Computational Astrophysics I: Introduction and basic concepts

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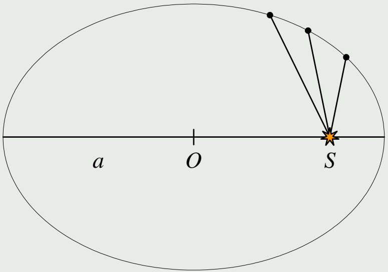
The two-body problem

We remember (?)

The Kepler's laws of planetary motion (1619)

1. Each planet moves in an elliptical orbit where the Sun is at one of the foci of the ellipse.
2. The velocity of a planet increases with decreasing distance to the Sun such, that the planet sweeps out equal areas in equal times. (*Consequence of which law?*)
3. The ratio P^2/a^3 is the same for all planets orbiting the Sun, where P is the orbital period and a is the semimajor axis of the ellipse. (*What defines value of ratio?*)



The 1. and 3. Kepler's law describe the shape of the orbit (Copernicus: circles), but not the time dependence $\vec{r}(t)$. This can in general not be expressed *analytically* by elementary mathematical functions (see below).
Therefore we will try to find a *numerical* solution.

Equations of motion II

Earth-Sun system

Step 1: $\rightarrow$ two-body problem $\rightarrow$ one-body problem via reduced mass of lighter body (partition of motion) via Newton's 3. & 2. law:

$$\vec{F}_{12} = -\vec{F}_{21} \Rightarrow m_1 \vec{a}_1 = -m_2 \vec{a}_2 \Rightarrow \vec{a}_2 = -\frac{m_1}{m_2}\vec{a}_1 \tag{1}$$

$$\vec{a}_{\mathrm{rel}} := \vec{a}_1 - \vec{a}_2 = \left(1 + \frac{m_1}{m_2}\right)\vec{a}_1 = \frac{m_2 + m_1}{m_1 m_2} m_1 \vec{a}_1 = \mu^{-1}\vec{F}_{12} \tag{2}$$

$$= \frac{d^2 \vec{x}_{\mathrm{rel}}}{dt^2} = \frac{d^2}{dt^2}(\vec{x}_1 - \vec{x}_2) \tag{3}$$

$$\Rightarrow \mu = \frac{M\, m}{m + M} = \frac{m}{\frac{m}{M} + 1} \tag{4}$$

as $m_{\mathrm{E}} \ll M_{\odot}$ is $\mu \approx m$, i.e. motion is relative to the center of mass $\equiv$ only motion of m. Set point of origin $(0,0)$ to the source of the force field of M.

Equations of motion III

Hence: Newton's 2. law (with $m \approx \mu$):

$$m\frac{d^2\vec{r}}{dt^2} = \vec{F} \tag{5}$$

$$m\frac{d^2}{dt^2}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} \tag{6}$$

and force field according to Newton's law of gravitation :

$$\vec{F} = -\frac{GMm}{r^3}\,\vec{r} \tag{7}$$

$$\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = -\frac{GMm}{r^3}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{8}$$

Equations of motion IV

Kepler's laws, as well as the assumption of a *central force* imply → *conservation of angular momentum* → motion is only in a *plane* (→ Kepler's 1st law).
So, we use Cartesian coordinates in the xy-plane:

$$F_x = -\frac{GMm}{r^3}x \qquad (9)$$

$$F_y = -\frac{GMm}{r^3}y \qquad (10)$$

The equations of motion are then:

$$\frac{d^2x}{dt^2} = -\frac{GM}{r^3}x \qquad (11)$$

$$\frac{d^2y}{dt^2} = -\frac{GM}{r^3}y \qquad (12)$$

$$\text{where} \quad r = \sqrt{x^2+y^2} \qquad (13)$$

Excursus: Analytic solution of the Kepler problem I

To derive the *analytic* solution for equation of motion $\vec{r}(t) \rightarrow$ use polar coordinates: ϕ, r

1. use conservation of angular momentum ℓ:

$$\mu r^2 \dot{\phi} = \ell = \text{const.} \tag{14}$$

$$\dot{\phi} = \frac{\ell}{\mu r^2} \tag{15}$$

2. use conservation of total energy ($\vec{v} = \dot{r}\vec{e}_r + r\dot{\phi}\vec{e}_\phi \rightarrow E_{\text{kin}} = \frac{\mu}{2}(\dot{r}^2 + r^2\dot{\phi}^2)$):

