulations how many iterations to choose of course, those are details we shall come to it when we actually implement it I am implement the code. So, at the end of the simulation you analyze the physics using either stat physics or if you

are doing suppose some solving the Newton's equation for suppose the planets in the solar system ah.

So, we could not do it you want the trajectory which we could use astronomy you could look at interaction between galaxies. Again as I said I mean what you want to do with it what potential you use whether it is big galaxies be is your unit or planet or smaller particles, nanoparticles or interacting liquids that is decided by the physics decides the V of r . But the molecular dynamics simulations just tells you how to integrate Newton's equation of motion efficiently and in a reliable manner right that is all that is there to it actually.

But you will see those will sound so simple there are complications which you will have to be aware of, if you just do it naively you will soon get infinity the simulation is not going to work. So, the reasons molecular dynamics simulations is being taught at the end of the course, is because it there is a lot of scope for error it is more complicated than any of the things that you have learned before. In principle it is simple it is just you have to be a bit more careful about various aspects you will come to it as we go along the course.

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→ So we are solving $3N$ differential Equations. for $x_i(t)$.
 $3N$ " " " for $v_i(t)$.

→ Calculating $x_i(t+\Delta t) = x_i(t) + \dots$
 $v_i(t+\Delta t) = v_i(t) + \dots$] Easy. → Choose suitably small Δt

→ Calculating the force → Difficult and Expensive. → $N \times N$ Calculation

→ Comparison with Off-lattice Monte Carlo Simulation.

N particles



REPEAT N times

- Randomly choose particle i → Calculate E_i
- Give a displacement $\Delta \vec{r}_i$ in a random direction.
- Calculate E_f
- If $\Delta E < 0$ → accept move.
- else accept with prob $e^{-\Delta E/k_B T}$.
- Repeat N times. → 1 MCS

So, message we are essentially solving $3 N$ differential equations for position $3 N$ differential equations for velocity in molecular dynamics and keep calculating force and with this new force keep updating these quantities right. So, that is all that is there. Now updating the expression for the position and velocity of the particles right. This is a

relatively very easy step all that one has to do is calculate a suitably small value of Δt , the Δt basically here you are discretizing time right when you solve the differential equation you continuously in analytic course.

So, then time is nearly continuous Δt goes to 0, but here you want to take finite you have to take a finite you are discretizing time and saying ok. I am looking at the positions at time t_1 at time t_2 at time t_3 $t_2 - t_1$ is constant $t_3 - t_2$ is constant and so on so forth. And Δt that the value of Δt or Δt has to be small enough, that the Newton's equations are integrated correctly and of course, we will check whether they are being integrated correctly or not.

But though Δt has to be small enough if you want to look at a very long trajectory you also want it to be large enough. I mean you do really do not want to look at take the smallest possible Δt , you want to take the largest possible a permissible Δt which allows you to integrate Newton's equation of motion correctly right. If you have a too large a Δt then your nutrients equation would not be calculated correctly it would not be updated correctly you would not to get the right solution to the Newton's equation of motion interacting by a potential.

If you take very small Δt then to have a large trajectory you will have an extremely long number of iterations you will have to wait for days for the simulation to complete. So, you want to really take a small enough Δt , but large is permissible right. So, that your simulation runs quickly and you can get your even lesser down to analyze your physics results. What I was saying is that the calculation of positions and velocities update of this there is a relatively very cheap and cheap computationally cheap process.

It is a easy process, however calculating the force is relatively difficult and computationally expensive. And why is that because you have to calculate the force for between a particle N all other end particles. Because in practical impact is the interaction could go to infinity right. Of course, there are steps to handle this aspect you were especially for short range forces, you own do not want an N cross N calculation you want to reduce it we will discuss that.

But in principle here for each calculation of force or to calculate the force between each pair of particles which is a N cross N process and then you were to calculate the distance and the expression. Whereas, this part if you have N particles you have N steps or rather

3 N steps to update position and update velocity right. So, large part when I say that we will be discussing molecular dynamics simulation, a large part of the discussion will actually be about this aspect and not this aspect this is trivial you should see. At the beginning at the introduction even before I go get down to the details.

