

Content



0. Introduction

1. Differential equations

- 1.1 Classical equation of motion (classical mechanics, pendulum)
- 1.2 Partial differential equation relaxation methods (electromagnetism, diffusion)
- 1.3 Partial differential equation in space-time (traffic flow, tsunami)

2. Eigenvalue problem

- 2.1 Schrödinger equation and Hamiltonian (Harmonic oscillator, wave package)
- 2.2 Quantum lattice model and Hilbert space (Heisenberg model)
- 2.3 Exact diagonalization of spin chain (Spin wave, Haldane conjecture, topology)
- 2.4 Matrix product state and density matrix renormalization group (DMRG)

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

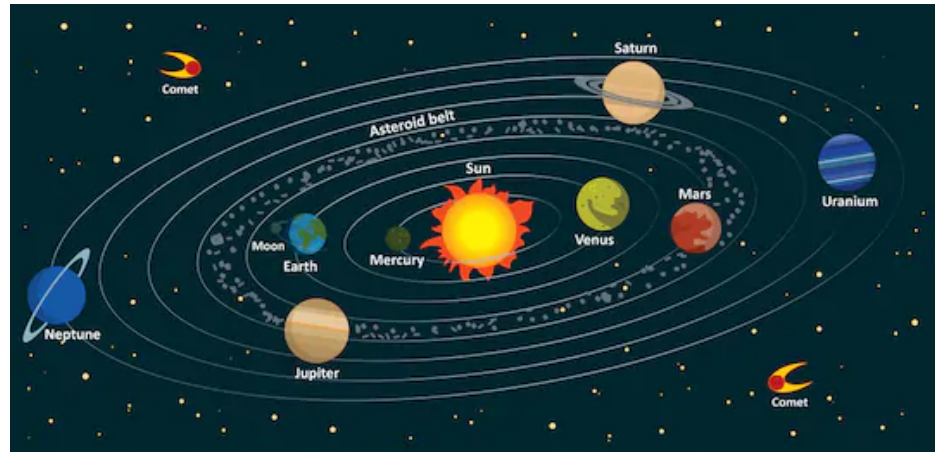
4.1 AI in quantum physics

4.2 HPC and parallelism

4.3 ...

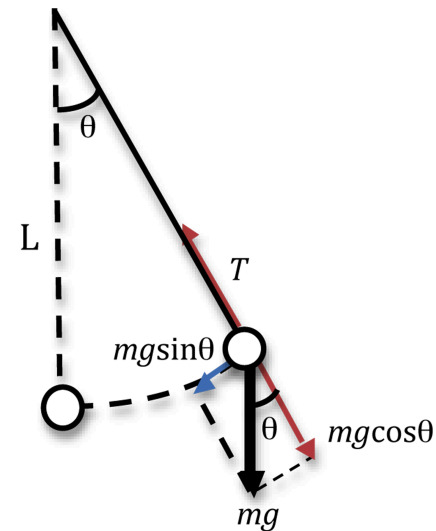
Differential equations

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



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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