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{\ell^2}{2\mu r^2} - \frac{GM\mu}{r} \tag{16}$$

$$\dot{r}^2 = \frac{2E}{\mu} - \frac{\ell^2}{\mu^2 r^2} + \frac{2GM}{r} \tag{17}$$

$\rightarrow$ two coupled equations for r and ϕ

3. decouple Eq. (15), use the orbit equation $r = \frac{\alpha}{1+e\cos\phi}$ with numeric eccentricity e ($= \overline{f_1\, O}/a$, *Value for circle?*) and $\alpha \equiv \frac{\ell^2}{GM\mu^2}$ gives separable equation for $\dot{\phi}$

$$\dot{\phi} = \frac{d\phi}{dt} = \frac{G^2M^2\mu^3}{\ell^3}(1+e\cos\phi)^2 \tag{18}$$

$$t = \int_{t_0}^{t} dt' = k\int_{\phi_0}^{\phi} \frac{d\phi'}{(1+e\cos\phi')^2} = f(\phi) \tag{19}$$

right-hand side integral can be looked up in, e.g., Bronstein:

$$t/k = \frac{e\sin\phi}{(e^2-1)(1+e\cos\phi)} - \frac{1}{e^2-1}\int \frac{d\phi}{1+e\cos\phi} \tag{20}$$

$\rightarrow e \neq 1$: parabola excluded; the integral can be further simplified
for the hyperbola ($e > 1$):

$$\int \frac{d\phi}{1+e\cos\phi} = \frac{1}{\sqrt{e^2-1}} \ln \frac{(e-1)\tan\frac{\phi}{2} + \sqrt{e^2-1}}{(e-1)\tan\frac{\phi}{2} - \sqrt{e^2-1}} \tag{21}$$

for the ellipse ($0 \leq e < 1$):

$$\int \frac{d\phi}{1 + e\cos\phi} = \frac{2}{\sqrt{1-e^2}} \arctan \frac{(1-e)\tan\frac{\phi}{2}}{\sqrt{1-e^2}} \qquad (22)$$

→ Eq. (20) with Eqn. (22) & (21): $t(\phi)$ must be inverted to get $\phi(t)$!

(e.g., by numeric root finding)

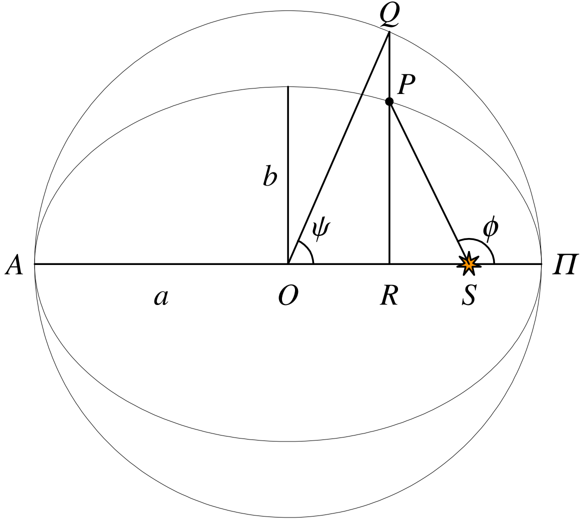
→ only easy for $e = 0$ → circular orbit

$$t = k \int d\phi' = k\phi \rightarrow \ \phi(t) = k^{-1} t = \frac{G^2 M^2 \mu^3}{\ell^3} t \qquad (23)$$

and from orbit equation (for $e = 0$) $r = \alpha = \frac{\ell^2}{GM\mu^2} = \text{const.}$

For the general case, it is much easier to solve the equations of motion numerically.

Alternative formulation for time dependency in case of an ellipse ($0 \leq e < 1$):



Orbit, circumscribed by auxiliary circle with radius a (= semi-major axis); true anomaly ϕ, eccentric anomaly ψ. Sun at S, planet at P, circle center at O. Perapsis (perhelion) Π and apapsis (aphelion) A:

- consider a line normal to $\overline{A\Pi}$ through P on the ellipse, intersecting circle at Q and $\overline{A\Pi}$ at R.
- consider an angle ψ (or E, eccentric anomaly) defined by $\angle \Pi O Q$

