Computational Physics

PHYS4150/8150 (6 credits)

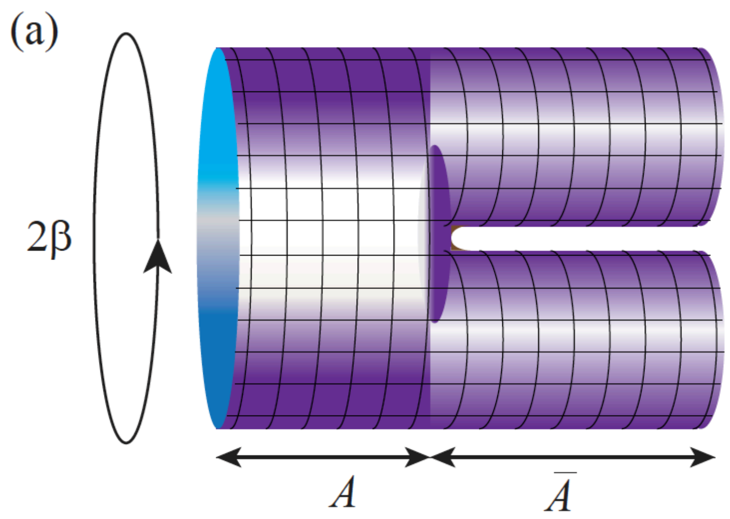
Place: KKL 201

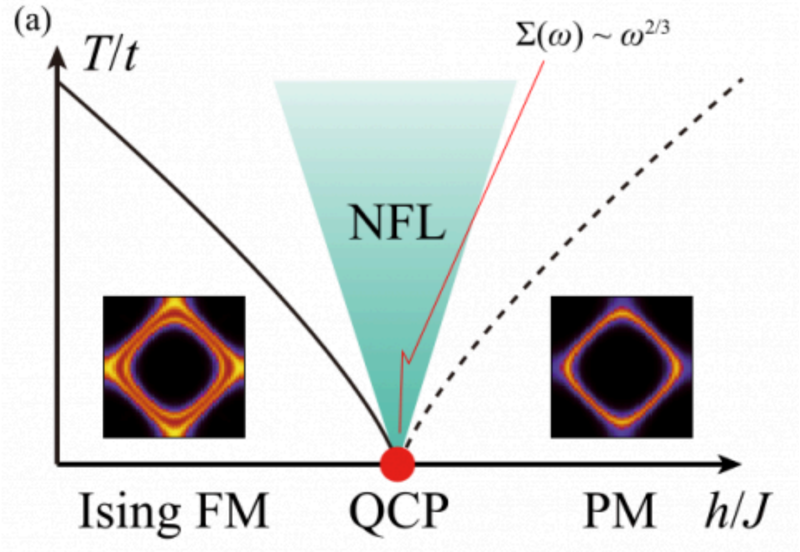
Time : Mon 17:30-18:20
Thu 16:30-17:20; 17:30-18:20

https://quantummc.xyz/teaching/hku-phys4150-8150-computational-physics-2024/

Teacher: Zi Yang Meng (zymeng@hku.hk)

Tutor: Tim-Lok Chau (Justin) (justintlchau@connect.hku.hk)
Min Long (minlo@connect.hku.hk)





Content

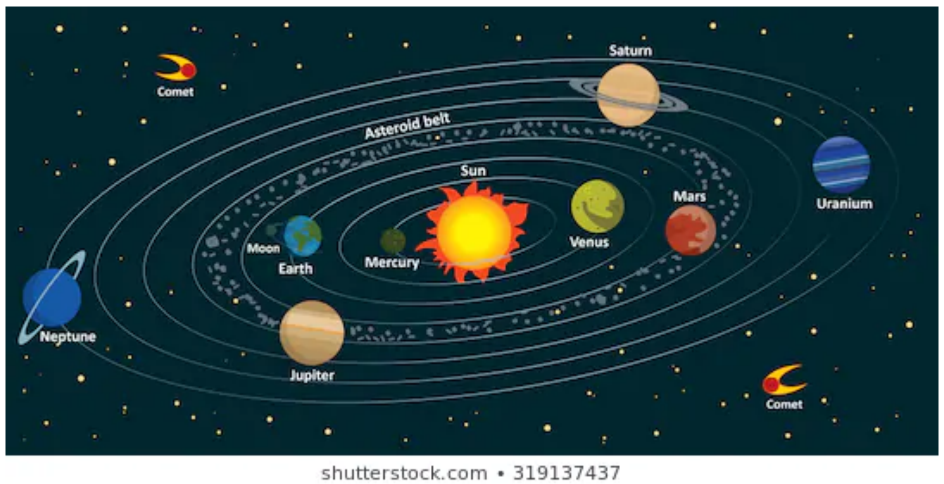
Content

3. Statistical and many-body physics
   3.1 Classical Monte Carlo and phase transitions (Ising model and critical phenomena)
   3.2 Quantum Monte Carlo methods (Path-integral and cluster update)

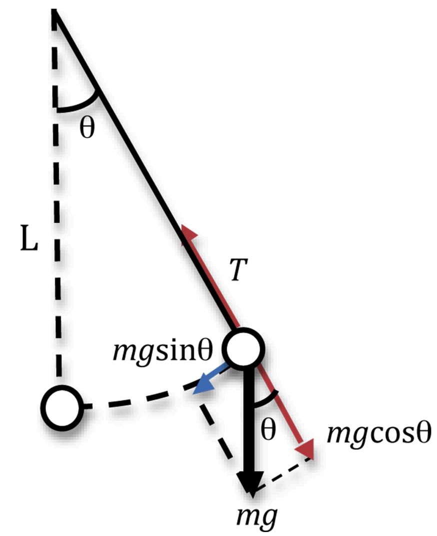
4. Machine learning in physics and High performance computation
   4.1 AI in quantum physics
   4.2 HPC and parallelism
   4.3 …

Differential equations

- Initial value problems: time-dependent equations with given initial conditions



Solar system



Pendulum

浮世绘，葛饰北斋，神奈川冲浪里

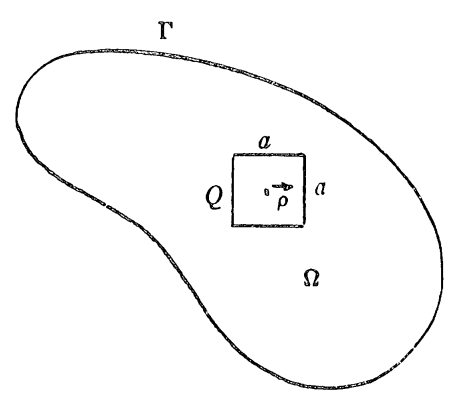
- Boundary value problems: differential equations with specific boundary values

CAN ONE HEAR THE SHAPE OF A DRUM?

MARK KAC, The Rockefeller University, New York

To George Eugene Uhlenbeck on the occasion of his sixty-fifth birthday

- Am. Math. Mon. 73, 1 (1966)



Eigenvalues of Dirichlet problem for Laplacian

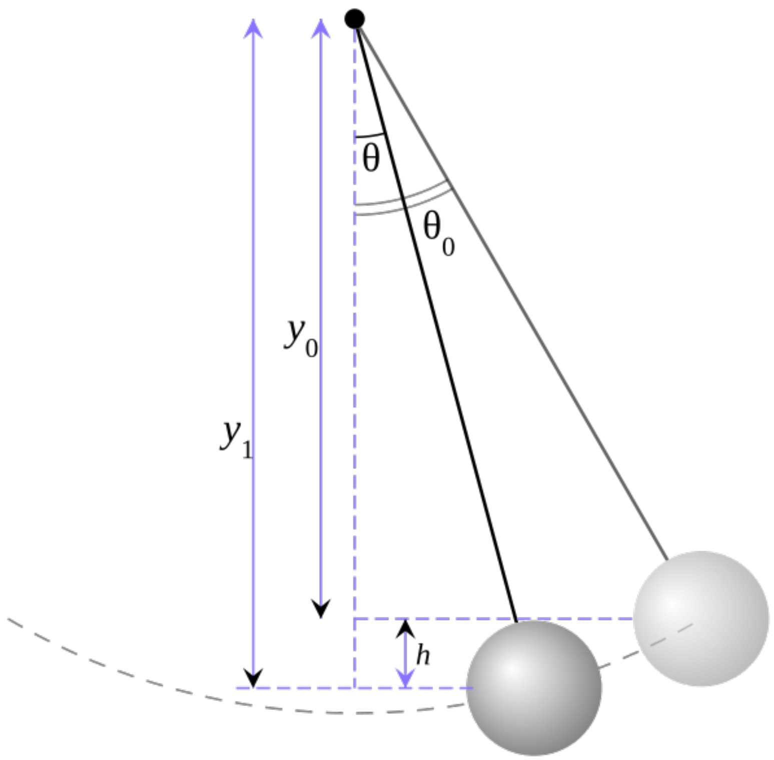
$$\tfrac{1}{2}\nabla^2 U + \lambda U = 0 \text{ in } \Omega,$$
$$U = 0 \text{ on } \Gamma.$$

