

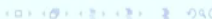

An Introduction to Programming through C++
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Lecture 27 Part-2 - Cosmological Simulation - Second-order Euler method

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What we discussed

- ▶ The basic cosmological simulation problem
- ▶ First order (Euler) method

Next: A second order method



Welcome back. In the previous segment, we discussed the basic cosmological simulation problem and we discussed the first-order Euler method for it. In this segment we will talk about a second-order method which is going to be a lot more accurate.

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A second order method

A better approximation is obtained by using 3 Taylor series terms:



$$f(t + \Delta) \approx f(t) + f'(t)\Delta + f''(t)\frac{\Delta^2}{2}$$

Can be written differently:

$$\begin{aligned} & f'(t)\Delta + f''(t)\frac{\Delta^2}{2} \\ & \approx \left\{ f'(t) + f''(t)\frac{\Delta}{2} \right\} \Delta \\ & \approx f'\left(t + \frac{\Delta}{2}\right)\Delta \end{aligned}$$

First order approx for $f'(t + \frac{\Delta}{2})$

Alternate statement:

$$f(t + \Delta) \approx f(t) + f'\left(t + \frac{\Delta}{2}\right)\Delta$$


So the idea is simple. Instead of using two terms of the Taylor series we are going to use three terms. So $f(t + \Delta)$, f is the variable we want to estimate at time $t + \Delta$ we are given

the value at time t , so $f(t) + \Delta$ is $f(t) + f'(t) \cdot \Delta$ and in the previous method we had stopped at this point.

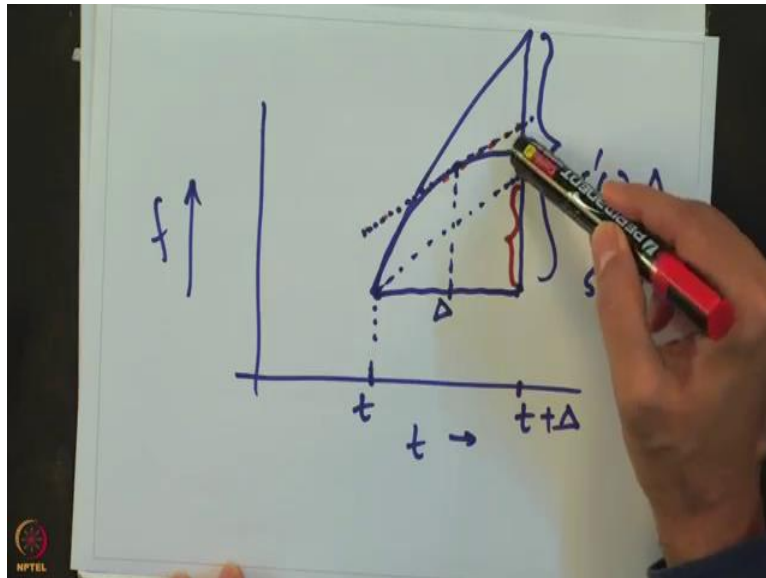
But here we are going to add one more term, so $+ f''(t) \cdot \Delta^2/2$. So this is still approximately equal to because as we know the Taylor series just keeps going and we are not taking all the terms of the series. We are just taking powers, second powers of Δ . And therefore, by the way it is called second-order method. Now this can be written in a different manner, so let us look at this part just this part. So I have so this is what I have written down over here and I am going to rewrite it by taking Δ common because Δ is there in both.

So this I brought out this Δ so here I just get $f'(t)$ and here I get $f''(t) \cdot \Delta/2$. Now if you look at this you may observe that this is actually a quantity which can be written differently. So in what way? Well I can write it this way. Why is that? So this is just a first order approximation of this. How? Well, if I want to know the value of variable at $t + \text{something}$, if I want to know the value of the variable at $t + \text{something}$, how do I get it? Well, I write it as the value of the variable at t , then plus the derivative of this plus this something in the multiplication.

So indeed in this parenthesis what I have is the first-order approximation of this, we are going in other way of course that we are saying. So we are going to substitute this for this over here. So instead of this we are going to get this term. So here is the alternate statement of the second-order method. So we have same thing $f(t) + \Delta$ is equal to the first term does not change but this second term looks like this because this taken first-order approximation is exactly what this is.

This alternate statement is nice in many ways. Why? First of all, there are only two terms, so that is good. Second, the second derivative has gone away so it is a simpler thing and that almost looks like the first-order method. The only difference is that in the second term we had, we had t over here $f'(t) \cdot \Delta$. So here we have $t + \Delta/2$, so that is the only difference but this is still essentially the same expression and therefore in terms of error, this is going to be as good but because it is simpler we are going to use this in our algorithm. So we will use this form but before we get to that, I want to look at what is geometrically just as to just so that you get a better intuition of what is going on over here.