Let me tell you what molecular dynamics simulation gives, you know you have position and velocity at each instant in time. But you can also study a system with a so called of lattice Monte Carlo simulations. We did a lattice Monte Carlo simulations in the rising model right in the previous module of the course. But you could also look at a system of interacting particles by Monte Carlo simulations and if you have potentials and particles can move around in space you can happen off lattice Monte Carlo simulations as well.

So, let me compare what advantages you have with Monte Carlo simulations, what advantages you have with molecular dynamics simulations when should one do a molecular dynamics simulations. And not be happy enough with a off lattice Monte Carlo simulations. Typically Monte Carlo simulations are much faster than molecular dynamics simulations. But before I compare I have to briefly tell you what is an off lattice Monte Carlo simulation right, only then can it can you compare there only then can I compare and only then can you take a judicious decision whether you want to do your you on a study system by Monte Carlo or by molecular dynamics.

So, what one does not know Monte Carlo simulation is one takes a box, just like in molecular dynamics and these red dots are essentially a large number of particles which are distributed in space. So, if for each you have an x coordinate no v coordinate no velocities in Monte Carlo simulations. So, what you have is the x coordinate of each of these particles right and in and space is continuous.

So, the particles can occupy any point in space not that they have to occupy certain discrete point in space. If that is true then you would call that you would call that essentially a lattice, so here particles can move around in space. Even if the even if they are sitting in a lattice, we are looking at a crystal they might be sitting on a lattice, but maybe they might be jiggling around due to thermal energy right.

So, then space is again continuous I mean they can move in continuous space about it is average lattice position that is what atoms do right, I mean in a crystal. And in a liquid or in a gas basically they move all around the space, I mean it is not that they can occupy

only discrete points on a lattice and move around that right. So, coming back to Monte carol simulations these particles are basically occupying different points in space they are not overlapping and to perform a Monte carlo simulation what one does is randomly choose particle as in ising model we were choosing a randomly choosing a spin in the lattice here.

We are just randomly choosing a particle using a random number generator if you want to give it a displacement. So, in ising model we were giving a flip. So, if the spin was pointing up we are giving a flip we are basically changing them by chain giving the spins of flip we were changing the microstate of the system. And then we would decide whether we would accept or reject the trial spin flipped here what we are going to do is give a displacement in a random direction to particle i right.

So, we will give a trial displacement of particle i in a random direction by this Δr_i . But before we give the random displacement we calculate the initial energy of the system right. Just like we calculated the initial energy in rising modeled case then after giving a random displacement so, suppose this particle this particle would have moved somewhere here.

So, that would change that would result in a change of the interaction between this particle and the other particles a change in the potential energy of the system and so, we calculate E_f the new energy after the displacement trial displacement. Now just as in the rising model if ΔE if the change in energy is less than 0 if the energy decreases then we accept the move, else we accept this trial displacement move with probability it is all minus ΔE by kBT .

If ΔE is positive then we accept it with probability it is all minus ΔE by kBT . And if we repeat this choosing a particle N times where N is the total number of particles in the system, then you say that you have done one Monte carol step right. So, basically you choose a random particle try to move it choose another random particle or choose another particle randomly try to move it. And you do this N times and you have essentially generated a different microstate with a different position of particles a different value of the energy. And whether high energy micro states will be accessed or not will depend upon the statistical physics.

This is of course, in only in equilibrium and if we repeat this N MCS times you would have basically generated so many different microstates of the system and you can calculate your statistical averages. Note while we were discussing all of this never once have I been mentioning the word velocity, never mentioned the word kinetic energy. It is just a position based you are changing the position what is the change in energy the whether the new microstate

We will be accessed or not with probability $e^{-\beta \Delta E}$ to the power ΔE by $k_B T$ rather $e^{-\beta E_i}$, i being the energy of the microstate by the partition function this is the importance of sampling.

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Monte Carlo (MC) $\rightarrow x_i(t)$

Mol. Dyn. (MD) $\rightarrow x_i(t) \quad v_i(t) \rightarrow$ Velocity profile in Shear flow/Poiseuille flow. or if you need exact trajectory in space.