Length of circumference

Number of holes

$$\sum_{n=1}^{\infty} e^{-\lambda_n t} \sim \frac{|\Omega|}{2\pi t} - \frac{L}{4}\frac{1}{\sqrt{2\pi t}} + \frac{1}{6} \qquad (1-r)\frac{1}{6}$$

- Eigenvalue problems



$$\frac{1}{2}mv^2 = mgh \qquad v = \sqrt{2gh} \qquad v = \ell\frac{d\theta}{dt}$$

$$\frac{d\theta}{dt} = \frac{\sqrt{2gh}}{\ell} = \sqrt{\frac{2g}{\ell}(\cos(\theta) - \cos(\theta_0))}$$

$$\sqrt{\frac{2g}{\ell}}\int_0^{T/4} dt = \int_0^{\theta_0} \frac{d\theta}{\sqrt{(\cos(\theta) - \cos(\theta_0))}}$$

$$\cos(\theta) = 1 - \frac{\theta^2}{2} + \cdots \qquad \theta = \theta_0 \sin(\phi) \quad \phi \in [0, \frac{\pi}{2}]$$

$$T = 4\sqrt{\frac{\ell}{g}}\int_0^{\theta_0} \frac{d\theta}{\sqrt{\theta_0^2 - \theta^2}} = 4\sqrt{\frac{\ell}{g}}\int_0^{\pi/2} d\phi = 2\pi\sqrt{\frac{\ell}{g}}$$

$$\frac{d}{dt}\frac{d\theta}{dt} = \frac{d}{dt}\sqrt{\frac{2g}{\ell}(\cos(\theta) - \cos(\theta_0))} = \frac{1}{2}\frac{\frac{-2g}{\ell}\sin(\theta)}{\sqrt{\frac{2g}{\ell}(\cos(\theta) - \cos(\theta_0))}}\frac{d\theta}{dt} = -\frac{g}{\ell}\sin(\theta)$$

$$\frac{d^2\theta}{dt^2} = -\frac{g}{\ell}\sin(\theta)$$

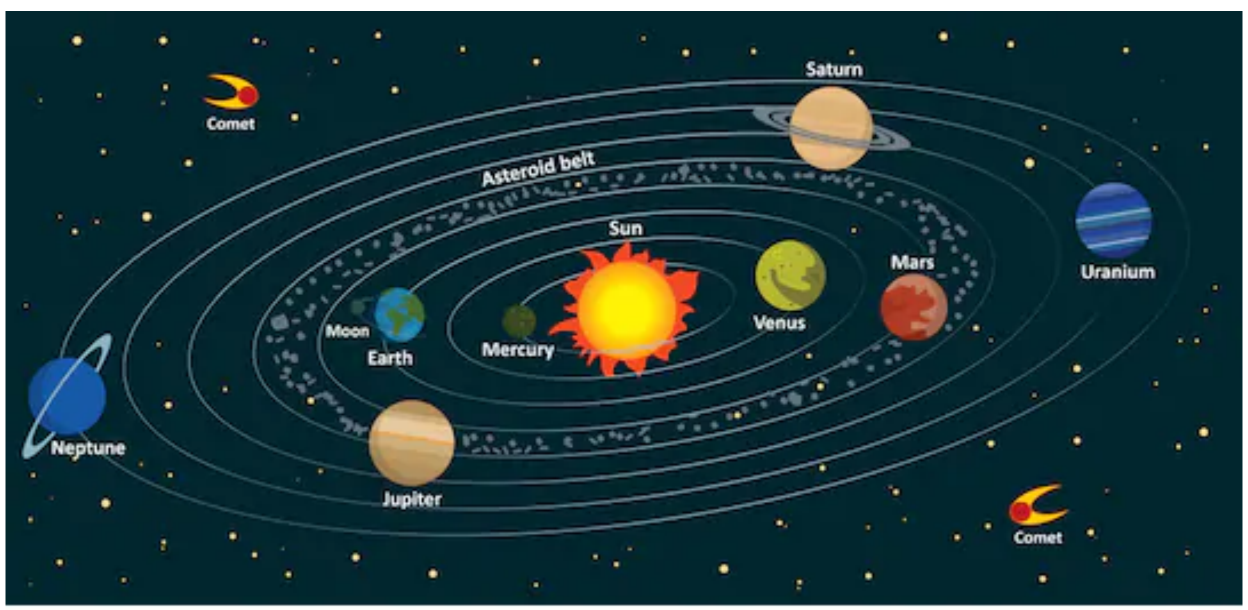
Classical equation of motion

Differential equations $\dot{\vec{v}}_i(t) = \vec{a}_i(\vec{x}_0(t), \vec{x}_1(t), \cdots, \vec{x}_{N-1}; \vec{v}_0(t), \vec{v}_1(t), \cdots, \vec{v}_{N-1}(t); t)$

State of dynamical system $\dot{\vec{x}}_i(t) = \vec{v}_i(t), \quad i = 0,1,\cdots,N-1$

Gravitation (such as solar system) $\vec{a}_i(\vec{x}_0(t), \cdots, \vec{x}_{N-1}(t)) = G \sum_{j \neq i} \frac{m_j}{|\vec{x}_j(t) - \vec{x}_i(t)|^3} [\vec{x}_j(t) - \vec{x}_i(t)]$

G Gravitational constant



shutterstock.com • 319137437

Discretization

$$t = t_0, t_1, t_2, \cdots \qquad \tau = t_{n+1} - t_n$$

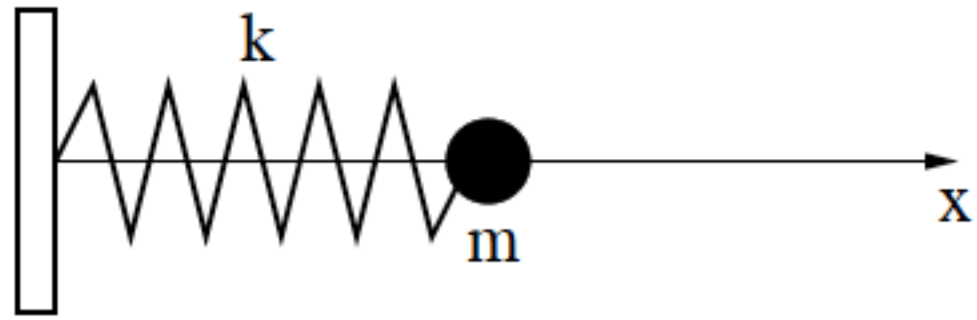
$$\vec{x}(t) = \begin{pmatrix} \vec{x}_0(t) \\ \vec{x}_1(t) \\ \vdots \\ \vec{x}_{N-1}(t) \end{pmatrix} \quad \vec{v}(t) = \begin{pmatrix} \vec{v}_0(t) \\ \vec{v}_1(t) \\ \vdots \\ \vec{v}_{N-1}(t) \end{pmatrix} \quad \vec{a}(t) = \begin{pmatrix} \vec{a}_0(t) \\ \vec{a}_1(t) \\ \vdots \\ \vec{a}_{N-1}(t) \end{pmatrix}$$