$$\frac{1}{2} \nabla^2 U + \lambda U = 0 \text{ in } \Omega,$$

$$U = 0 \text{ on } \Gamma.$$

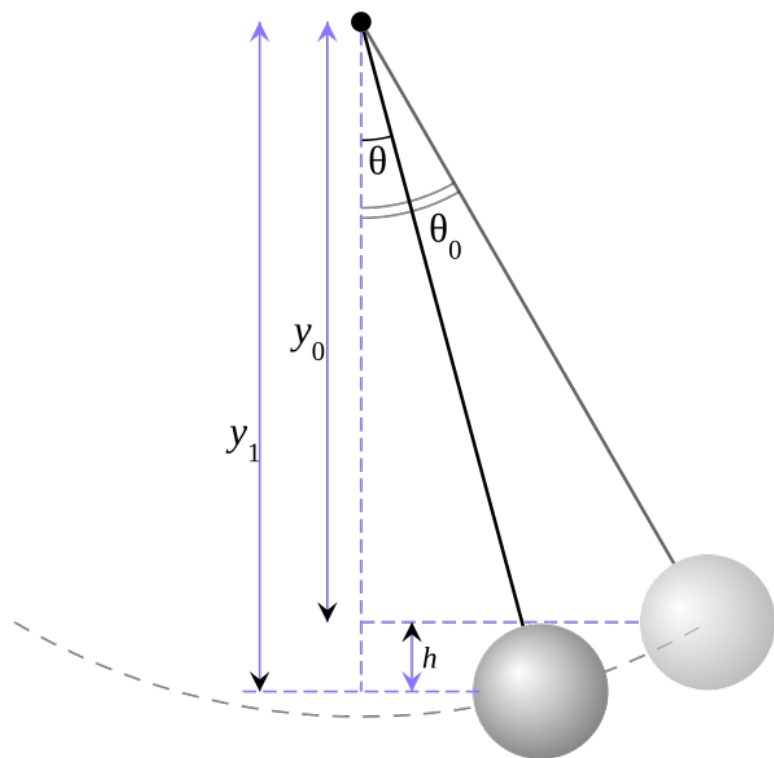
Length of circumference

Number of holes

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

$$(1-r) \frac{1}{6}$$

- Eigenvalue problems



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

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

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

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

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

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

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

Classical equation of motion

Differential equations

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

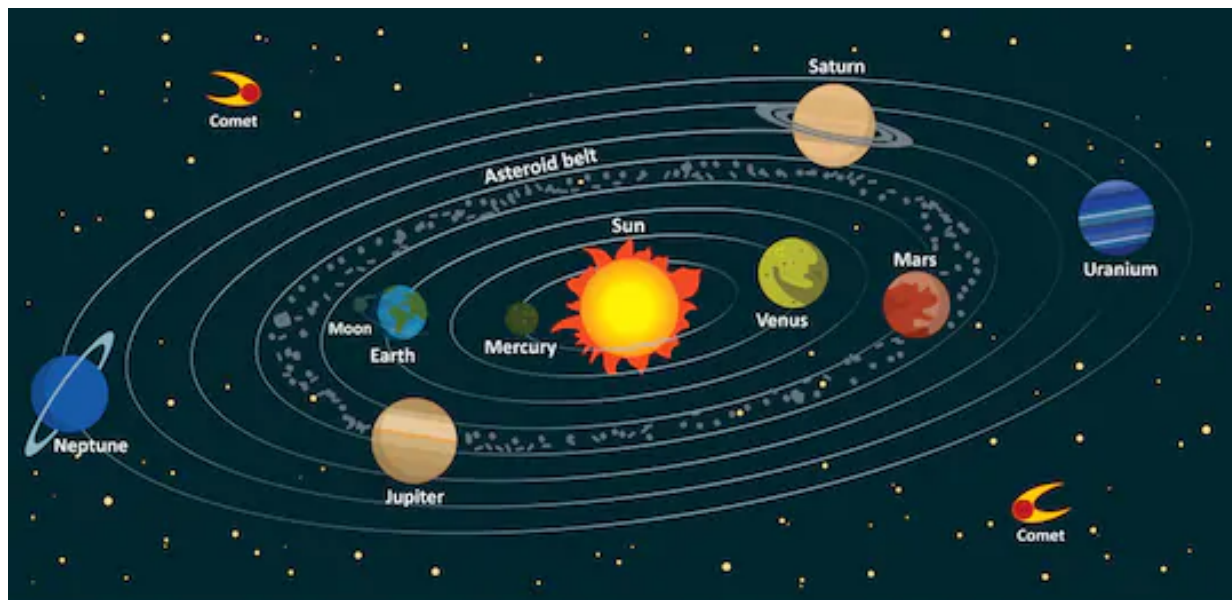
State of dynamical system

$$\dot{\vec{x}}_i(t) = \vec{v}_i(t), \quad i = 0, 1, \dots, N-1$$

Gravitation (such as solar system)

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

G Gravitational constant



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Discretization

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

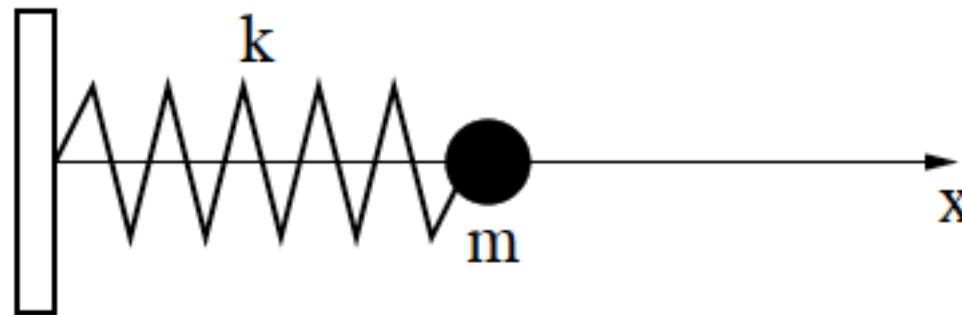
$$\vec{x}(t) = \begin{pmatrix} \vec{x}_0(t) \\ \vec{x}_1(t) \\ \vdots \\ \vec{x}_{N-1}(t) \end{pmatrix} \quad \vec{v}(t) = \begin{pmatrix} \vec{v}_0(t) \\ \vec{v}_1(t) \\ \vdots \\ \vec{v}_{N-1}(t) \end{pmatrix} \quad \vec{a}(t) = \begin{pmatrix} \vec{a}_0(t) \\ \vec{a}_1(t) \\ \vdots \\ \vec{a}_{N-1}(t)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

