

Solving Newton's equations of motion

• Verlet method.

The 2nd order ODE =

$$\frac{d^2x}{dt^2} = F(x, t) \quad (1)$$

h as the discretized step. Let us expand x with Taylor expansion.

$$\text{add } \left\{ \begin{array}{l} x(h) = x(0) + h \frac{dx(0)}{dt} + \frac{h^2}{2!} \frac{d^2x(0)}{dt^2} + \frac{h^3}{3!} \frac{d^3x(0)}{dt^3} + O(h^4) \quad (2) \\ x(-h) = x(0) - h \frac{dx(0)}{dt} + \frac{h^2}{2!} \frac{d^2x(0)}{dt^2} - \frac{h^3}{3!} \frac{d^3x(0)}{dt^3} + O(h^4) \quad (3) \end{array} \right.$$

$\nearrow F(x, 0)$
 $\searrow F(x, 0)$

gives $x(h) = 2x(0) - x(-h) + h^2 F(x, 0) + O(h^4) \quad (4)$

This is the basic algorithm. However, we don't know $x(-h)$ in the first place, so the very first point has to be approximated by (3):

$$x(-h) \approx x(0) - h v(0) + \frac{h^2}{2} F(x, 0)$$

We can also have

$$v(h) \approx v(0) + \frac{F(h) + F(0)}{h} h$$

\nwarrow average

This is called velocity Verlet.

Leapfrog (Störmer) Method

$$\text{For } x, \quad x(h) \sim x(0) + v(0) \cdot h + \frac{1}{2} F(0) h^2$$

$$\text{For } v, \quad v(h) \sim v(0) + \frac{F(h) + F(0)}{2} h \quad (\text{same as Verlet})$$