$$\dot{\vec{v}}(t) = \vec{a}(\vec{x}(t), \vec{v}(t), t)$$

$$\dot{\vec{x}}(t) = \vec{v}(t)$$

Classical equation of motion

Harmonic Oscillator



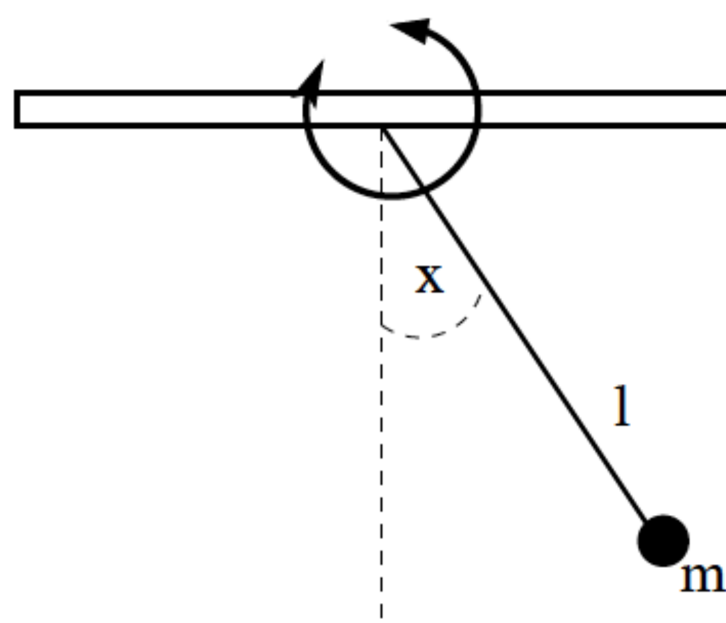
$$\dot{v}(t) = -\frac{k}{m}x$$

$$\dot{x}(t) = v$$

$$\gamma = 0, \, Q = 0$$

goes back to harmonic oscillator at small x

Driven Pendulum



$g = 9.81 m/s^2$

γ friction coefficient

Q strength of periodic driving force

Ω driving frequency

$$\dot{v}(t) = -\frac{g}{l}\sin(x) - \gamma\dot{x} + Q\sin(\Omega t)$$

acceleration depends on velocity

$$\dot{x}(t) = v$$

Numerical Differentiation

$$f(t_{n+1}) = f(t_n) + \tau f'(t_n) + \frac{\tau^2}{2} f''(t_n) + O(\tau^3)$$

$$f(t_{n-1}) = f(t_n) - \tau f'(t_n) + \frac{\tau^2}{2} f''(t_n) + O(\tau^3)$$

Two-point formula

$$f'(t_n) = \frac{f(t_{n+1}) - f(t_n)}{\tau} + O(\tau) \qquad f'(t_n) = \frac{f(t_n) - f(t_{n-1})}{\tau} + O(\tau)$$

$$f(t_{n+1}) - f(t_{n-1}) = 2\tau f'(t_n) + O(\tau^3)$$

$$f(t_{n+1}) + f(t_{n-1}) = 2f(t_n) + \tau^2 f''(t_n) + O(\tau^4)$$

be careful here, the 3rd order cancels,
the error is at the 4th order

three-point formula

$$f'(t_n) = \frac{f(t_{n+1}) - f(t_{n-1})}{2\tau} + O(\tau^2) \qquad f''(t_n) = \frac{f(t_{n+1}) - 2f(t_n) + f(t_{n-1})}{\tau^2} + O(\tau^2)$$

Euler method

2-point formula for 1st derivative

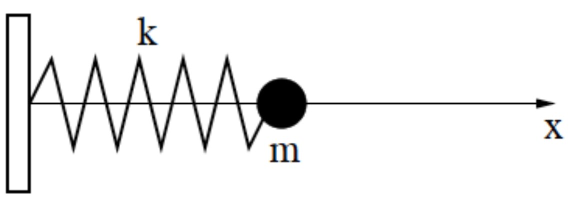
$$\dot{\vec{x}}(t) = \frac{\vec{x}(t+\tau) - \vec{x}(t)}{\tau} + O(\tau)$$

$$\dot{\vec{v}}(t) = \frac{\vec{v}(t+\tau) - \vec{v}(t)}{\tau} + O(\tau)$$

Leonhard Euler (1707-1783)
Mathematician, physicist, astronomer

$$\overrightarrow{x}(n+1) = \overrightarrow{x}(n) + \tau\overrightarrow{v}(n) + O(\tau^2)$$

$$\overrightarrow{v}(n+1) = \overrightarrow{v}(n) + \tau\overrightarrow{a}(n) + O(\tau^2)$$



$$E(n+1) = \frac{1}{2}k[x(n)+\tau v(n)]^2 + \frac{1}{2}m[v(n)+\tau a(n)]^2$$

$$= \frac{1}{2}k[x(n)+\tau v(n)]^2 + \frac{1}{2}m[v(n)-\tau\frac{k}{m}x(n)]^2$$

$$= E(n) + \frac{1}{2}\tau^2 k v^2(n) + \frac{1}{2}\tau^2\frac{k^2}{m}x^2(n)$$

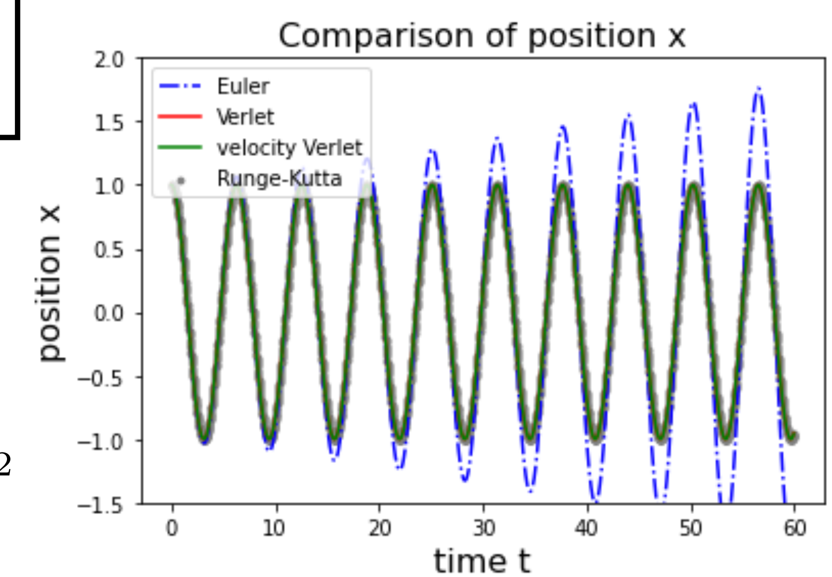
$$= E(n) + \tau^2\frac{k}{m}\underbrace{[\frac{1}{2}mv^2(n) + \frac{1}{2}kx^2(n)]}_{E(n)}$$

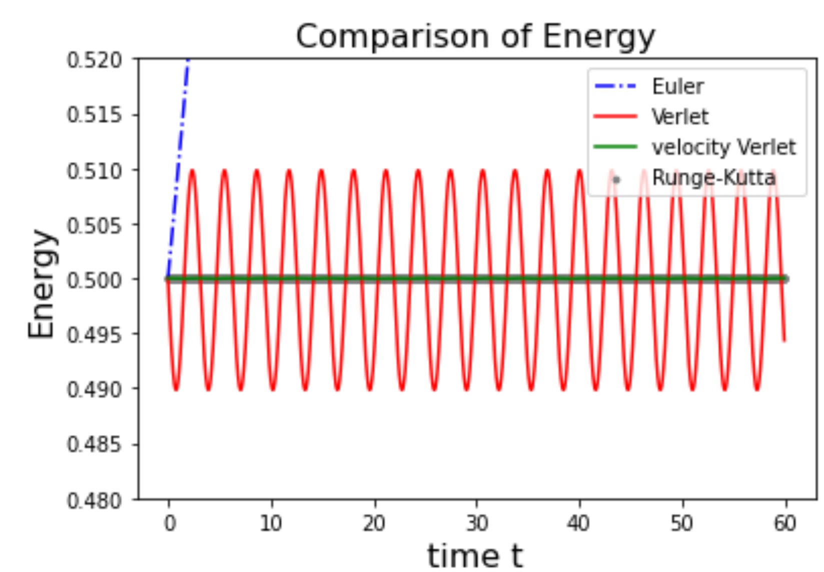
$k = m = 1 \quad x(0) = 1, v(0) = 0$

$$\ddot{x} = -x \rightarrow x(t) = \cos(t)$$

draw x and v ?