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

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

Classical equation of motion

Harmonic Oscillator



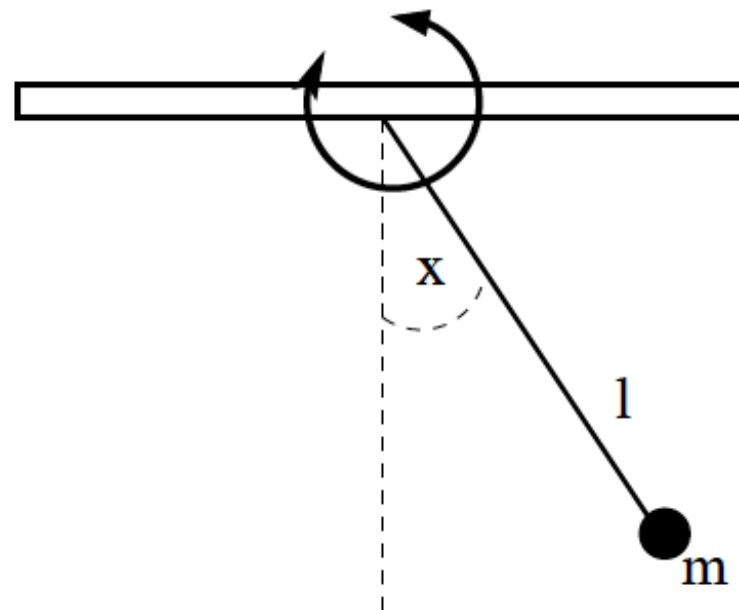
$$\ddot{x}(t) = -\frac{k}{m}x$$

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

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

goes back to harmonic oscillator at small x

Driven Pendulum



$$g = 9.81 \text{ m/s}^2$$

γ friction coefficient

Q strength of periodic driving force

Ω driving frequency

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

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

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

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

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

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

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

three-point formula

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

Euler method

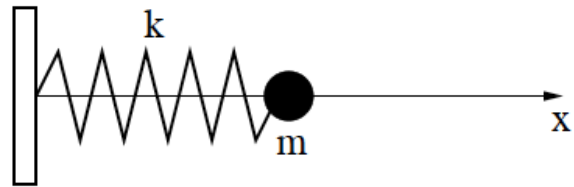
2-point formula for 1st derivative

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

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

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

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



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

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

draw x and v ?

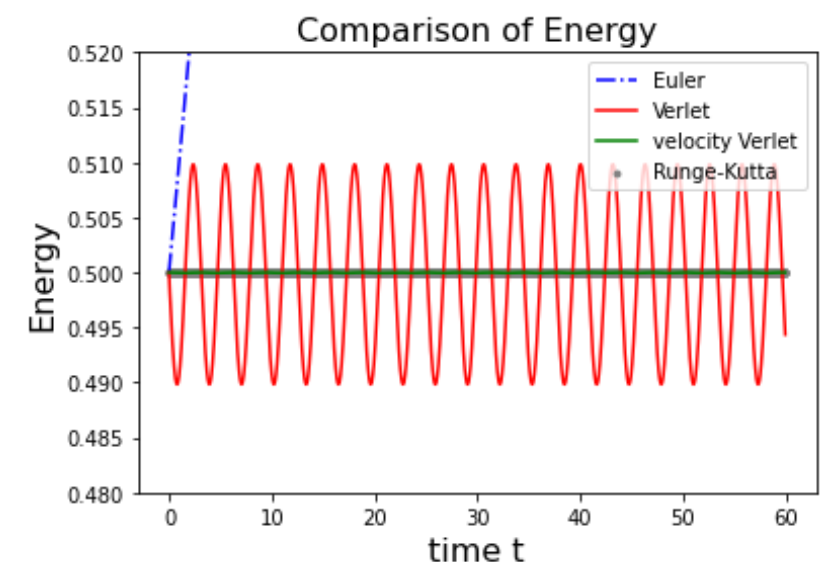
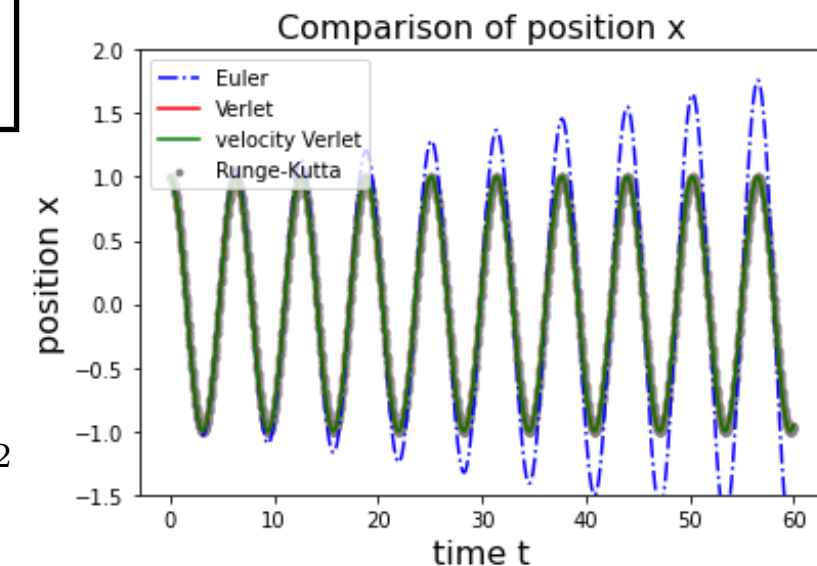
$$E(t) = \frac{1}{2}kx^2 + \frac{1}{2}mv^2 = \frac{1}{2}$$

$$\begin{aligned} E(n + 1) &= \frac{1}{2}k[x(n) + \tau v(n)]^2 + \frac{1}{2}m[v(n) + \tau a(n)]^2 \\ &= \frac{1}{2}k[x(n) + \tau v(n)]^2 + \frac{1}{2}m[v(n) - \tau \frac{k}{m}x(n)]^2 \\ &= E(n) + \frac{1}{2}\tau^2 kv^2(n) + \frac{1}{2}\tau^2 \frac{k^2}{m}x^2(n) \\ &= E(n) + \tau^2 \frac{k}{m} \underbrace{\left[\frac{1}{2}mv^2(n) + \frac{1}{2}kx^2(n) \right]}_{E(n)} \end{aligned}$$