VERLET ALGORITHM.

Taylor series: $x_i(t + \Delta t) = x_i(t) + \frac{dx_i}{dt} \Delta t + \frac{1}{2} \frac{d^2x_i}{dt^2} (\Delta t)^2 + \dots$

$x_i(t - \Delta t) = x_i(t) - \frac{dx_i}{dt} \Delta t + \frac{1}{2} \frac{d^2x_i}{dt^2} (\Delta t)^2 + \dots$

Adding $x_i(t + \Delta t) + x_i(t - \Delta t) = 2x_i(t) + a(t)(\Delta t)^2$

Subtracting: $x_i(t + \Delta t) - x_i(t - \Delta t) = 2v_i(t) \Delta t$

Velocity Verlet Algorithm

But in all of this there is no mention of velocity is just a position based. So, in Monte Carlo simulation and the degree of freedom which you have which you are working with two different different microstates be different microstates of the N symbol is $x_i(t)$. Whereas, in molecular dynamics simulations which I denote by MD molecular dynamics and Monte Carlo is MC Monte Carlo. You have in molecular dynamics we have access to both position and velocities, so this is the key difference.

So, if you want the exact trajectory of a spaceship in space you do molecular dynamics, the interaction might be the same $1/r$. But you cannot do a Monte Carlo because there do you are trying out random moves, if you want the exact trajectory of Neptune or a spaceship or some galaxies then you do molecular dynamics. Even when you are looking

at suppose solid liquid gas where you are interested in statistical properties of the system and not an astronomical system.

Say then where if you need to understand the physics of your system the velocity degree of freedom then you cannot do a Monte Carlo, Monte Carlo has only positions right. Now suppose you want to calculate the velocity profile of a fluid in shear flow or say in moisture flow, then you have to do molecular dynamics. Though Monte Carlo as I told you is faster it gives you statistical properties faster, but if you want some dynamical properties or you want to look at the approach from a non equilibrium system to a equilibrium system how the system is relaxing.

Then you would typically do a molecular dynamics simulations. Having said that let me tell you though we would not discuss it in great detail one also at times looks at Monte Carlos simulations to look at dynamics or the evolution of a system that is also done. But you do not have access to the velocity degree of freedom right.

So, this has been a general introduction to what and when should we use molecular dynamics, what is the basic ideas of molecular dynamics. Now slowly let me enter a more (Refer Time: 29:46) detail ok. As I told you there is the update of positions and velocities and this is the calculation of force right. The simple part is update of velocities and position and whereas one can also use the Runge Kutta method which was discussed in the differential equation module and what we will discuss in this module is another method is the so called Verlet algorithm ok.

One can also use the Runge Kutta, but we will discuss the Verlet algorithm and the Verlet algorithm has the advantage that the equations of motion that we use to update or to calculate Newton's equation of motion, the trajectory of the particles they are time reversible. So, that is implicitly their I mean the way this and the way this Verlet algorithm or the update of position and velocity is arranged.

So, in the Verlet algorithm all that we are using is nothing more than the Taylor series, the Taylor series expansion. Suppose you have the access to the position and velocity of all the particles, you have initializes the velocity and position of all the particles at time t . Then you can calculate well if you have the position you have also calculated the force, from force you get the acceleration. Then using Taylor series you can write down the position of particle i at time t plus Δt using $x_i t$.

So, you need to know the position of the particle at time t plus $\frac{dx}{dt}$ right, that is what the Taylor series expansion says calculated at time t into Δt plus half d^2x/dt^2 double derivative calculated at time t . So, this is nothing but the acceleration, acceleration can be calculated from the force into Δt whole square plus higher order terms right. Similarly you can write x_i at t minus Δt at time previous as $x_{i,t}$ you are doing just a Taylor series expansion nothing more than that.