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A second order method

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Can be written differently:

$$\begin{aligned} & f'(t)\Delta + f''(t)\frac{\Delta^2}{2} \\ & \approx \{f'(t) + f''(t)\frac{\Delta}{2}\}\Delta \\ & \approx f'(t + \frac{\Delta}{2})\Delta \end{aligned}$$

First order approx for $f'(t + \frac{\Delta}{2})$

Alternate statement:

$$f(t + \Delta) \approx f(t) + f'(t + \frac{\Delta}{2})\Delta$$

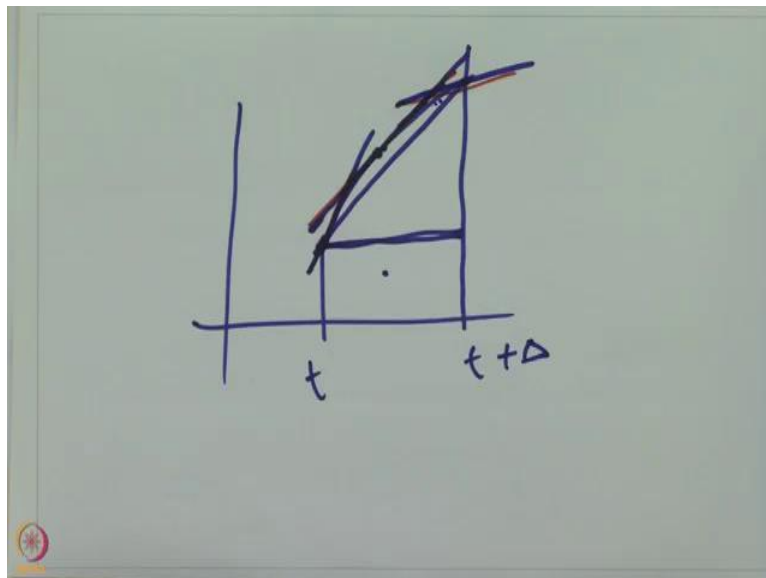
So, again, let me draw a picture, so this is time and say let us say this is t and let us say this is $t + \Delta$ and on this axis we have f . So let say so I am plotting the curve let say something like this, okay? So this is the plot of f , now what does the first order approximation say? The first-order approximation. The first-order approximation says that the increment that you are going to get is going to be the distance, so this distance is Δ so the time difference which is Δ times the slope and what is the slope? The slope of the tangent, so the slope of the tangent is going to be something like this.

So this whole thing is going to be $f'(t) \cdot \Delta$ because this f' is nothing but the slope of the tangent, all right. So what is the second-order term, the second-order method say? The second-order method is saying that look, do not take the slope at time t sorry, do not take the slope at time t but take it at time $t + \Delta/2$.

So take it somewhere over here. So take it somewhere over here and now the slope looks something like this, okay. So I want to multiply this slope by this delta and then add that up. So to do that, I am just going to make it appear somewhere over here, so this slope I have just dragged it down, now I am going to multiply it by the delta and what has now happened is that the product is going to get me this.

So this is this slope multiplied by this delta, this whole thing is this slope see that the slope is going really sharp. So now it turns out that taking the slope in the middle is a good idea. In this picture also you can see that what I am getting to over here is much closer to the actual curve than this is. And there is, there is a different way of there is a different reason different way of thinking about it and that is that...

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To go from here to here, if I take the so when I multiply this distance by the slope I am sort of assuming that the slope is going to be the same inside this entire interval. So if the slope was really the same in the entire interval then it would be just a straight line. In that case multiplying it would give me the exact answer.

But the slope is not the same, so should I take the slope at the beginning, should I take the slope at the end or should I take slope in the middle? Well, the slope in the middle is likely to be closer to the average slope and therefore we should be taking the slope in the middle. So that is really the intuition behind this formula. It comes out from the Taylor series but the intuition is this.

That I want the slope I want to multiply delta by the slope but I should pick a value which is sort of close to all the values in this interval. So this is t , this is $t + \Delta$. I should pick a value of the slope which is close to all the values. So what are the values? Well, the slope starts like this then it goes like this and it finally comes like this. So the slope in the middle which is this, is kind of like this, kind of like this, it is closer to both and therefore we get less error. So we just did this, we got the geometric interpretation and this is just to informally see why this method should be doing better.