Energy and position are not conserved, needs better method



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



Verlet method

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

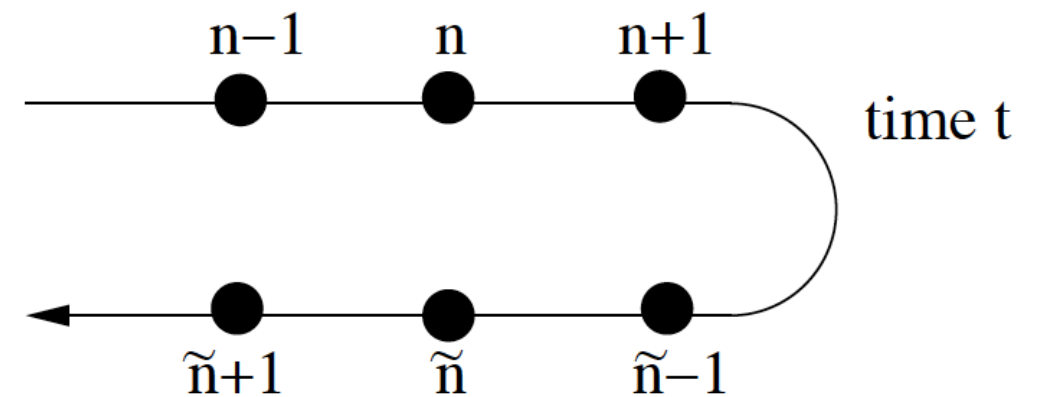
$$\ddot{\vec{x}}(t) = \frac{\vec{x}(t + \tau) + \vec{x}(t - \tau) - 2\vec{x}(t)}{\tau^2} + O(\tau^2)$$

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

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

acceleration does not depend on velocity

Time reversal symmetry



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

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

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

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

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

PHYSICAL REVIEW

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

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(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.

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 does 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

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

Define velocities at half-steps

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

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

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

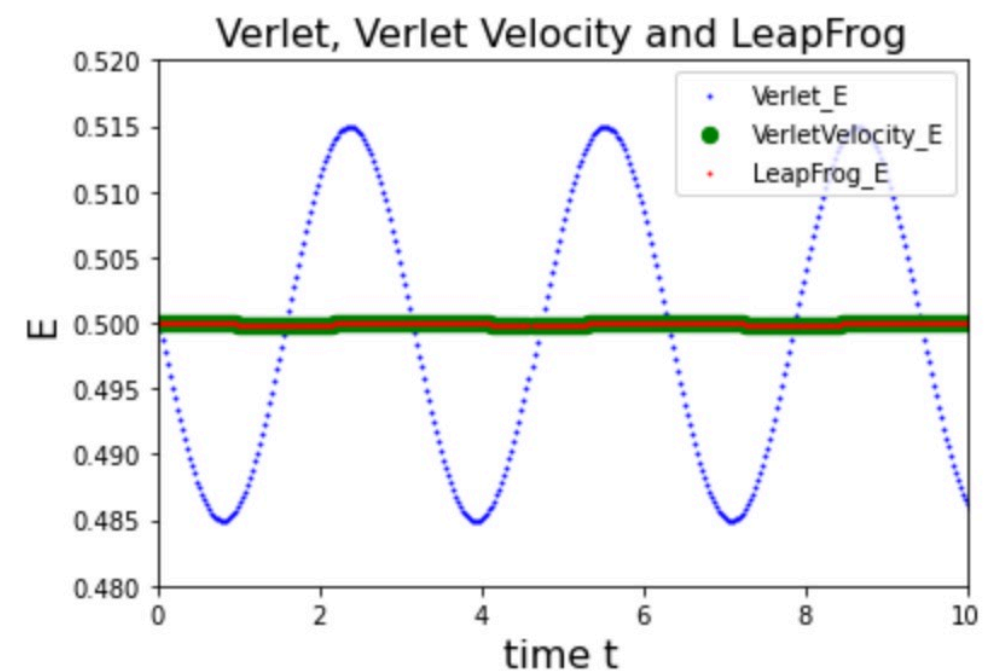
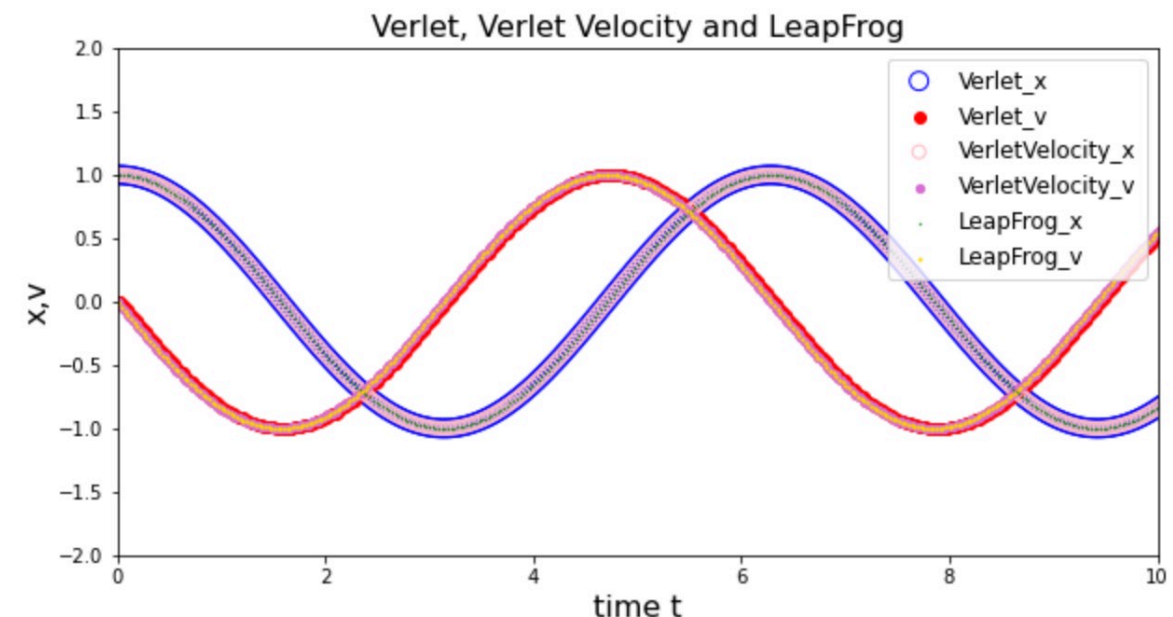
$$= \vec{x}(n) + \underbrace{\tau \vec{v}(n - \frac{1}{2})}_{\tau \vec{v}(n+\frac{1}{2})} + \tau^2 \vec{a}(n) + O(\tau^4)$$

