Thermodynamics for Biological Systems: Classical and Statistical Aspects

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Lecture – 82
Integration Algorithms

So as I said that due to complex nature of U it is very difficult to obtain an analytical solution of the equation of motion. So, we often use numerical methods to get a solution of, of rt of equation of motion as we shown in equation number 1.

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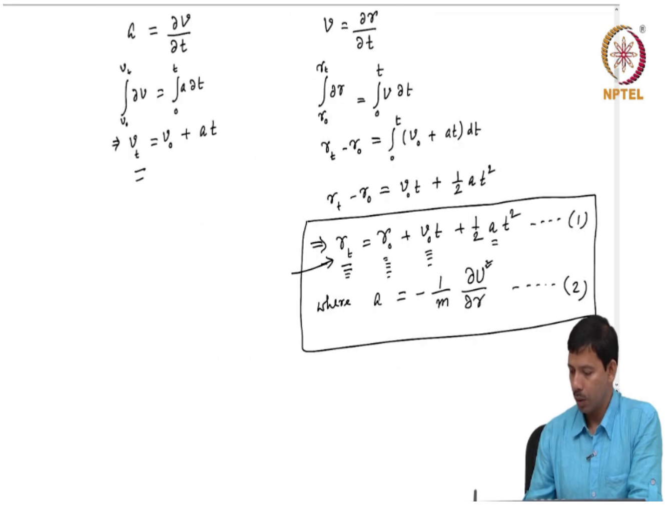

So, as I said that this rt we will now be obtained by using numerical methods and those numerical methods are called integration algorithms.

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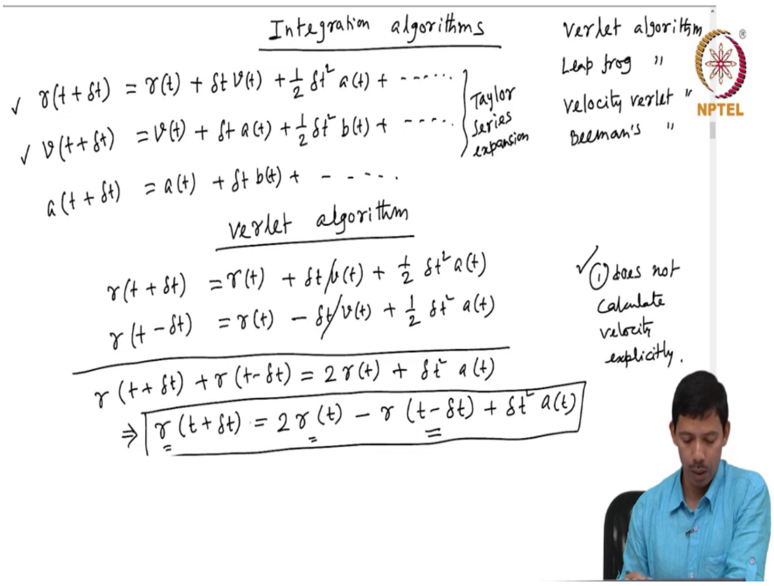

And there are several integration algorithms to obtain the new set of coordinates. And some of those very well known integration algorithms are Verlet algorithm, Leapfrog algorithm, we have velocity Verlet algorithm, we have Beeman's algorithm and so on. But all these algorithms they rely upon the Taylor series expansion.

So what is Taylor series expansion? Taylor series expansion tells that my position at time t plus delta-t would depend my position at time t plus delta t vt plus half del t square a t. And the series continuous so this is a Taylor series expansion Taylor series expansion.

$$r(t+\delta t) = r\,(t) + \ \delta t\, v(t) + \frac{1}{2}\,\delta t^2\, a(t) + \ \dots\dots$$

Likewise my velocity at time t plus delta-t could depend on my velocity at time t plus delta-t a t plus half del t square V t and so on, so forth.

$$v(t+\delta t) = v\,(t) + \ \delta t\, a(t) + \frac{1}{2}\,\delta t^2\, b(t) + \ \dots\dots$$

Likewise my acceleration also will depend on acceleration at time t plus del t bt and so on, so forth.

$$a(t+\delta t) = a\,(t) + \ \delta t\, b(t) + \ \dots\dots$$

So, all these algorithms they rely upon Taylor series expansion and how they differ from each other is where they truncate this series. So, so at some point, we have to truncate the series. And so these algorithms differ from one to each other where they truncate the series and as well as whether they explicitly calculate velocity and r or they calculate r and implicitly calculate V.