But of course, this thing is nothing but the velocity this thing is nothing but the acceleration and if you have $x_{i,t-\Delta t}$ the only difference that you get is you have a negative sign here instead of a positive sign. Now the terms to remain that, see now if you add this equation and the this equation right. If you add these two equations then you essentially get $x_{i,t+\Delta t}$ the position of particle i at time t plus Δt . You get two $x_{i,t}$ the calculator at time t , acceleration at time t into Δt whole square and basically if you add it I bring this term to the right hand side of the equation, so this is your expression.

So, using Taylor series if you want the position of time at t plus Δt , you need the position at time t the position at time t right, the acceleration at time t . Moreover you need the position at time t minus Δt right two steps back. So, this is how you would calculate it, if you subtract this equation from this equation then you would get $x_{i,t+\Delta t}$ plus Δt . So, here you would get $x_{i,t+\Delta t}$ minus $x_{i,t-\Delta t}$, so which is our subtracting and then these terms would cancel. And what you would have is $\frac{dx}{dt}$ I have written as velocity intentionally this that is what it is calculated at time t into Δt .

So, you are basically you have just managed to calculate v_i at time t right. So, here you have position and which depends upon $x_{i,t+\Delta t}$ and here you can calculate the velocity at any time. But then what you need is the position at time t plus Δt and the position at t time t minus Δt . So, you need these two positions are two different times to be able to calculate this in general. Now doing a bit of algebra and some mathematical jugglery, you can also write Verlet algorithm into the velocity Verlet algorithm is just a bit more algebra and then that.

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Velocity Verlet Algorithm

$$z(t+\Delta t) = z(t) + v(t)\Delta t + \frac{1}{2}a(t)(\Delta t)^2$$
$$v(t+\Delta t) = v(t) + \frac{1}{2} \frac{F(t) + F(t+\Delta t)}{m}$$

→ Update Position.
Update Force.
Update Velocity.
Repeat.

And in the velocity Verlet algorithm what you do is $x(t + \Delta t)$ and Verlet and velocity Verlet are absolutely equivalent. You can even use this or you can use the Verlet algorithm I have a bias towards the velocity Verlet algorithm because I use it, but there is nothing holy about it you can use either of them. So, the velocity Verlet algorithm what you do is $x(t + \Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$.

So, you see that this is a time t this is a time t this is at time t right and then you get the position at time $t + \Delta t$. And the velocity can be written as $v(t + \Delta t)$ can be written as the velocity as time t , so the previous time the force or rather I should write the acceleration $F(t)/m$ is acceleration. So, the acceleration at time t and the acceleration at time $t + \Delta t$.

So, you see here again to calculate the velocity at time $t + \Delta t$ you need the force at two different times, including the force at time $t + \Delta t$ right. In the previous case to calculate velocity you were needing the position at time $t - \Delta t$, same here to calculate the position the new position of the particle after time t you were needing the position of the particle at $t - \Delta t$.

Whereas, this has simplified a bit and here all you need to update the position is the position velocity in oscillation at time t . However, to calculate the velocity at time $t + \Delta t$ you need the force or the oscillation at the previous time as well as the

acceleration at the current instant in time at time t plus Δt . So, in the Verlet algorithm you have to update the position first using this equation.

Once you have $x_{t+\Delta t}$ you can calculate $F_{t+\Delta t}$ right. Because you have the new position of with the new positions you can calculate the new forces save the old force in some other array. So, you have to update the force save the old force and with these new two forces update velocity and that is all that is there to molecular dynamics repeat. So, you basically you keep on doing this you have the position the new position the new force and the new velocity.

So, with that you can calculate the position at time $t+2\Delta t$, then you calculate the force at time $t+2\Delta t$ and then you calculate the velocity at time $t+2\Delta t$. You have access to these three immediately you can go to this step and calculate the position at $t+3\Delta t$. So, what are you getting? You are getting position velocity and force at incremental values of time.

You are getting essentially the trajectory in space x as a function of t as it in as t changes as the particles move around as time progresses. You have the velocity of particles as time progresses a t_1 t_2 t_3 t_4 t_3 being greater than t_2 t_2 being greater than t_1 right. So, that is all that is there in the update of position and velocity. However, you will see that the calculation the force calculation step we will take much more time.