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

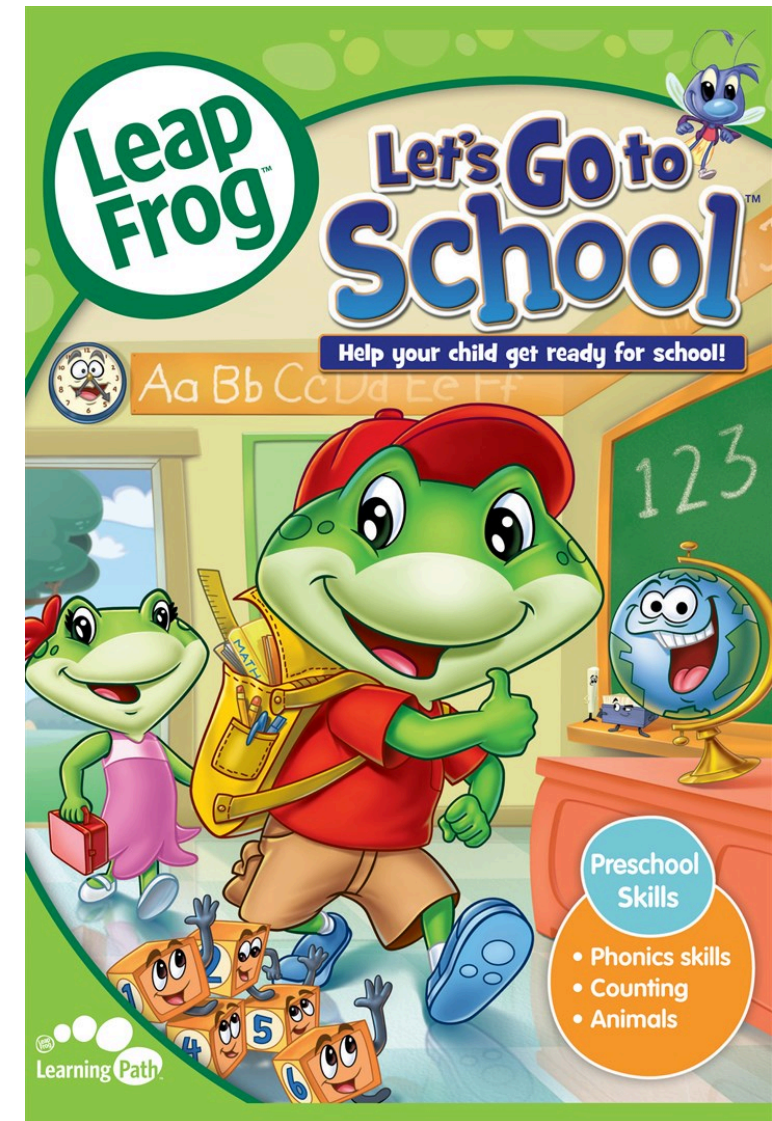


Notice no τ^2 term in iteration

Less roundoff errors

Initial value problem

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

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

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

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

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

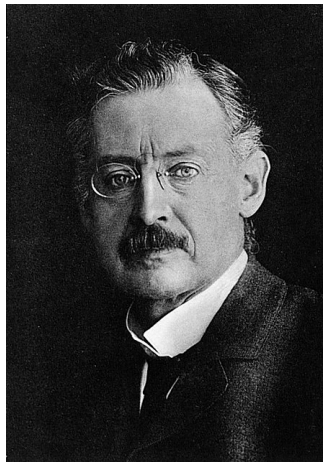
requires $\tau^2 \frac{k}{m} \ll 4$ for stable solution