We will see two of them. So, first we will be talking about the Verlet algorithm. So in the Verlet algorithm, r is expanded up to third term and then it has been truncated. So, it has been truncated in the third term. So it also okay so if r t plus delta t is this what is your rt minus delta t. So, r t minus delta t I am sorry this is r, so rt minus delta t is your rt minus delta t VT plus half del t square a t.

$$r(t+\delta t) = r\,(t) + \ \delta t\, v(t) + \frac{1}{2}\,\delta t^2\, a(t) \qquad eqn\ (1)$$

$$r(t-\delta t) = r\,(t) - \ \delta t\, v(t) + \frac{1}{2}\,\delta t^2\, a(t) \qquad eqn\ (2)$$

If you sum the equation (1) and (2)

$$r\ (t+\ \delta t)+r\ (t-\delta t)=2r\ (t)+\ \delta t^2\ a(t)$$
$$r\ (t+\ \delta t)=2r\ (t)-r\ (t-\delta t)+\ \delta t^2\ a(t)$$

This is the Verlet algorithm. This is how we get the new confirmation $r\ (t+\ \delta t)$ starting from the information of r (t). So, what is the disadvantage of this algorithm?

Number one disadvantage is you need to have r at (t – δt) so that means you have to have an approximate set of coordinates of r which is a preceding time of (t – δt). The second and the major disadvantage of verlet is that it does not calculate velocity explicitly. So, it has advantage and disadvantage both since it does not calculate the velocity explicitly, this algorithm is faster. So that is an advantage but the disadvantage is that you do not have the velocity very accurately calculated in Verlet algorithm.

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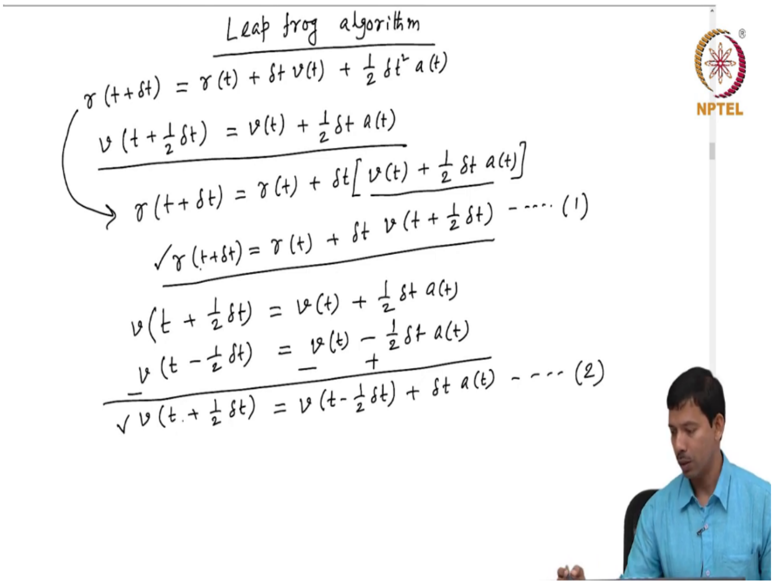

And therefore some scientists prefer to use leapfrog algorithm. So, in the leapfrog algorithm the velocity is computed explicitly. So, in leapfrog algorithm the r, the new set of coordinates is again obtained by truncating the series at third term.

$$r\ (t+\delta t)=r(t)+\ \delta t\ v(t)+\frac{1}{2}\delta t^2\ a(t)$$

In leapfrog algorithm, velocity is calculated at t plus half delta t.

$$v\left(t+\frac{1}{2}\delta t\right)=v(t)+\frac{1}{2}\ \delta t\ a(t)$$

So if using this expression I can rewrite this equation as

$$r\,(t+\,\delta t) = r\,(t) +\,\delta t\,[v(t) + \frac{1}{2}\delta t\,a(t)]$$

$$r\,(t+\,\delta t) = r\,(t) +\,\delta t\,v\left(t+\frac{1}{2}\delta t\right) \qquad eqn\,(1)$$

this is how the coordinates are obtained.