Excursus: The Kepler equation II

Then: position in polar coordinates (r, ϕ) of the body P can be described in terms of ψ:

$$x_S(P) = r\cos\phi = a\cos\psi - ae \qquad (ae = \overline{OS}) \tag{24}$$

$$y_S(P) = r\sin\phi = a\sin\psi\sqrt{1-e^2} \qquad (= \overline{PR} = \overline{QR}\sqrt{1-e^2} = a\sin\psi\sqrt{1-e^2}) \tag{25}$$

(with $\overline{PR}/\overline{QR} = b/a = \sqrt{1-e^2}$), square both equations and add them up:

$$r = a(1 - e\cos\psi) \tag{26}$$

Now, to find $\psi = \psi(t)$, need relationship between $d\phi$ and $d\psi$, so combine Eqn. (25) & (26)

$$\sin\phi = \frac{b\sin\psi}{a(1-e\cos\psi)} \quad |d/dt \text{ \& quotient rule } \left(\frac{u}{v}\right)' = \frac{u'v - v'u}{v^2} \tag{27}$$

$$\cos\phi d\phi = \frac{b}{a}\frac{(\cos\psi(1-e\cos\psi)d\psi - e\sin^2\psi d\psi)}{(1-e\cos\psi)^2} \tag{28}$$

$$d\phi = \frac{b}{a(1-e\cos\psi)}d\psi \tag{29}$$

together with the angular momentum $d\phi = \frac{\ell}{\mu r^2} dt$, where r is replaced by Eq. (26):

$$(1 - e\cos\psi)d\psi = \frac{\ell}{\mu ab} dt \tag{30}$$

$$= \text{set } t = 0 \rightarrow \psi(0) = 0, \text{ integration:} \tag{31}$$

$$\psi - e\sin\psi = \frac{\ell t}{\mu ab} \tag{32}$$

use Kepler's 2nd law $\frac{\pi ab}{P} = \frac{\ell}{2\mu}$ with πab the area of the ellipse, we get $\ell/(\mu ab) = 2\pi/P \equiv \omega$ (orbital angular frequency), so:

Kepler's equation for the eccentric anomaly ψ (or E)

$$\psi - e\sin\psi = \omega t \tag{33}$$

$$E - e\sin E = M \quad \text{(astronomer's version)} \tag{34}$$

M: mean anomaly = angle for constant angular velocity $= 2\pi \frac{t - t_\Pi}{P}$

Kepler's equation $E(t) - e \sin E(t) = M(t)$

- is a transcendental equation for the eccentric anomaly $E(t)$
- can be solved by, e.g., Newton's method
- because of $E = M + e \sin E$, also (Banach) fixed-point iteration possible (slow, but stable), already used by Kepler (1621):

```
E = M ;
for (int i = 0 ; i < n ; ++i)
   E = M + e * sin(E) ;
```

- can be solved, e.g., by Fourier series $\rightarrow$ Bessel (1784-1846):

$$E = M + \sum_{n=1}^{\infty} \frac{2}{n} J_n(ne) \sin(nM) \tag{35}$$

$$J_n(ne) = \frac{1}{\pi} \int_0^{\pi} \cos(nx - ne \sin x) dx \tag{36}$$

Circular orbits

A special case as a solution of the equations of motion (11) & (12) is the circular orbit. Then:

$$\ddot{r} = \frac{v^2}{r} \tag{37}$$

$$\frac{mv^2}{r} = \frac{GMm}{r^2} \quad \text{(equilibrium of forces)} \tag{38}$$

$$\Rightarrow \quad v = \sqrt{\frac{GM}{r}} \tag{39}$$

The relation (39) is therefore the condition for a circular orbit.
Moreover, Eq. (39) yields together with

$$P = \frac{2\pi r}{v} \tag{40}$$

$$\Rightarrow \quad P^2 = \frac{4\pi^2}{GM}\, r^3 \tag{41}$$

Astronomical units

For our solar system it is useful to use astronomical units (AU):

$$1\,\mathrm{AU} = 1.496 \times 10^{11}\,\mathrm{m}$$

and the unit of time is the (Earth-) year

$$1\,\mathrm{a} = 3.156 \times 10^{7}\,\mathrm{s} \quad (\approx \pi \times 10^{7}\,\mathrm{s}),$$

so, for the Earth $P = 1\,\mathrm{a}$ and $r = 1\,\mathrm{AU}$
Therefore it follows from Eq. (41):

$$GM = \frac{4\pi^2 r^3}{P^2} = 4\pi^2\,\mathrm{AU}^3\,\mathrm{a}^{-2} \tag{42}$$