$$E(t) = \frac{1}{2}kx^2 + \frac{1}{2}mv^2 = \frac{1}{2}$$





Energy and position are not conserved, needs better method

Verlet method

$$\ddot{\vec{x}}(t) = \vec{a}(\vec{x}(t), t)$$ 3-point formula for 2nd derivative

acceleration does not depend on velocity

$$\ddot{\vec{x}}(t) = \frac{\vec{x}(t+\tau) + \vec{x}(t-\tau) - 2\vec{x}(t)}{\tau^2} + O(\tau^2)$$

$$\vec{x}(t+\tau) = 2\vec{x}(t) - \vec{x}(t-\tau) + \tau^2 \vec{a}(\vec{x}(t), t) + O(\tau^4)$$

$$\vec{v}(t) = \dot{\vec{x}}(t) = \frac{\vec{x}(t+\tau) - \vec{x}(t-\tau)}{2\tau} + O(\tau^2)$$

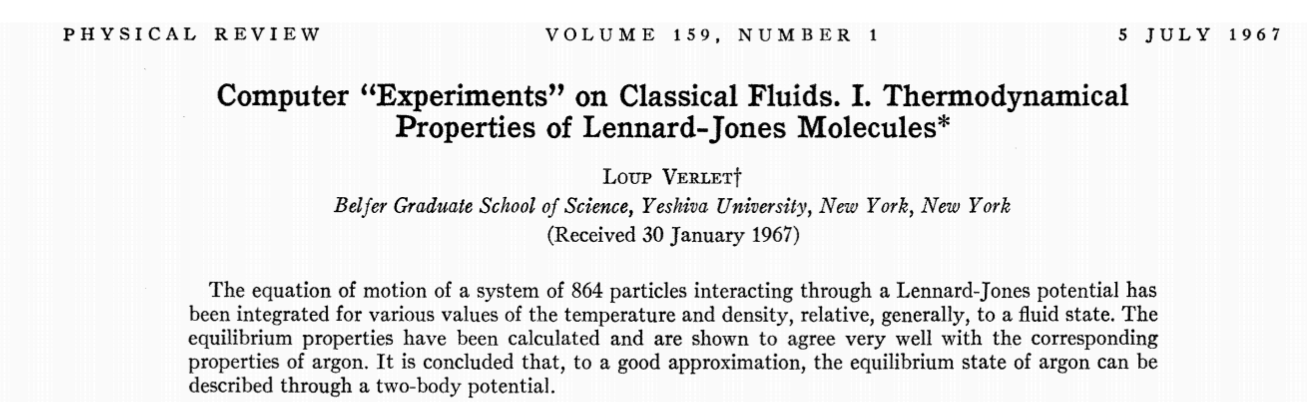
Verlet

$$\vec{x}(n+1) = 2\vec{x}(n) - \vec{x}(n-1) + \tau^2 \vec{a}(n) + O(\tau^4)$$

$$\vec{v}(n) = \frac{\vec{x}(n+1) - \vec{x}(n-1)}{2\tau} + O(\tau^2)$$

not self-starting $\vec{x}(0)$ and $\vec{v}(0)$ need $\vec{x}(-1)$

Taylor expansion $$\vec{x}(-1) = \vec{x}(0) - \tau\vec{v}(0) + \frac{\tau^2}{2}\vec{a}(0)$$

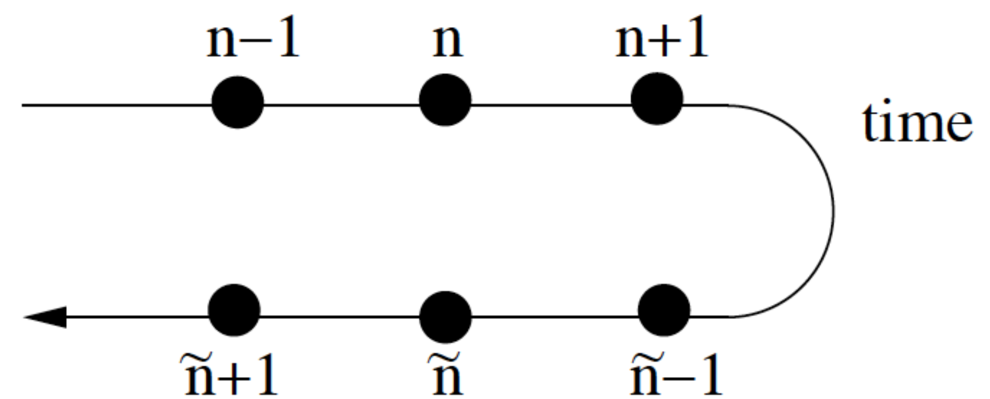

PHYSICAL REVIEW VOLUME 159, NUMBER 1 5 JULY 1967

Computer "Experiments" on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*

LOUP VERLET†
Belfer Graduate School of Science, Yeshiva University, New York, New York
(Received 30 January 1967)

The equation of motion of a system of 864 particles interacting through a Lennard-Jones potential has been integrated for various values of the temperature and density, relative, generally, to a fluid state. The equilibrium properties have been calculated and are shown to agree very well with the corresponding properties of argon. It is concluded that, to a good approximation, the equilibrium state of argon can be described through a two-body potential.

Time reversal symmetry



$$\vec{x}(\tilde{n}+1) = 2\vec{x}(\tilde{n}) - \vec{x}(\tilde{n}-1) + \tau^2\vec{a}(\tilde{n})$$
$$= 2\vec{x}(n) - \vec{x}(n+1) + \tau^2\vec{a}(n) = \vec{x}(n-1)$$

$$\vec{v}(\tilde{n}) = \frac{\vec{x}(\tilde{n}+1) - \vec{x}(\tilde{n}-1)}{2\tau}$$
$$= \frac{\vec{x}(n-1) - \vec{x}(n+1)}{2\tau} = -\vec{v}(n)$$

Travel backwards the trajectory, return to the initial state, apart from the roundoff errors

Laws of thermodynamics

- The 0th law: if two systems are each in thermal equilibrium with a third system, then they are in equilibrium with each other.

  defines thermal equilibrium and forms a basis for the definition of T.

- The 1st law: when energy passes into or out of a system (as work, heat or matter), the system's internal energy changes in accord with the law of conservation of energy. $\Delta U_{system} = Q - W$

- The 2nd law: in a natural thermodynamic process, the sum of the entropies of the systems never decreases.

  heat doest not spontaneously pass from a colder body to a warmer body

$$\delta Q = TdS$$

$$S = k \log W$$

- The 3rd law: a system's entropy approaches a constant value as the temperature approaches absolute zero.

Variants of Verlet I: Velocity Verlet

$$\vec{x}(n+1) = 2\vec{x}(n) - \vec{x}(n-1) + \tau^2\vec{a}(n) \quad (1)$$

add $\vec{x}(n+1)$ to (1)

$$2\vec{x}(n+1) = 2\vec{x}(n) + \vec{x}(n+1) - \vec{x}(n-1) + \tau^2\vec{a}(n)$$

using $\vec{v}(n) = \frac{\vec{x}(n+1) - \vec{x}(n-1)}{2\tau}$

$$\vec{x}(n+1) = \vec{x}(n) + \tau\vec{v}(n) + \frac{1}{2}\tau^2\vec{a}(n)$$

$$\vec{x}(n) = 2\vec{x}(n-1) - \vec{x}(n-2) + \tau^2\vec{a}(n-1) \quad (2)$$

add (1) to (2)

$$\vec{x}(n+1) - \vec{x}(n-1) = \vec{x}(n) - \vec{x}(n-2) + \tau^2(\vec{a}(n-1) + \vec{a}(n))$$

divide by 2τ

$$\vec{v}(n) = \vec{v}(n-1) + \frac{1}{2}\tau(\vec{a}(n-1) + \vec{a}(n))$$

shift n to $n+1$

Velocity Verlet

$$\vec{x}(n+1) = \vec{x}(n) + \tau\vec{v}(n) + \frac{1}{2}\tau^2\vec{a}(n)$$

$$\vec{v}(n+1) = \vec{v}(n) + \frac{1}{2}\tau(\vec{a}(n) + \vec{a}(n+1))$$

Implies acceleration does not depend on the velocity

given $\vec{x}(0)$ and $\vec{v}(0)$ self-starting.