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Using $f(t + \Delta) \approx f(t) + f'(t + \frac{\Delta}{2})\Delta$


Suppose $f = r_i$, i.e. position of star i . Then $f' = v_i$, i.e. velocity. Let $t = 0$.

$$r_i(\Delta) \approx r_i(0) + v_i(\frac{\Delta}{2})\Delta$$

Suppose $f = v_i$, velocity of star i . Then $f' = a_i$, i.e. acceleration. Let $t = \frac{\Delta}{2}$.

$$v_i(\frac{\Delta}{2} + \Delta) \approx v_i(\frac{\Delta}{2}) + a_i(\Delta)\Delta = v_i(\frac{\Delta}{2}) + \left(\sum_{j \neq i} G \frac{m_j(r_j(\Delta) - r_i(\Delta))}{|r_j(\Delta) - r_i(\Delta)|^3} \right)$$

If we know $r_i(0)$, $v_i(\frac{\Delta}{2})$, we can calculate $r_i(\Delta)$, $v_i(\Delta + \frac{\Delta}{2})$.



All right, so let us now try to apply this in the context of cosmological simulation. So we will do exactly like how we proceeded before. So let say f is r_i , so this f is r_i and r_i as we know is the position of star i . So what is f' ? Well, f' is the derivative of position which is the velocity. Again, we are going to let t be 0. So what does this give us? So this tells us that the position at time Δ is the initial position plus the velocity at the middle of the interval times Δ . Now this may be another way to see why this new method is better.

Because what we are saying over here is that we are multiplying Δ by the velocity in the middle. So we are saying yes, the velocity might be changing and we are hoping that the velocity in the middle is a better representative of the velocities in the entire interval. Intuitively the velocity gets lots of time to change from our selected velocity if we select at the middle but if we select it at the beginning. If we select it in the middle, then the initial velocity or the final velocity is not too far in time from the middle.

And therefore, the middle is a better representative, so that is as far as the position is concerned. So if we know the position at time 0 and we know the velocity at time Δ by 2 then we can calculate the position at time Δ . Next let say let see what happens if f is the velocity, so then f' is the acceleration and again let us take time equal to 0, sorry this time we are going to take time equal to Δ by 2, you will see why, Okay.

So what becomes of this? So t is $\Delta/2$, so we are going to get $\Delta/2 + \Delta$. This is going to be v_i of Δ by 2, remember we are substituting v_i for f and t and $\Delta/2$ for t . And f' is acceleration and t is $\Delta/2$ so this whole thing becomes $\Delta \cdot \Delta$.

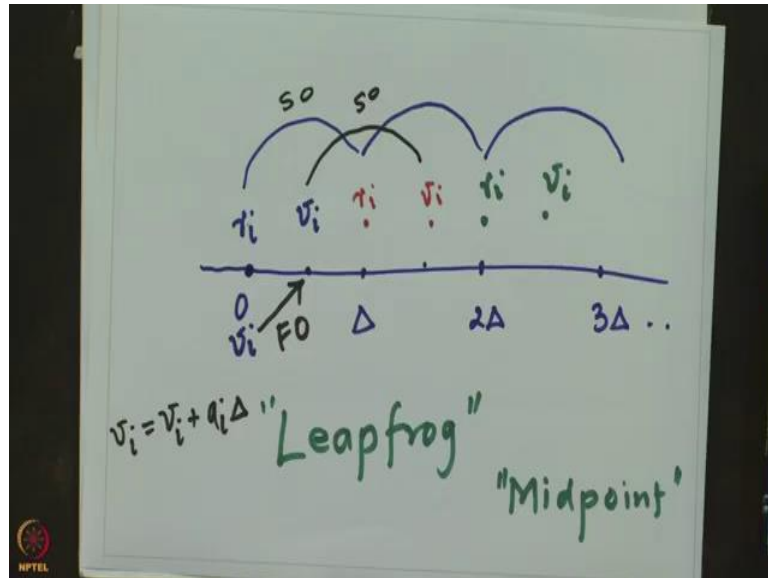
So this tells us how we could calculate the velocity at time $\Delta/2 + \Delta$ and for that we need to know the velocity at time Δ by 2 and then the acceleration at time Δ . Do you know the acceleration at time Δ ? Well, as it happens we do, so this is the velocity term, this is the for the acceleration what I am going to get. Well, for the acceleration we already know that it depends only on the position oh, I think I need a Δ over here, so there is a Δ over here which I have which I need to add.