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

one shall use $\tau \ll T$

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 $O(\tau^5)$

$$x(0) = x_0$$

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

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

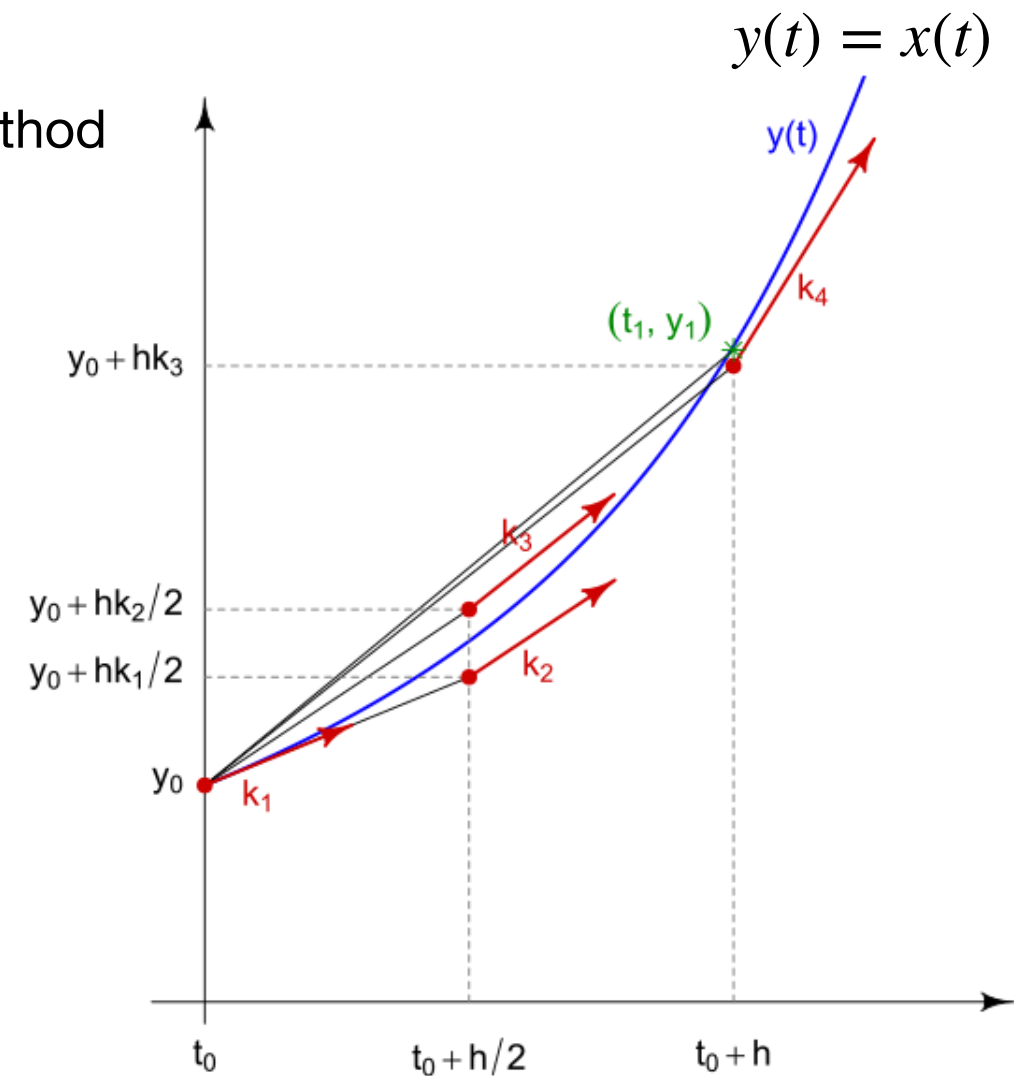
$$k_1 = f(x(n), n)$$

Euler method

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

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

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



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

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

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

$$x(t + \tau) = x(t) + \sum_{i=1}^p w_i k_i, \quad \text{with}$$

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

$$k_i = \tau f \left(x(t) + \sum_{j < i} \alpha_{ij} k_j, t + \sum_{j < i} \alpha_{ij} \tau \right), \quad i \geq 2$$

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

$$w_1 + w_2 = 1$$

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

$$p = 2 \quad x(t + \tau) = x(t) + w_1 k_1 + w_2 k_2$$

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

$$\downarrow$$

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

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

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

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

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

$$p = 3 \quad x(t + \tau) = x(t) + w_1 k_1 + w_2 k_2 + w_3 k_3$$

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

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

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

this morning

$$\begin{aligned}
 x(t+\tau) &= x(t) + w_1 k_1 + w_2 k_2 + w_3 k_3 + w_4 k_4 + O(\tau^5) \\
 \frac{dx}{dt} &= f(x,t) \\
 \frac{d}{dt} f(x,t) &= \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial t} = f_x f + f_t
 \end{aligned}$$

$$\begin{aligned}
 &= x(t) + \tau \frac{dx}{dt} + \frac{\tau^2}{2} \frac{d^2 x}{dt^2} + \frac{\tau^3}{3!} \frac{d^3 x}{dt^3} + \frac{\tau^4}{4!} \frac{d^4 x}{dt^4} + O(\tau^5) \\
 &\quad k_1 = \tau f(x,t) \\
 &\quad k_2 = \tau f\left(x + \frac{1}{2} k_1, t + \frac{1}{2} \tau\right) = \tau \left\{ f(x,t) + \frac{\tau}{2} \frac{d}{dt} f(x,t) + O(\tau^2) \right\} \\
 &\quad \quad = \tau \left\{ f(x,t) + \frac{\tau}{2} (f_t + f_x f) + O(\tau^2) \right\} \\
 &\quad k_3 = \tau f\left(x + \frac{1}{2} k_2, t + \frac{1}{2} \tau\right) = \tau f\left(x + \frac{\tau}{2} f\left(x + \frac{1}{2} k_1, t + \frac{\tau}{2}\right), t + \frac{\tau}{2}\right) \\
 &\quad \quad = \tau f\left(x + \frac{\tau}{2} \left(f(x,t) + \frac{\tau}{2} (f_t + f_x f)\right), t + \frac{\tau}{2}\right) \\
 &\quad \quad = \tau \left\{ f(x,t) + \frac{\tau}{2} \frac{d}{dt} \left[f(x,t) + \frac{\tau}{2} (f_t + f_x f) \right] \right\} \\
 &\quad k_4 = \tau f(x + k_3, t + \tau) = \tau f\left(x + \tau f\left(x + \frac{1}{2} k_2, t + \frac{\tau}{2}\right), t + \tau\right) \\
 &\quad \quad = \tau f\left(x + \tau f\left(x + \frac{\tau}{2} f\left(x + \frac{1}{2} k_1, t + \frac{\tau}{2}\right), t + \frac{\tau}{2}\right), t + \tau\right) \\
 &\quad \quad = \tau \left\{ f(x,t) + \tau \frac{d}{dt} \left[f(x,t) + \frac{\tau}{2} \frac{d}{dt} \left[f(x,t) + \frac{\tau}{2} (f_t + f_x f) \right] \right] \right\} \\
 &\quad \quad + \frac{\tau^2}{2} (w_2 + w_3 + 2w_4) \frac{d^2 f}{dt^2} + \frac{\tau^3}{4} (w_3 + 2w_4) \frac{d^3 f}{dt^3} + \frac{\tau^4}{4} w_4 \frac{d^4 f}{dt^4}
 \end{aligned}$$

