SUMMARY FOURTH LECTURE

CONTENTS

I. EQUATIONS OF MOTION

Consider a particle of mass m moving along the x-axis, the equations of motion are

$$\begin{cases} \dot{x} &= \dfrac{p(t)}{m} \\ \dot{p} &= F(t) \end{cases} . \tag{1}$$

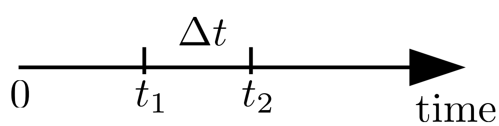
II. EULER INTEGRATOR

Suppose we know the position $x(t)$, momentum $p(t)$, and force $F(t)$ at a specific time t. Let's rewrite the equations of motion by using the definition of time derivative:

$$\begin{cases} \dot{x} &= \dfrac{d}{dt}x = \lim\limits_{\Delta t \to 0} \dfrac{x(t+\Delta t) - x(t)}{\Delta t} = \dfrac{p(t)}{m} \\ \dot{p} &= \dfrac{d}{dt}p = \lim\limits_{\Delta t \to 0} \dfrac{p(t+\Delta t) - p(t)}{\Delta t} = F(t) \end{cases} . \tag{2}$$

Time derivatives are defined for time intervals Δt infinitely small.

Consider instead finite time intervals, e.g. let Δt t be the difference between two specific moments t_2 and t_1 on the timeline.



Then, we rewrite the equations of motion without the limit:

$$\begin{cases} \dfrac{x(t+\Delta t) - x(t)}{\Delta t} = \dfrac{p(t)}{m} \\ \dfrac{p(t+\Delta t) - p(t)}{\Delta t} = F(t) \end{cases} . \tag{3}$$

Multiplying by Δt, and rearranging the equations, we obtain the position and the momentum at time $t + \Delta t$:

$$\begin{cases} x(t+\Delta t) = x(t) + \dfrac{p(t)}{m}\Delta t \\ p(t+\Delta t) = p(t) + F(t)\Delta t \end{cases} . \tag{4}$$

We observe that, by applying the definitions $\dot{x}(t) = \frac{p(t)}{m}$ and $\dot{p}(t) = F(t)$, we obtain

$$\begin{cases} x(t+\Delta t) = x(t) + \dot{x}(t)\Delta t \\ p(t+\Delta t) = p(t) + \dot{p}(t)\Delta t \end{cases} . \tag{5}$$

Then, the Euler approximation is equivalent to truncating the Taylor series of position and momentum at the second term. Unfortunately, this is not a good approximation, because it does not conserve the total energy

$$E = \frac{p^2}{2m} + V(x)\,. \tag{6}$$

III. SEMI-IMPLICIT EULER INTEGRATOR

To correct the Euler integrator, we simply replace the momentum $p(t)$ at time t, with the momentum $p(t + \Delta t)$ at time $t + \Delta t$ in the first equation:

$$\begin{cases} x(t+\Delta t) = x(t) + \dfrac{p(t+\Delta t)}{m}\Delta t \\ p(t+\Delta t) = p(t) + F(t)\Delta t \end{cases}. \tag{7}$$

Inserting the second equation into the first equation yields

$$\begin{cases} x(t+\Delta t) = x(t) + \dfrac{p(t) + F(t)\Delta t}{m}\Delta t \\ p(t+\Delta t) = p(t) + F(t)\Delta t \end{cases}, \tag{8}$$

and finally

$$\begin{cases} x(t+\Delta t) = x(t) + \dfrac{p(t)}{m}\Delta t + \dfrac{F(t)}{m}\Delta^2 t \\ p(t+\Delta t) = p(t) + F(t)\Delta t \end{cases}. \tag{9}$$

Consider now a time interval $[0,\,\tau]$, and a time-discretization into N_τ sub-intervals $[t_k, t_{k+1}]$ of equal length Δt such that

$$\begin{aligned} t_0 &= 0 \\ t_1 &= \Delta t \\ t_2 &= 2\Delta t \\ &\dots \\ t_{N_\tau} &= \tau = N_\tau \Delta t \end{aligned} \tag{10}$$

The semi-implicit Euler integrator is generalized as

$$\begin{cases} F(t_k) = -\dfrac{d}{dx}V(x(t_k)) \\ x(t_{k+1}) = x(t_k) + \dfrac{p(t_k)}{m}\Delta t + \dfrac{F(t_k)}{m}\Delta t^2 \\ p(t_{k+1}) = p(t_k) + F(t_k)\Delta t \end{cases}. \tag{11}$$

where we added a line for the computation of the force at time t_k provided a potential energy function $V(x)$.