So this acceleration term is this term and this is the acceleration at time Δ . Do you know this term? Well, we do if we know r_i of Δ and by the way when I say we can calculate r_i , I mean we can do it for all stars. So we can know it for r_j and everything as well, all right. So yeah, there is a Δ term over here.

Basically what where, what has this led us to? So this says that if we know $r_i(0)$ and v_i of Δ then we can calculate r_i of Δ and v_i of $\Delta + \Delta$ by 2, okay let us just check again. So can we calculate r_i of Δ ? Well, here is r_i of Δ , well we have $r_i + 0$, yes we said if we know $r_i(0)$, do we know v_i of Δ by 2? Yes, if we, we said if we know $v_i(\Delta/2)$. So yes, if we know these two things, we will be able to calculate r_i of Δ . Will we be able to calculate v_i of $\Delta + \Delta/2$?

Well, v_i of $\Delta + \Delta$ by 2 we are going to update as $v_i(\Delta/2)$. Do we know this? Well, yes we said if we know $v_i(\Delta/2)$, do we know these things? Well, all $r_i(\Delta)$ we have calculated in this step over here. So therefore, we know these terms as well and therefore we can calculate this. So what does this mean, what have we exactly accomplished? So I am going to draw a timeline over here.

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Okay, so this is 0, then this is Δ then this is 2Δ , then this is 3Δ and so on. So at this point we know r_i and at this middle point we know v_i . And what that tells us that knowing these two things knowing this and this, we can calculate this and this but now we can apply the same argument or let me let me write it down properly. We can calculate r_i for this point and v_i for this point. Now I can apply the same argument to these two terms the same calculation. So I will be able to calculate the r_i over here and the v_i over here and I can keep going. So it is like the previous thing but r_i and v_i values are not at the same time, at the same time instant.

Okay, so they are at these staggered time instants. In fact what is going on is that the r_i values are calculated at integral multiples of Δ , odd multiples of $\Delta/2$. So these are the r_i calculations and these are the v_i calculations. So you can fancifully think of the r_i values sort of jumping across the v_i values and in fact this method is also called the Leapfrog method or it is also called the Midpoint method.

But anyway so this is how the updates were. We calculate these two first, from these two we can calculate these two, from these two we can calculate these two and so on. So that is exactly our algorithm. What I am going to write down now is just this in a little bit more like code first of all.

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Using $f(t + \Delta) \approx f(t) + f'(t + \frac{\Delta}{2})\Delta$

Suppose $f = r_i$, i.e. position of star i . Then $f' = v_i$, i.e. velocity. Let $t = 0$.

$$r_i(\Delta) \approx r_i(0) + v_i(\frac{\Delta}{2})\Delta$$

Suppose $f = v_i$, velocity of star i . Then $f' = a_i$, i.e. acceleration. Let $t = \frac{\Delta}{2}$.

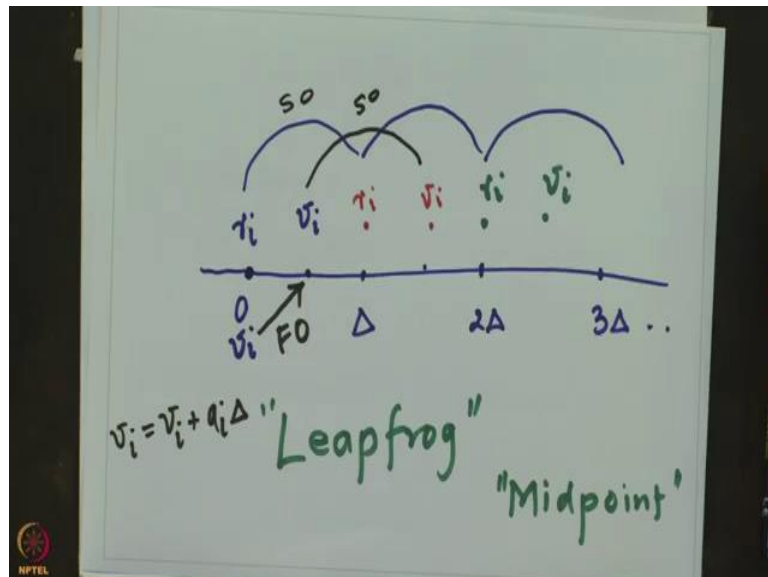
$$v_i(\frac{\Delta}{2} + \Delta) \approx v_i(\frac{\Delta}{2}) + a_i(\Delta)\Delta = v_i(\frac{\Delta}{2}) + \left(\sum_{j \neq i} G \frac{m_j(r_j(\Delta) - r_i(\Delta))}{|r_j(\Delta) - r_i(\Delta)|^3} \right)$$

If we know $r_i(0), v_i(\frac{\Delta}{2})$, we can calculate $r_i(\Delta), v_i(\Delta + \frac{\Delta}{2})$.