Variants of Verlet II: Leap-Frog

With better performance

Define velocities at half-steps

$$\vec{v}(t_n + \frac{1}{2}\tau) = \frac{\vec{x}(t_n + \tau) - \vec{x}(t_n)}{\tau}$$

3-point formula in half-steps

$$\vec{a}(t_n) = \dot{\vec{v}}(t_n) = \frac{\vec{v}(t_n + \frac{1}{2}\tau) - \vec{v}(t_n - \frac{1}{2}\tau)}{\tau} + O(\tau^2)$$

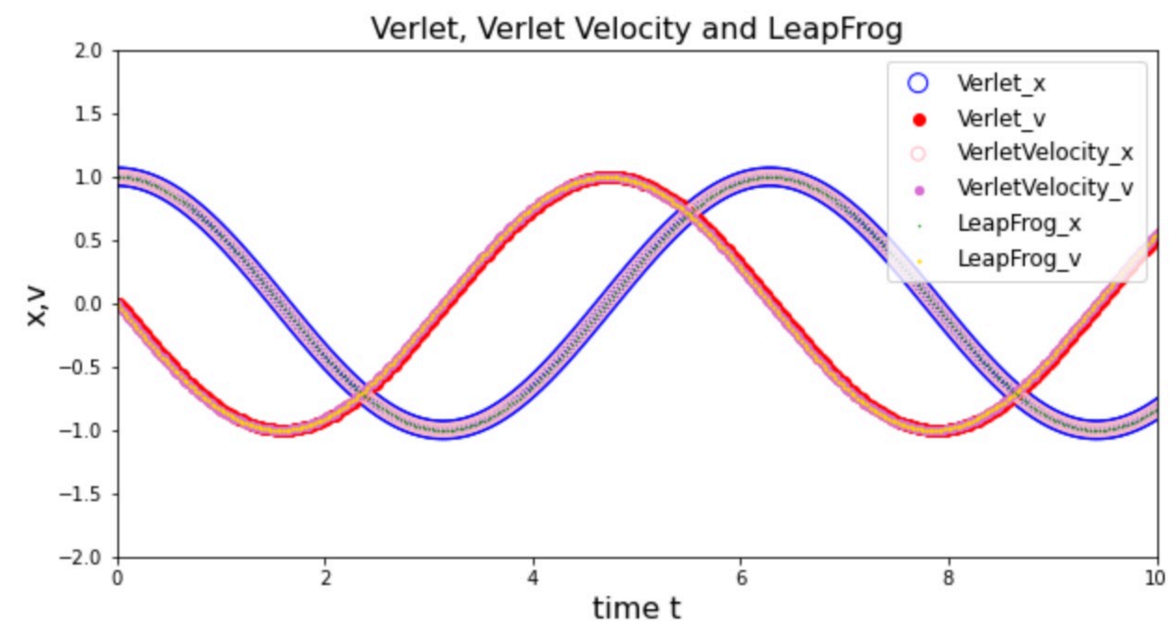
$$\vec{v}(t_n + \frac{1}{2}\tau) = \vec{v}(t_n - \frac{1}{2}\tau) + \tau\vec{a}(t_n) + O(\tau^3)$$

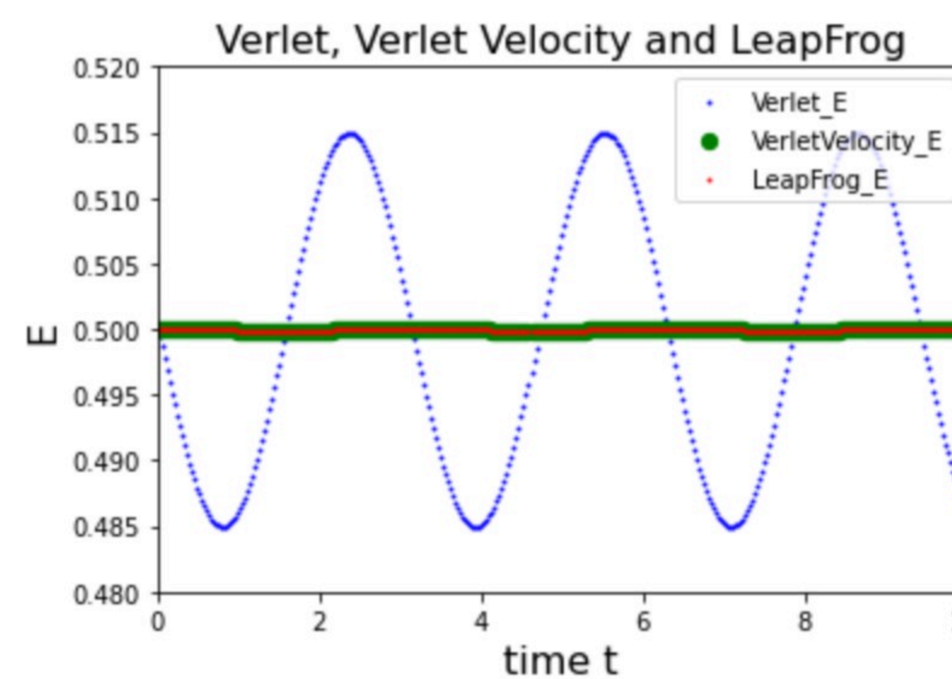
From Verlet

$$\vec{x}(n+1) = 2\vec{x}(n) - \vec{x}(n-1) + \tau^2\vec{a}(n) + O(\tau^4)$$

$$= \vec{x}(n) + \underbrace{\vec{x}(n) - \vec{x}(n-1)}_{\tau\vec{v}(n-\frac{1}{2})} + \tau^2\vec{a}(n) + O(\tau^4)$$

$$= \underbrace{\vec{x}(n) + \tau\vec{v}(n - \frac{1}{2}) + \tau^2\vec{a}(n)}_{\tau\vec{v}(n+\frac{1}{2})} + O(\tau^4)$$





Leap-Frog

$$\vec{v}(n + \frac{1}{2}) = \vec{v}(n - \frac{1}{2}) + \tau\vec{a}(n) + O(\tau^3)$$

$$\vec{x}(n+1) = \vec{x}(n) + \tau\vec{v}(n + \frac{1}{2}) + O(\tau^4)$$

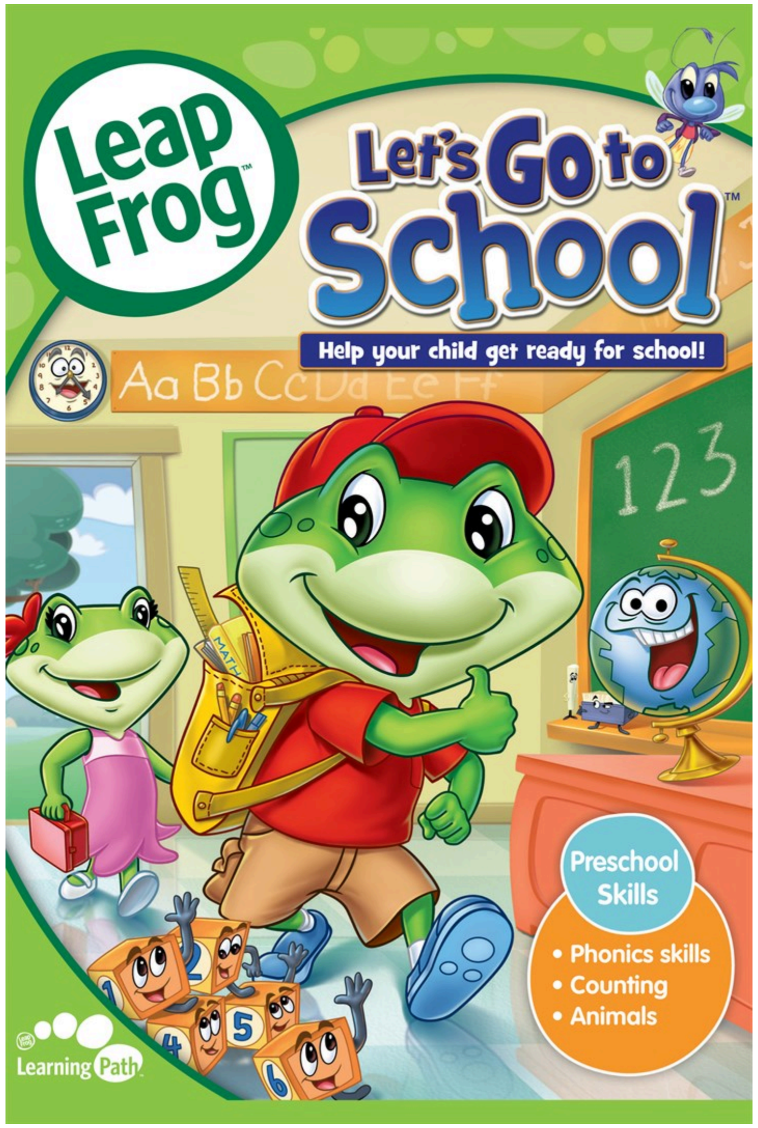
start the iteration $\vec{v}(-\frac{1}{2}) = \vec{v}(0) - \frac{1}{2}\tau\vec{a}(0)$