I.e. we set $GM \equiv 4\pi^2$ in our calculations.
Advantage: handy numbers!
Thus, e.g. $r = 2$ is approx. $3 \times 10^{11}\,\mathrm{m}$ and $t = 0.1$ corresponds to $3.16 \times 10^{6}\,\mathrm{s}$, and $v = 6.28$ is roughly 30 km/s.
cf.: our `rcalc` program with "solar units" for R, T, L; natural units in particle physics $\hbar = c = k_\mathrm{B} = \epsilon_0 = 1 \rightarrow$ unit of m, p, T is eV (also for E)

The equations of motion (11) & (12):

$$\frac{d^2\vec{r}}{dt^2} = -\frac{GM}{r^3}\vec{r} \tag{43}$$

are a system of differential equations of 2nd order, that we shall solve now.
Formally: *integration* of the equations of motion to obtain the *trajectory* $\vec{r}(t)$.

Step 1: reduction

Rewrite Newton's equations of motion as a system of differential equations of *1st order* (here: 1d):

$$v(t) = \frac{dx(t)}{dt} \quad \& \quad a(t) = \frac{dv(t)}{dt} = \frac{F(x,v,t)}{m} \tag{44}$$

The Euler method II

Step 2: Solving the differential equation

Differential equations of the form (initial value problem)

$$\frac{dx}{dt} = f(x,t), \quad x(t_0) = x_0 \tag{45}$$

can be solved numerically (discretization[1]) by as simple method:

Explicit Euler method ("Euler's polygonal chain method")

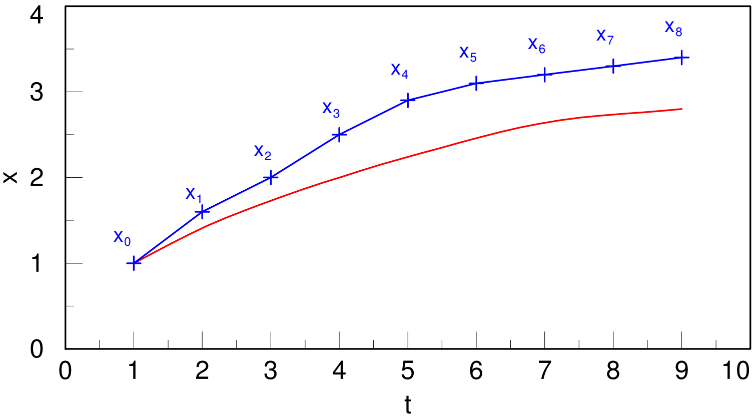
1. choose step size $\Delta t > 0$, so that $t_n = t_0 + n\Delta t, \quad n = 0, 1, 2, \ldots$
2. calculate the values (iteration):
   $x_{n+1} = x_n + f(x_n, t_n)\Delta t$ where $x_n = x(t_n)$ etc.

Obvious: The smaller the step size Δt, the more steps are necessary, but also the more accurate is the result.

[1] I.e. we change from calculus to algebra, which can be solved by computers.

The Euler method III

Why "polygonal chain method"?



Exact solution (–) and numerical solution (–).

Derivation from the Fundamental theorem of calculus

$$\text{integration of the ODE} \quad \frac{dx}{dt} = f(x,t) \quad \text{from } t_0 \text{ till } t_0 + \Delta t \tag{46}$$

$$\int_{t_0}^{t_0+\Delta t} \frac{dx}{dt} dt = \int_{t_0}^{t_0+\Delta t} f(x,t) dt \tag{47}$$

$$\Rightarrow x(t_0+\Delta t) - x(t_0) = \int_{t_0}^{t_0+\Delta t} f(x(t),t) dt \tag{48}$$

apply rectangle rule for the integral:

$$\int_{t_0}^{t_0+\Delta t} f(x(t),t) dt \approx \Delta t \, f(x(t_0),t_0) \tag{49}$$

Equating (48) with (49) yields Euler step

$$x(t_0+\Delta t) = x(t_0) + \Delta t \, f(x(t_0),t_0) \tag{50}$$

Derivation from Taylor expansion

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \, \frac{dx}{dt}(t_0) + \mathcal{O}(\Delta t^2) \tag{51}$$

$$\text{use} \quad \frac{dx}{dt} = f(x, t) \tag{52}$$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \, f(x(t_0), t_0) \tag{53}$$

while neglecting term of higher order in Δt

(*In which step did we neglect these higher order terms in the derivation from the fundamental theorem of calculus?*)