IV. VELOCITY VERLET INTEGRATOR

The Euler integrator is based on the truncation of the Taylor series at second term. To improve the accuracy of the solution, we can add the third term of the Taylor expansion of position and momentum:

$$\begin{cases} x(t+\Delta t) = x(t) + \dot{x}(t)\Delta t + \dfrac{1}{2}\ddot{x}(t)\Delta t^2 \\ p(t+\Delta t) = p(t) + \dot{p}(t)\Delta t + \dfrac{1}{2}\ddot{p}(t)\Delta t^2 \end{cases}. \tag{12}$$

At time t, we know all the terms but $\frac{1}{2}\ddot{p}(t)\Delta t^2$. To find an expression for this term, we Taylor-expand the time derivative of the momentum, and we truncate at the second term:

$$\dot{p}(t+\Delta t) = \dot{p}(t) + \ddot{p}(t)\Delta t\,. \tag{13}$$

We now multiply both sides by $\frac{1}{2}\Delta t$:

$$\frac{1}{2}\dot{p}(t+\Delta t)\Delta t = \frac{1}{2}\dot{p}(t)\Delta t + \frac{1}{2}\ddot{p}(t)\Delta t^2 \,. \tag{14}$$

Rearranging, we obtain an expression for the unknown term in eq. 12:

$$\frac{1}{2}\ddot{p}(t)\Delta t^2 = \frac{1}{2}\dot{p}(t+\Delta t)\Delta t - \frac{1}{2}\dot{p}(t)\Delta t \,. \tag{15}$$

Inserting eq. 15 into eq. 12 yields

$$\begin{cases} x(t+\Delta t) = x(t) + \dot{x}(t)\Delta t + \frac{1}{2}\ddot{x}(t)\Delta t^2 \\ p(t+\Delta t) = p(t) + \dot{p}(t)\Delta t + \frac{1}{2}\dot{p}(t+\Delta t)\Delta t - \frac{1}{2}\dot{p}(t)\Delta t \end{cases} . \tag{16}$$

In the second equation, we calculate the difference between the red terms, and obtain

$$\begin{cases} x(t+\Delta t) = x(t) + \dot{x}(t)\Delta t + \frac{1}{2}\ddot{x}(t)\Delta t^2 \\ p(t+\Delta t) = p(t) + \frac{1}{2}\dot{p}(t)\Delta t + \frac{1}{2}\dot{p}(t+\Delta t)\Delta t \end{cases} . \tag{17}$$

By applying the definitions of $\dot{x} = \frac{p}{m}$, $\ddot{x} = \frac{F}{m}$ and $\dot{p} = F$, we obtain:

$$\begin{cases} x(t+\Delta t) = x(t) + \frac{p(t)}{m}\Delta t + \frac{1}{2}\frac{F(t)}{m}\Delta t^2 \\ p(t+\Delta t) = p(t) + \frac{1}{2}F(t)\Delta t + \frac{1}{2}F(t+\Delta t)\Delta t \end{cases} , \tag{18}$$

and rearranging with square brackets

$$\begin{cases} x(t+\Delta t) = x(t) + \frac{p(t)}{m}\Delta t + \frac{1}{2}\frac{F(t)}{m}\Delta t^2 \\ p(t+\Delta t) = p(t) + \frac{1}{2}\left[F(t) + F(t+\Delta t)\right]\Delta t \end{cases} . \tag{19}$$

If we consider a time interval discretized as in eq. 10, then the velocity Verlet integrator is generalized as

$$\begin{cases} F(t_k) = -\frac{d}{dx}V(x(t_k)) \\ x(t_{k+1}) = x(t_k) + \frac{p(t_k)}{m}\Delta t + \frac{F(t_k)}{m}\Delta t^2 \\ F(t_{k+1}) = -\frac{d}{dx}V(x(t_{k+1})) \\ p(t_{k+1}) = p(t_k) + \frac{1}{2}\left[F(t_k) + F(t_{k+1})\right]\Delta t \end{cases} , \tag{20}$$

where we have made explicit the steps where the force is calculated. The main difference between velocity Verlet and Euler integrator is that the former is based on a third-order truncation of the Taylor series, whereas the latter is based on a second-order truncation. This makes velocity Verlet's integrator more accurate, but requires the force to be calculated twice, at time t_k and time t_{k+1}. Thus, the higher accuracy requires more computational effort.