Notice no τ^2 term in iteration

Less roundoff errors

Initial value problem

- Euler (tau^2)
- Verlet (tau^4, time-reversal)
- Velocity Verlet (variant of Verlet 1)
- Leap-frog (variant of Verlet 2, less roundoff error)
- Runge-Kutta (tau^5, workhorse)



LeapFrog Enterprises, Inc. is the leader in innovative solutions that encourage a child's curiosity and love of learning throughout their early developmental journey.

Stability Analysis $$\ddot{x} = -\frac{k}{m}x$$

According to Verlet $$x(t+\tau) = 2x(t) - x(t-\tau) - \tau^2 \frac{k}{m} x(t)$$

$$\text{assume } x(t) = Ae^{i\omega t}$$

$$e^{i\omega\tau} = 2 - e^{-i\omega\tau} - \tau^2 \frac{k}{m}$$

$$2\cos(\omega\tau) = 2 - \tau^2 \frac{k}{m}$$

requires $\tau^2 \frac{k}{m} \ll 4$ for stable solution

$$\text{period of harmonic oscillator } T = 2\pi\sqrt{\frac{m}{k}}$$

$$\text{one shall use } \tau << T$$

Runge-Kutta method

Developed around 1900 by

Carl Runge 1856-1927
German mathematician, physicist

Martin Kutta 1867-1944
German mathematician

4-th order Runge-Kutta (RK4) with an error $O(\tau^5)$

$$x(0) = x_0$$

$$\dot{x} = f(x, t)$$

$$x(n+1) = x(n) + \frac{1}{6}\tau(k_1 + 2k_2 + 2k_3 + k_4) + O(\tau^5)$$

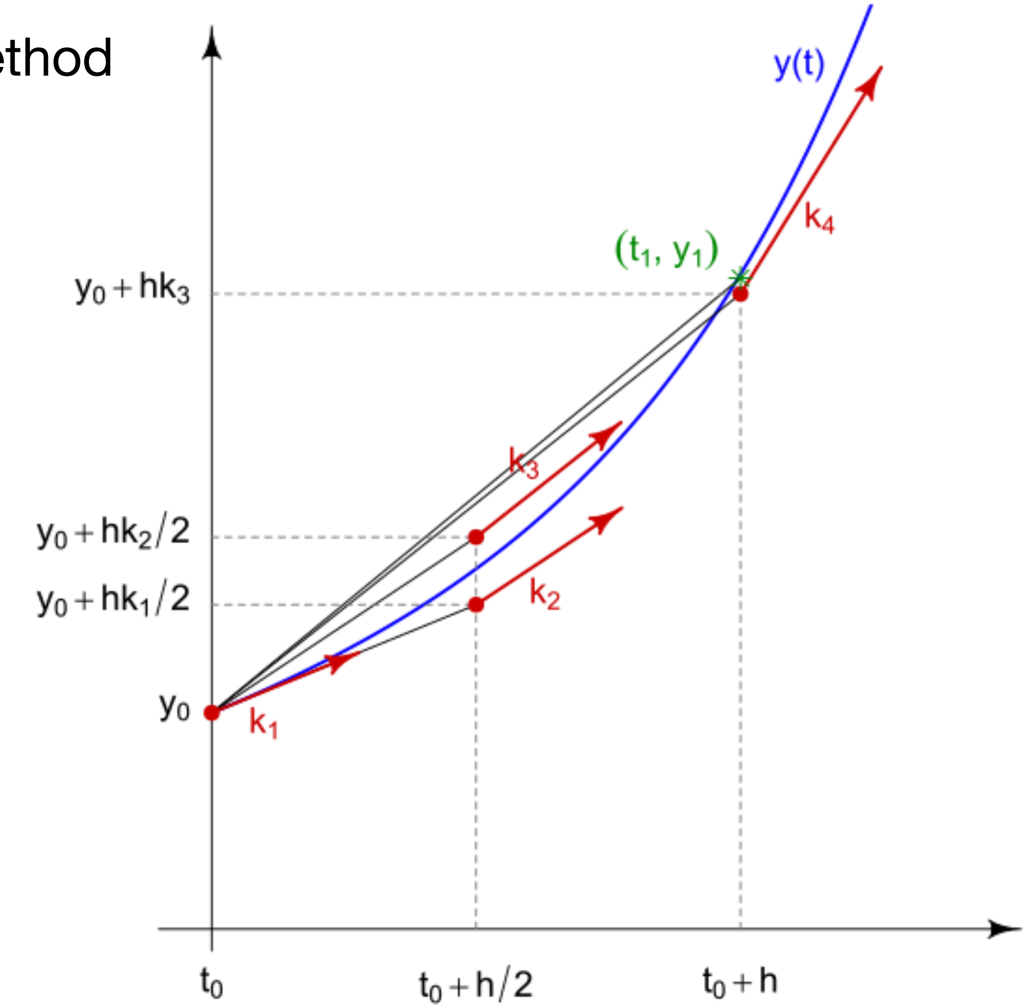
$$k_1 = f(x(n), n)$$ Euler method

$$k_2 = f(x(n) + \frac{\tau}{2}k_1, n + \frac{1}{2})$$

$$k_3 = f(x(n) + \frac{\tau}{2}k_2, n + \frac{1}{2})$$

$$k_4 = f(x(n) + \tau k_3, n + 1)$$

$y(t) = x(t)$



Taylor expansion in several variables $\dot{x} = f(x(t), t)$ $x(t+\tau) = x(t) + \tau\dot{x}(t) + \frac{\tau^2}{2}\ddot{x}(t) + \frac{\tau^3}{3!}\dddot{x}(t) + O(\tau^4)$

$$x(t+\tau) = x(t) + \tau f(x(t),t) + \frac{\tau^2}{2!}[\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt}] + \frac{\tau^3}{3!}[\frac{\partial^2 f}{\partial t^2} + 2\frac{\partial^2 f}{\partial t \partial x}\frac{dx}{dt} + \frac{\partial^2 f}{\partial x^2}(\frac{dx}{dt})^2 + (\frac{\partial f}{\partial x})^2\frac{dx}{dt} + \frac{\partial f}{\partial t}\frac{\partial f}{\partial x}] + O(\tau^4) + \cdots$$

$$x(t+\tau) = x(t) + \tau f(x,t) + \frac{\tau^2}{2}[f_t + f_x f] + \frac{\tau^3}{3!}[f_{tt} + 2f_{tx}f + f_{xx}f^2 + f_x^2 f + f_x f_t] + O(\tau^4)$$

p (=2) equations

p+p(p-1)/2 (=3) parameters

$$\begin{aligned} x(t+\tau) &= x(t) + \sum_{i=1}^{p} w_i k_i, \quad \text{with} \\ k_1 &= \tau f(x(t), t), \\ k_i &= \tau f\left(x(t) + \sum_{j<i}\alpha_{ij}k_j, t + \sum_{j<i}\alpha_{ij}\tau\right), \quad i \geq 2 \end{aligned}$$