$$\begin{aligned}
 &= x(t) + \tau (w_1 + w_2 + w_3 + w_4) f(x,t) \\
 &\quad \left\{ \begin{aligned} w_1 + w_2 + w_3 + w_4 &= 1 \\ w_2 + w_3 + 2w_4 &= 1 \\ \frac{w_3}{4} + \frac{w_4}{2} &= \frac{1}{6} \\ \frac{w_4}{4} &= \frac{1}{24} \end{aligned} \right. \Rightarrow \boxed{\begin{aligned} w_1 &= \frac{1}{6} \\ w_2 &= \frac{1}{3} \\ w_3 &= \frac{1}{3} \\ w_4 &= \frac{1}{6} \end{aligned}}
 \end{aligned}$$

$$x(t + \tau) = x(t) + \sum_{i=1}^p w_i k_i, \quad \text{with}$$

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

$$k_i = \tau f \left(x(t) + \sum_{j<i} \alpha_{ij} k_j, t + \sum_{j<i} \alpha_{ij} \tau \right), \quad i \geq 2$$

determine the $p + \frac{p(p-1)}{2}$ parameters $w_i, i = 1, \dots, p$ and $\alpha_{ij}, i, j = 1, \dots, p, j < i$ 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

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

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

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

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

$$x(t + \tau) = x(t) + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(\tau^5)$$

Our bible



Chap.17.1.

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

Runge-Kutta method on harmonic oscillator

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

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

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

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

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

$$\tau = 0.03$$

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

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

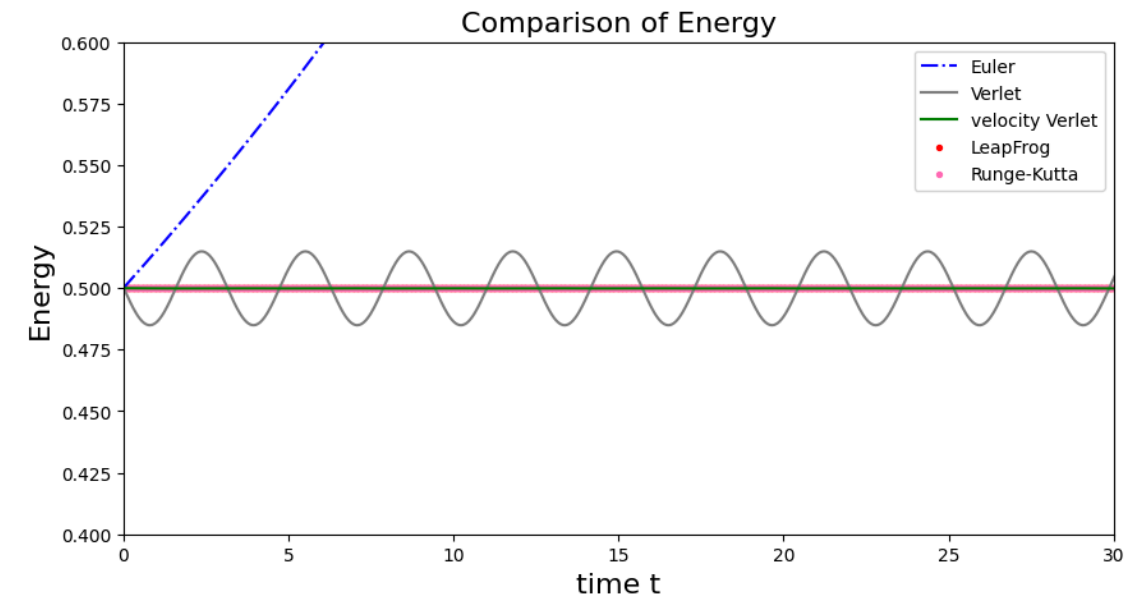
$$l_2 = \tau a(x(n) + \frac{1}{2}k_1, v(n) + \frac{1}{2}l_1, n + \frac{1}{2}) \rightarrow \tau a(x(n) + \frac{1}{2}k_1)$$

