Notas de aula

Introdução à Física Computacional

Prof. Gerson – UFU – 2019

Atendimento:

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- Horário: sextas-feiras 16:00 – 16:50

1st and 2nd order differential equations

→ While Euler and Runge-Kutta solve 1st order ODEs, in physics we often deal with 2nd order ODEs → Newton's law

1st order ODEs

$$\frac{d\vec{y}(t)}{dt} = \vec{f}(t, \vec{y})$$

$$\vec{y}(0) = \vec{y}_0$$

Runge-Kutta
[wikipedia]

reduction of order

2nd order ODEs

$$\frac{d^2\vec{r}(t)}{dt^2} = \vec{a}(t, \vec{r}(t))$$

$$\vec{r}(0) = \vec{r}_0$$

$$\dot{\vec{r}}(0) = \vec{v}_0$$

Verlet
[wikipedia]

Verlet integration

→ We want to solve: $\dfrac{d^2\vec{r}(t)}{dt^2} = \vec{a}(t, \vec{r}(t))$

How to discretize the second order derivative?
… Taylor …

forward: $r(t+\Delta t) \approx r(t) + \Delta t\, r'(t) + \dfrac{\Delta t^2}{2} r''(t) + \dfrac{\Delta t^3}{3!} r'''(t) + \mathcal{O}(\Delta t^4)$

backward: $r(t-\Delta t) \approx r(t) - \Delta t\, r'(t) + \dfrac{\Delta t^2}{2} r''(t) - \dfrac{\Delta t^3}{3!} r'''(t) + \mathcal{O}(\Delta t^4)$

Sum both to get...

$$r''(t) = \frac{r(t-\Delta t) - 2r(t) + r(t+\Delta t)}{\Delta t^2} + \mathcal{O}(\Delta t^2)$$

$$t \to t_n = n\Delta t$$

$$r''_n = \frac{r_{n-1} - 2r_n + r_{n+1}}{\Delta t^2}$$

Time-reversal invariant!!!

$$\Delta t \to -\Delta t$$

Noether: conservation of energy!

Verlet integration

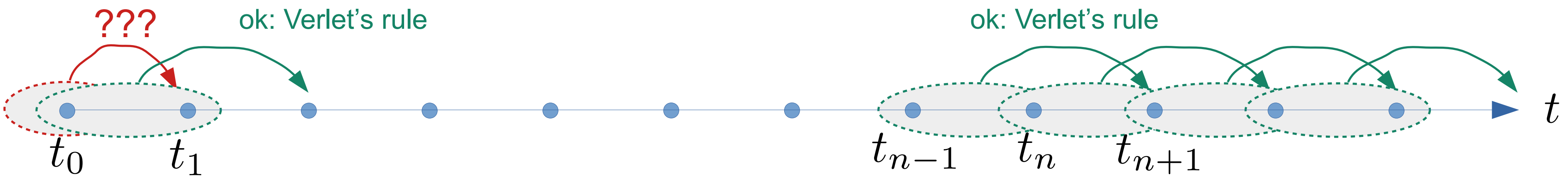
$$\frac{d^2\vec{r}(t)}{dt^2} = \vec{a}(t, \vec{r}(t))$$

$$r''_n = \frac{r_{n-1} - 2r_n + r_{n+1}}{\Delta t^2}$$

a simple recursion, just as complex as Euler's

$$\boxed{\vec{r}_{n+1} = 2\vec{r}_n - \vec{r}_{n-1} + \vec{a}(t_n, \vec{r}_n)\Delta t^2}$$

is it sufficient?



How to do the first step from n=0 to n=1?

We know r_0, v_0, and $a(t_0, r_0)$ → $\boxed{\vec{r}_1 = \vec{r}_0 + \vec{v}_0\Delta t + \frac{1}{2}\vec{a}(t_0, \vec{r}_0)\Delta t^2}$

small initialization error

Velocity-dependent forces

What if $\vec{a} \equiv \vec{a}(t, \vec{r}(t), \vec{v}(t))$?

answer 1: forget Verlet... use Runge-Kutta + reduction of order

answer 2:
→ use Euler to calculate the velocity

$$\vec{v}_1 = \vec{v}_0 + \vec{a}(t_0, \vec{r}_0, \vec{v}_0)\Delta t \quad \text{and} \quad \vec{v}_{n+1} = \vec{v}_{n-1} + \vec{a}(t_n, \vec{r}_n, \vec{v}_n)2\Delta t$$

Summary: the full Verlet recursion is:

Prototype

$$\frac{d^2\vec{r}(t)}{dt^2} = \vec{a}(t, \vec{r}(t), \vec{v}(t))$$

Initial conditions

$$\vec{r}(0) = \vec{r}_0$$
$$\dot{\vec{r}}(0) = \vec{v}_0$$

First step: 0 → 1

$$\vec{r}_1 = \vec{r}_0 + \vec{v}_0\Delta t + \frac{1}{2}\vec{a}(t_0, \vec{r}_0, \vec{v}_0)\Delta t^2$$
$$\vec{v}_1 = \vec{v}_0 + \vec{a}(t_0, \vec{r}_0, \vec{v}_0)\Delta t$$

Other steps: n → n+1

$$\vec{r}_{n+1} = 2\vec{r}_n - \vec{r}_{n-1} + \vec{a}(t_n, \vec{r}_n)\Delta t^2$$
$$\vec{v}_{n+1} = \vec{v}_{n-1} + \vec{a}(t_n, \vec{r}_n, \vec{v}_n)2\Delta t$$