And the velocity is obtained from

$$v\left(t+\frac{1}{2}\delta t\right) = v(t) + \frac{1}{2}\,\delta t\,a(t)$$

$$v\left(t-\frac{1}{2}\delta t\right) = v(t) - \frac{1}{2}\,\delta t\,a(t)$$

And subtracting these two, I get,

$$v\left(t+\frac{1}{2}\delta t\right) = v\left(t-\frac{1}{2}\delta t\right) +\,\delta t\,a(t) \qquad eqn\,(2)$$

Vt plus half delta t is equal to Vt minus half delta t plus delta t a t. So, these are the two equations (1 and 2) we solve in leapfrog algorithms. One is your new coordinates $r\,(t+\,\delta t)$ and the other is your velocity at $v\,\left(t+\frac{1}{2}\delta t\right)$. So, now if you look at the expressions of r and v, your r is having a jump from t to t plus delta t whereas my velocity is jumping from t to half delta t.

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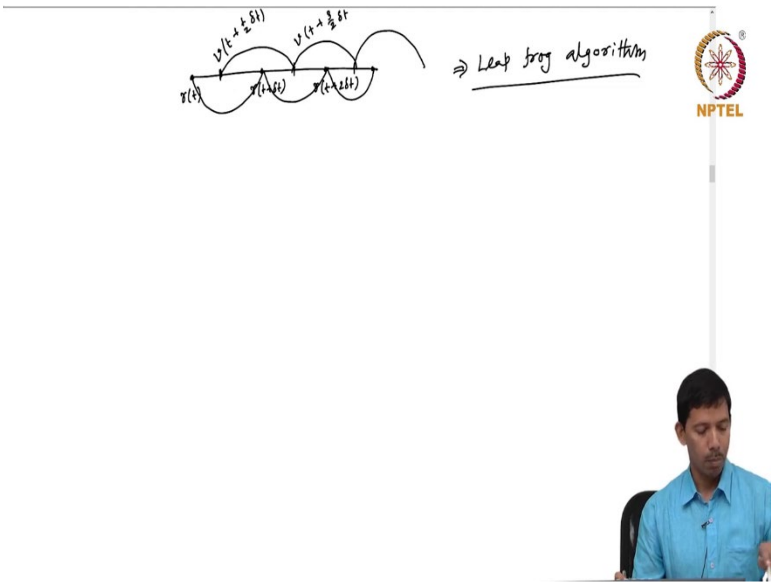

So, in other words, in leapfrog algorithm, this is your r (t), this is your r at time $(t+\,\delta t)$ if this is your coordinates. And this is your $r\,(t+\,2\delta t)$and so on, so forth whereas your velocity is being computed at here. Your velocity is being computed at V time $\left(t+\frac{1}{2}\delta t\right)$ it is again being computed at here, which is $\left(t+\frac{3}{2}\delta t\right)$. So, what you see here is basically position and the velocity they are leaping over the other.

So, since velocity and positions they are leaping over the other, this algorithm is called the leap, is like a frog, position is leaping over the velocity and velocity is leaping over the position and that is what is called leap frog algorithm. So, as you can easily see in the leapfrog algorithm that this is much more accurate, because it is explicitly calculating the velocity and it is also calculating velocity at every half delta t time step.

And therefore this method is much more accurate which is the advantage but the disadvantage again would be that the memory requirement would be much more because here you have to store both the positions and the velocity. And therefore your memory requirement for leapfrog algorithm will be more than the Verlet algorithm. So, I think these two algorithms given you some idea how you can make your system move starting from one structure to the other structure.