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

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

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

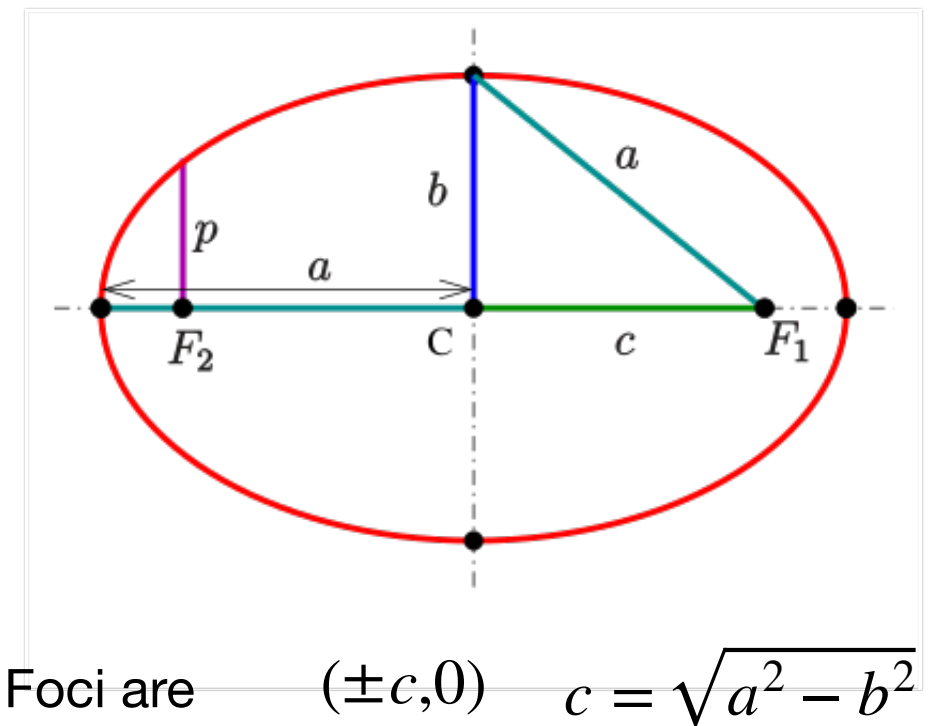
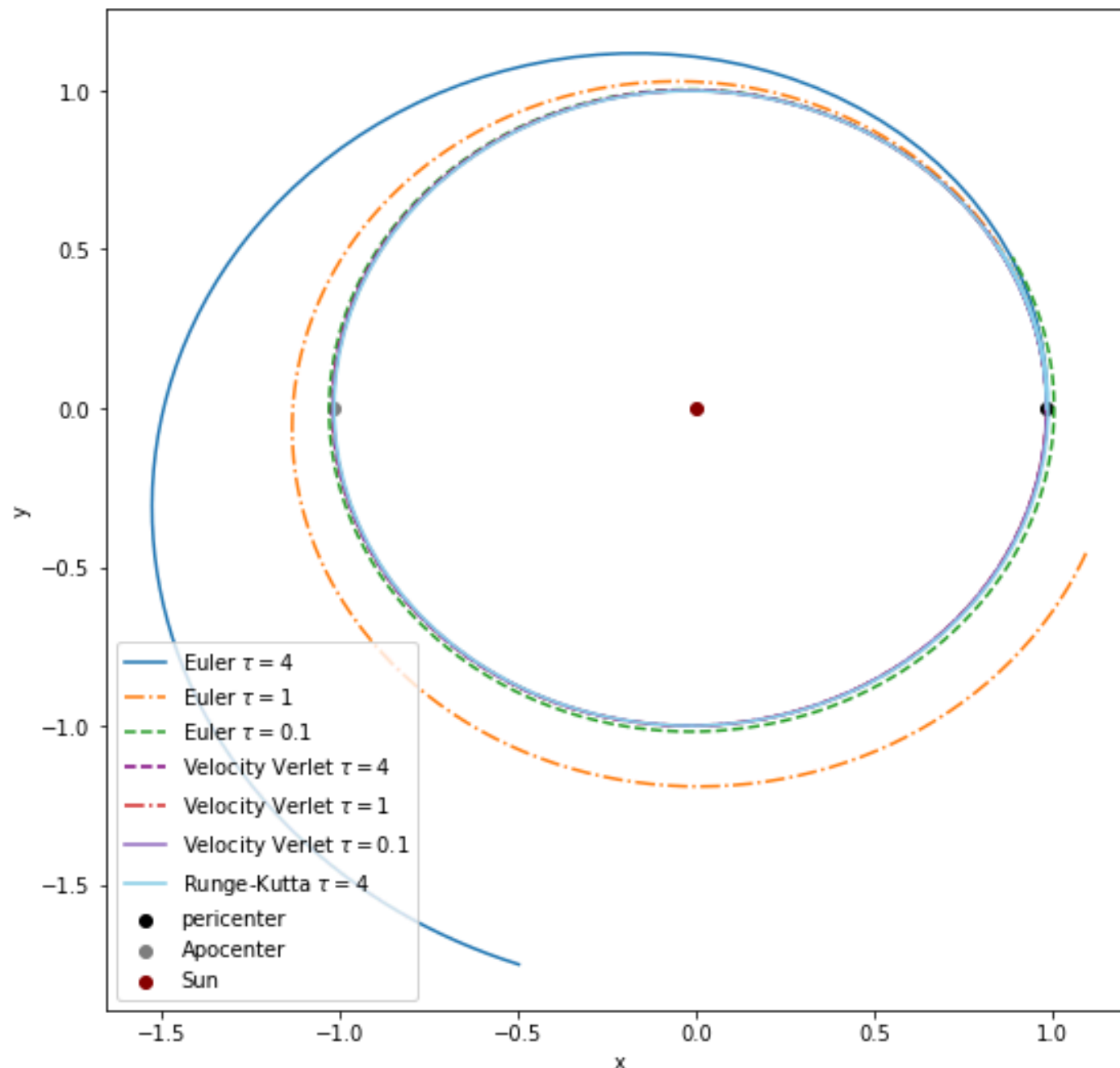
$$l_4 = \tau a(x(n) + k_3, v(n) + l_3, n + 1) \rightarrow \tau a(x(n) + k_3)$$



Earth Revolution

For the earth revolution due to the gravitational force, 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 around 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.



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