$$w_1 + w_2 = 1$$

$$w_2\alpha_{21} = \frac{1}{2}$$

$p = 2$ $\quad x(t+\tau) = x(t) + w_1k_1 + w_2k_2$

$$= x(t) + w_1\tau f(x,t) + w_2\tau f(x + \alpha_{21}k_1, t + \alpha_{21}\tau)$$

$$f(x,t) + \alpha_{21}\tau(f_t + f_x f) + O(\tau^2)$$

$$= x(t) + (w_1 + w_2)\tau f(x,t) + w_2\tau^2\alpha_{21}[f_t + f_x f] + O(\tau^3)$$

$$w_1 = \frac{1}{2}, w_2 = \frac{1}{2}, \alpha_{21} = 1$$

$$w_1 = 0, w_2 = 1, \alpha_{21} = \frac{1}{2}$$

$$w_1 = \frac{1}{3}, w_2 = \frac{2}{3}, \alpha_{21} = \frac{3}{4}$$

$p = 3$ $\quad x(t+\tau) = x(t) + w_1k_1 + w_2k_2 + w_3k_3$

$$k_1 = \tau f(x,t)$$

$$k_2 = \tau f(x + \alpha_{21}k_1, t + \alpha_{21}\tau)$$

$$k_3 = \tau f(x + \alpha_{31}k_1 + \alpha_{32}k_2, t + \alpha_{31}\tau + \alpha_{32}\tau)$$

this morning

$$x(t+\tau) = x(t) + w_1 k_1 + w_2 k_2 + w_3 k_3 + w_4 k_4 + O(\tau^5)$$

$$= x(t) + \tau \frac{dx}{dt} + \frac{\tau^2}{2}\frac{d^2x}{dt^2} + \frac{\tau^3}{3!}\frac{d^3x}{dt^3} + \frac{\tau^4}{4!}\frac{d^4x}{dt^4} + O(\tau^5)$$

$$\frac{dx}{dt} = f(x,t)$$

$$\frac{d}{dt} f(x,t) = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial t} = f_x f + f_t$$

$$k_1 = \tau f(x,t)$$

$$k_2 = \tau f\left(x + \tfrac{1}{2}k_1, t + \tfrac{1}{2}\tau\right) = \tau\left\{f(x,t) + \frac{\tau}{2}\frac{d}{dt}f(x,t) + O(\tau^2)\right\}$$

$$= \tau\left\{f(x,t) + \frac{\tau}{2}(f_t + f_x f) + O(\tau^2)\right\}$$

$$k_3 = \tau f\left(x + \tfrac{1}{2}k_2, t + \tfrac{1}{2}\tau\right) = \tau f\left(x + \tfrac{\tau}{2} f\left(x + \tfrac{1}{2}k_1, t + \tfrac{\tau}{2}\right), t + \tfrac{\tau}{2}\right)$$

$$= \tau f\left(x + \tfrac{\tau}{2}\left(f(x,t) + \tfrac{\tau}{2}(f_t + f_x f)\right), t + \tfrac{\tau}{2}\right)$$

$$= \tau\left\{f(x,t) + \frac{\tau}{2}\frac{d}{dt}\left[f(x,t) + \frac{\tau}{2}(f_t + f_x f)\right]\right\}$$

$$k_4 = \tau f(x + k_3, t + \tau) = \tau f\left(x + \tau f\left(x + \tfrac{1}{2}k_2, t + \tfrac{\tau}{2}\right), t + \tau\right)$$

$$= \tau f\left(x + \tau f\left(x + \tfrac{\tau}{2} f\left(x + \tfrac{1}{2}k_1, t + \tfrac{\tau}{2}\right), t + \tfrac{\tau}{2}\right), t + \tau\right)$$

$$= \tau\left\{f(x,t) + \tau\frac{d}{dt}\left[f(x,t) + \frac{\tau}{2}\frac{d}{dt}\left[f(x,t) + \frac{\tau}{2}(f_t + f_x f)\right]\right]\right\}$$

$$= x(t) + \tau(w_1 + w_2 + w_3 + w_4) f(x,t)$$

$$+ \frac{\tau^2}{2}(w_2 + w_3 + 2w_4)\frac{df}{dt} + \frac{\tau^3}{4}(w_3 + 2w_4)\frac{d^2f}{dt^2} + \frac{\tau^4}{4} w_4 \frac{d^3f}{dt^3}$$

$$\begin{cases} w_1 + w_2 + w_3 + w_4 = 1 \\ w_2 + w_3 + 2w_4 = 1 \\ \frac{w_3}{4} + \frac{w_4}{2} = \frac{1}{6} \\ \frac{w_4}{4} = \frac{1}{24} \end{cases} \Rightarrow \boxed{\begin{aligned} w_1 &= \tfrac{1}{6} \\ w_2 &= \tfrac{1}{3} \\ w_3 &= \tfrac{1}{3} \\ w_4 &= \tfrac{1}{6} \end{aligned}}$$

$$
\begin{aligned}
x(t+\tau) &= x(t) + \sum_{i=1}^{p} w_i k_i, \quad \text{with} \\
k_1 &= \tau f(x(t), t), \\
k_i &= \tau f\left(x(t) + \sum_{j<i} \alpha_{ij} k_j, t + \sum_{j<i} \alpha_{ij} \tau \right), \quad i \geq 2
\end{aligned}
$$

determine the $p + \frac{p(p-1)}{2}$ parameters $w_i, i = 1, ..., p$ and $\alpha_{ij}, i, j = 1, ..., p, j < i$ in such a way that the expression matches the Taylor expansion up to and including order p, so the error will be $O(\tau^{p+1})$. This condition provides p equations. One finds, that this procedure works only for $p \leq 4$, i.e. only for $p \leq 4$ does one indeed find solutions

$$
\begin{aligned}
k_1 &= \tau f(x(t), t), \\
k_2 &= \tau f(x(t) + \frac{k_1}{2}, t + \frac{\tau}{2}), \\
k_3 &= \tau f(x(t) + \frac{k_2}{2}, t + \frac{\tau}{2}), \\
k_4 &= \tau f(x(t) + k_3, t + \tau), \\
x(t+\tau) &= x(t) + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(\tau^5)
\end{aligned}
$$

Our bible

Chap.17.1.

https://en.wikipedia.org/wiki/Runge%E2%80%93Kutta_methods

Runge-Kutta method on harmonic oscillator

$$\dot{x} = v(x, v, t)$$

$$\dot{v} = a(x, v, t)$$

$$x(n+1) = x(n) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$v(n+1) = v(n) + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4)$$

$$\tau = 0.03$$

$$k_1 = \tau v(x(n), v(n), n) \rightarrow \tau v(n)$$

$$l_1 = \tau a(x(n), v(n), n) \rightarrow \tau a(x(n))$$

$$k_2 = \tau v(x(n) + \frac{1}{2}k_1, v(n) + \frac{1}{2}l_1, n + \frac{1}{2}) \rightarrow \tau(v(n) + \frac{1}{2}l_1)$$

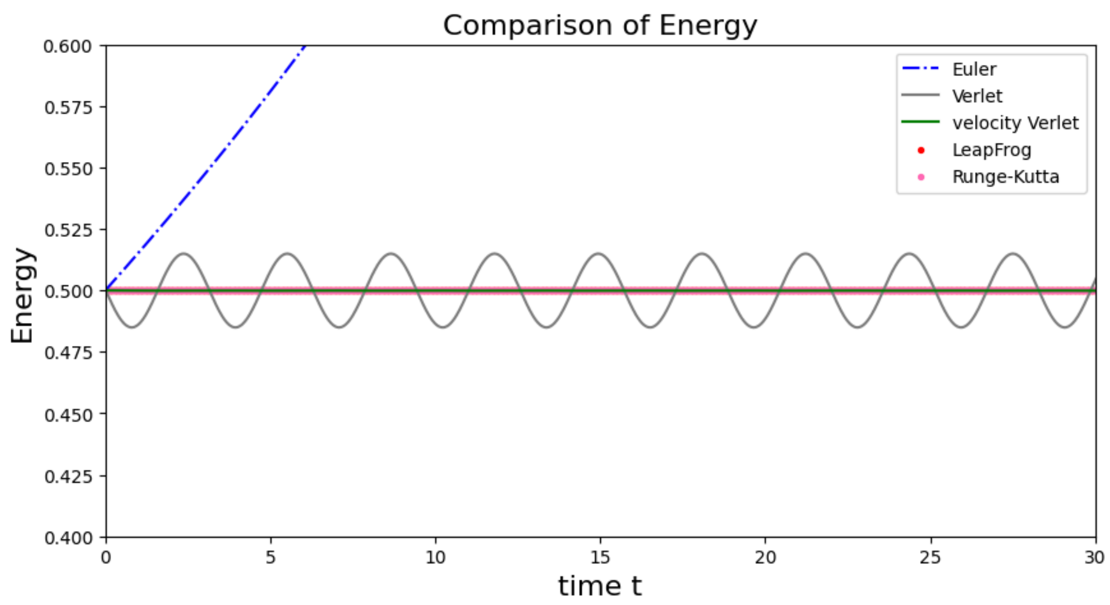
$$l_2 = \tau a(x(n) + \frac{1}{2}k_1, v(n) + \frac{1}{2}l_1, n + \frac{1}{2}) \rightarrow \tau a(x(n) + \frac{1}{2}k_1)$$

