MD-1

Molecular Dynamics

Galaxy formation
Nanoclusters (QM-force classical-move nuclei)
↓ Protein folding

A powerful and widely used research tool (yet very simple)

$$v = \frac{dx}{dt} \longrightarrow dx = v\,dt \longrightarrow x = x + v\,dt$$

$$a = \frac{F(x,v)}{m} = \frac{dv}{dt} \rightarrow dv = \frac{F(x,v)}{m}\,dt \rightarrow v = v + \frac{F(x,v)}{m}\,dt$$

CODE:

1) start with x_0 v_0

2) get x_1 v_1 ← iterate (not unlike Fibonacci code)

→ $x(t)$ $v(t)$ ✗ dt must be small

Slight subtlety

$$x_1 = x_0 + v_0\,dt$$

$$v_1 = v_0 + \frac{F(x_0, v_0)}{m}\,dt \quad \text{vs} \quad v_1 = v_0 + \frac{F(x_1, v_0)}{m}\,dt$$

"Euler" ↑ "Leapfrog" ↑

Leapfrog is much more stable

HW 1) $F(x,v) = -kx$ ← HW 2

2) $= -kx - \gamma v$ ← OPTIONAL

3) $= -kx - qx^3 - \gamma v$ ← HW 3