But we can repeat the step to get $r_i(2\Delta), v_i(2\Delta + \frac{\Delta}{2})$

And so on.

We know $r_i(0)$. How do we get $v_i(\Delta/2)$?



We can repeat the steps to get things for 2Δ and $2\Delta + \Delta/2$ and so on. Well, there is a little bit of problem though. So we said if we know these two things, but do we know these two things? Well, we do not, what was given to us were the positions and the velocities at time 0. So we know v_i at this time and r_i at this time, so our input specification said that we are given the positions and the velocity at time 0, we were not given this. So can we get this? Well, by now you should be able to guess this, can we get this? Well, given the velocity over here we can always get this if we know the acceleration because that is we can do this by a first-order Euler expression, we have update. So to go from here to here we will use a first-order update but note that happens only once. So before we get the whole process started, we are going to do this first-order update to get the velocity at this point. So what is the expression needed over here? So we are going to have v_i equals the original v_i + acceleration times Δ , so that is the first-order update. So that is what we are going to use here.

So we were given these two things, from that we got the velocity over here and r_i already we have and now we are going to use the method on this slide to get these, these, these and how are we getting these? So this is a second-order update. This is also a second-order update, so all of these are second-order updates. So we do one first-order update at the very beginning and subsequently we only do second-order updates. All right, so that is what the code or the algorithm is going to have.

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The algorithm

1. Read simulation duration, step size, number of stars into T, Δ, n .
2. For $i = 0..n-1$: Read initial position, velocity, mass into $r[i], v[i], m[i]$
3. For all i : $v[i] = v[i] + \left(\sum_{j \neq i} G \frac{m[j](r[j]-r[i])}{|r[j]-r[i]|^3} \right) \frac{\Delta}{2}$ First order update for $v[i]$
 $v[i]$ now hold velocities for time $\Delta/2$
4. For $s = 1, \dots, T/\Delta$:
 $r[i]$ holds position at time $(s-1)\Delta$, $v[i]$ holds velocities at $(s-0.5)\Delta$
5. For $i = 0..n-1$: $r[i] = r[i] + v[i]\Delta$ Position at $s\Delta$
6. For $i = 0..n-1$: $a[i] = \sum_{j \neq i} G \frac{m[j](r[j]-r[i])}{|r[j]-r[i]|^3}$ Acceleration at $s\Delta$
7. For $i = 0..n-1$: $v[i] = v[i] + a[i]\Delta$ Velocity at $(s+0.5)\Delta$
8. end for

First order update used only in step 3.
 Second order updates used in loop steps 5, 7.

Overall accuracy is high.



So as before we will read simulation duration, step size, number of stars into T, Δ, n . Then we will read the initial position, velocity, mass into those arrays and then this is going to be the first-order update that we talked about, so calculating v_i at this position. So at time $\Delta/2$ and you can see that that is why we are multiplying by time $\Delta/2$ and the values over here

are at time 0. So these are values at time 0 and from that we are now getting v_i at time $\Delta/2$.

And now we are just going to do this t/Δ times and at the beginning of the loop r_i will hold position at time $(s - 1)\Delta$, v_i will hold velocities at time $s - \Delta/2$. So we are effectively at this point in our execution. So at this point we have advanced to this point, so r_i is going to be over here, we have not got to the red values. So at this point r_i is holding the positions at 0 and v_i is going to be holding the positions at half.

But s is 1 over here, so this is $1 - \Delta/2$, so that is exactly the right thing. So exactly as we said, we will calculate the updated values of the position and that will get us the position at this time. So from this we got to this time. And then we will use the acceleration calculated earlier to go from this point to this point, so that will take us to acceleration sorry it should be no, yeah. So this is really the acceleration at $s\Delta$ not earlier. We are going to calculate the acceleration at this point. So we calculated the acceleration at this point and this acceleration we are going to add, so that will bring us to this point.

So as a result our velocity will be available at this point which is $s + \Delta/2$, $s + \Delta/2$ times Δ . That is it, that is the entire algorithm. So as we said earlier, the first-order update is used only in this step and over here and over here we are using second-order updates. So as a result the overall accuracy is high. This does turn out to be a good algorithm, all right.

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So what have we discussed in this segment? So we have discussed the second-order method and we have discussed sort of the details of the entire algorithm based on the second-order method. In the next segment I will show you the program but we will take a short break.