$$k_3 = \tau v(x(n) + \frac{1}{2}k_2, v(n) + \frac{1}{2}l_2, n + \frac{1}{2}) \rightarrow \tau(v(n) + \frac{1}{2}l_2)$$

$$l_3 = \tau a(x(n) + \frac{1}{2}k_2, v(n) + \frac{1}{2}l_2, n + \frac{1}{2}) \rightarrow \tau a(x(n) + \frac{1}{2}k_2)$$

$$k_4 = \tau v(x(n) + k_3, v(n) + l_3, n + 1) \rightarrow \tau(v(n) + l_3)$$

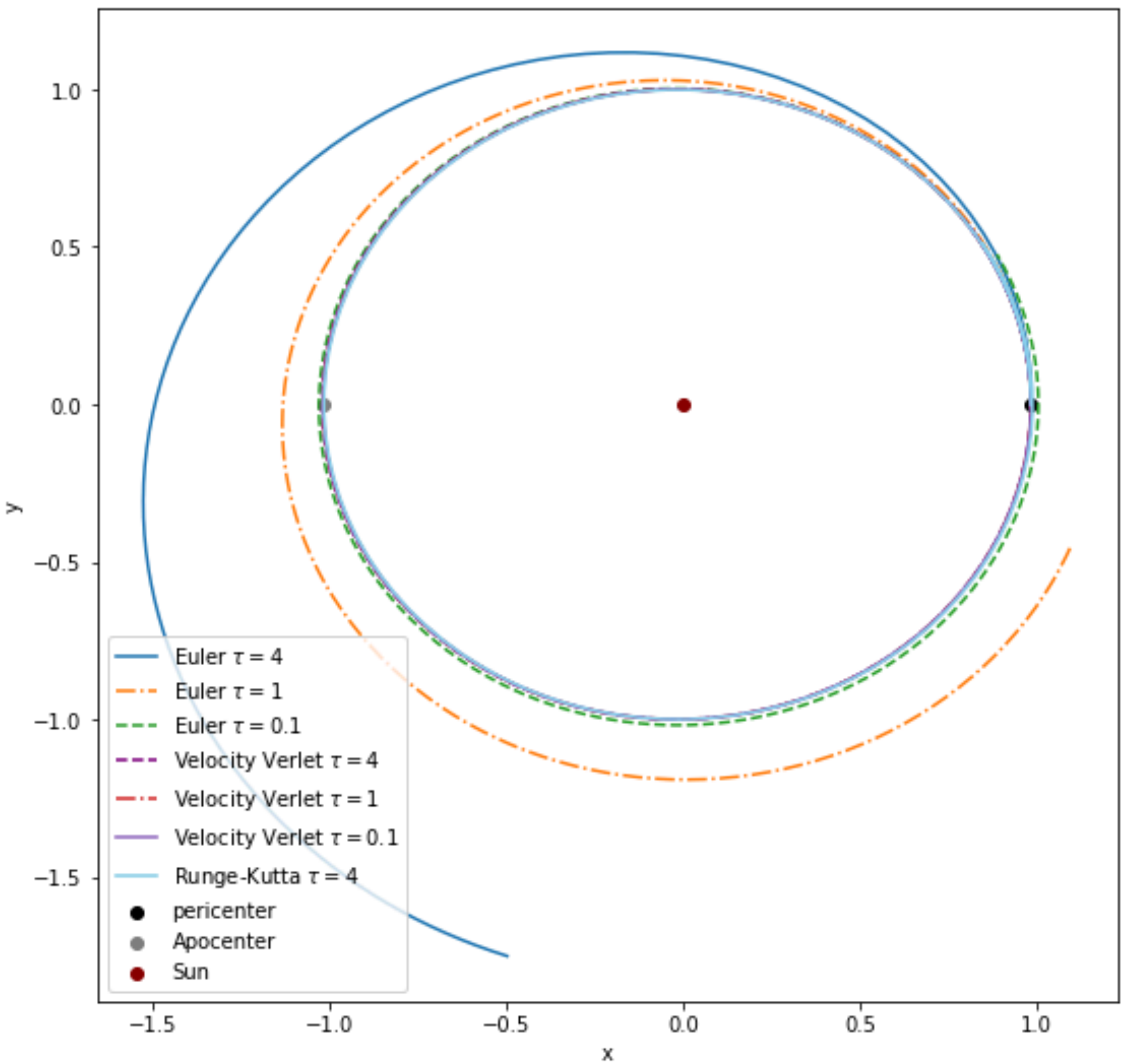
$$l_4 = \tau a(x(n) + k_3, v(n) + l_3, n + 1) \rightarrow \tau a(x(n) + k_3)$$

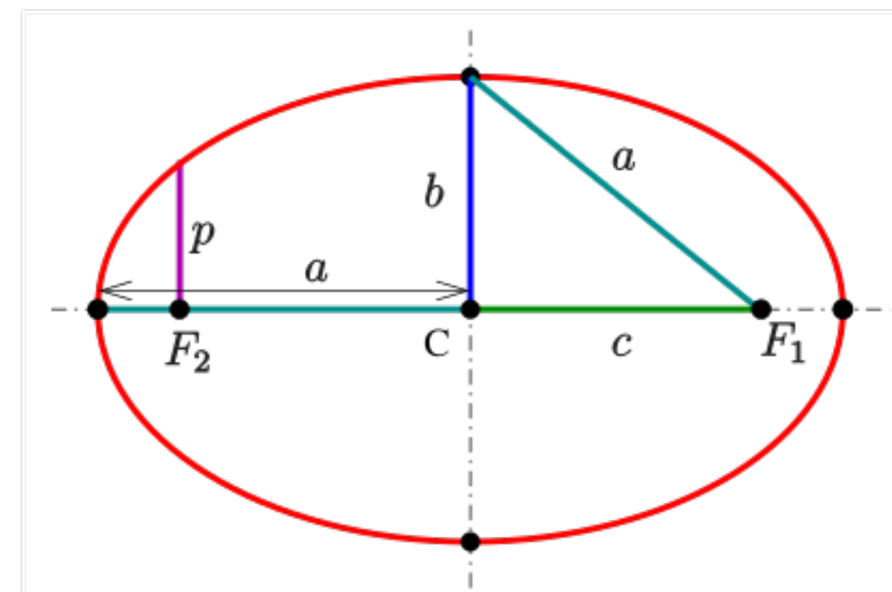


Earth Revolution

For the earth revolution due to the gravitational fore, the equation of motion is: $\frac{d^2\vec{r}}{dt^2} = -\frac{\mu}{r^3}\vec{r}$, where $\mu = G(M+m) \approx GM$. We already know that the earth moves in an ellipse aroung the sun, and now we can test the methods introduced before to numerically solve the differential equations and plot the trajectory to see the performance of the methods (here we consider the best Runge-Kutta method, the velocity Verlet method and the worst Euler method.).

The initial condition is: $x = a(1-e), y = 0, v_x = 0, v_y = \sqrt{\mu(1+e)/[a(1-e)]}$. we take $\mu = 2.958 \times 10^{-4}$, semi-major axis $a = 1.00000011$, and eccentricity $e = 0.01671022$. We take the unit of t to be 1 day.





Foci are $(\pm c, 0)$ $c = \sqrt{a^2 - b^2}$

Eccentricity $e = \frac{c}{a} = \sqrt{1 - (\frac{b}{a})^2}$