For the system Eqn. (44)

$$v(t) = \frac{dx(t)}{dt} \quad \& \quad a(t) = \frac{dv(t)}{dt} = \frac{F(x,v,t)}{m}$$

this means

Euler method for solving Newton's equations of motion

$$v_{n+1} = v_n + a_n \Delta t = v_n + a_n(x_n, t)\Delta t \quad (54)$$

$$x_{n+1} = x_n + v_n \Delta t \quad (55)$$

We note:

- the velocity at the end of the time interval v_{n+1} is calculated from a_n, which is the acceleration at the beginning of the time interval
- analogously x_{n+1} is calculated from v_n

Example: Harmonic oscillator $F = ma = -kx$

```
#include <iostream>
#include <cmath>
using namespace std ;

// set k = m = 1
int main () {

  int n = 10001, nout = 500 ;
  double t, v, v_old, x ;
  double const dt = 2. * M_PI / double(n-1) ;

  x = 1. ; t = 0. ; v = 0. ;

  for (int i = 0 ; i < n ; ++i) {
    t = t + dt ; v_old = v ;
    v = v - x * dt ;
    x = x + v_old * dt ;
    if (i % nout == 0) // print out only each nout step
      cout << t << " " << x << " " << v << endl ;
  }

  return 0 ;
}
```

The Euler-Cromer method

We will slightly modify the explicit Euler method, but such that we obtain the same differential equations for $\Delta t \to 0$.
For this new method we use v_{n+1} for calculating x_{n+1}:

Euler-Cromer method (semi-implicit Euler method)

$$v_{n+1} = v_n + a_n \Delta t \quad \text{(as for Euler)} \tag{56}$$

$$x_{n+1} = x_n + v_{n+1} \Delta t \tag{57}$$

Advantage of this method:

- as for Euler method, x, v need to be calculated only once per step
- especially appropriate for oscillating solutions, as energy is conserved much better (see below)

Proof of stability (Cromer 1981):

$$v_{n+1} = v_n + F_n \Delta t \quad (= v_n + a(x_n)\Delta t,\ m = 1) \tag{58}$$

$$x_{n+1} = x_n + v_{n+1} \Delta t \tag{59}$$

Without loss of generality, let $v_0 = 0$. Iterate Eq. (58) n times:

$$v_n = (F_0 + F_1 + \ldots + F_{n-1})\Delta t = S_{n-1} \tag{60}$$

$$x_{n+1} = x_n + S_n \Delta t \tag{61}$$

$$S_n := \Delta t \sum_{j=0}^{n} F_j \tag{62}$$

Note that for explicit Euler Eq. (61) is $x_{n+1} = x_n + S_{n-1}\Delta t$.

The change in the kinetic energy K between $t_0 = 0$ and $t_n = n\Delta t$ is because of Eq. (58) and $v_0 = 0$

$$\Delta K_n = K_n - K_0 = K_n = \frac{1}{2} S_{n-1}^2 \tag{63}$$

The change in the potential energy U:

$$\Delta U_n = -\int_{x_0}^{x_n} F(x) dx \tag{64}$$

Excursus: Proof of stability for the Euler-Cromer method III

Now use the trapezoid rule for this integral

$$\Delta U_n = -\frac{1}{2}\sum_{i=0}^{n-1}(F_i + F_{i+1})(x_{i+1} - x_i) \tag{65}$$

$$= -\frac{1}{2}\Delta t\sum_{i=0}^{n-1}(F_i + F_{i+1})S_i \qquad (\rightarrow \text{ Eq. 61}) \tag{66}$$

$$= -\frac{1}{2}\Delta t^2\sum_{i=0}^{n-1}\sum_{j=0}^{i}(F_i + F_{i+1})F_j \qquad (\rightarrow \text{ Eq. 62}) \tag{67}$$

As j runs from 0 to i (instead of $i-1$):
$\rightarrow \Delta U_n$ has same squared terms as ΔK_n, using $S_n = \Delta t \sum_{j=0}^{n} F_j$:

$$\Delta U_n = -\frac{1}{2}\Delta t^2 \left(\sum_{i=0}^{n-1} F_i^2 + \sum_{i=0}^{n-1}\sum_{j=0}^{i-1} F_i F_j + \sum_{i=1}^{n}\sum_{j=0}^{i-1} F_i F_j \right) \tag{68}$$

$$= -\frac{1}{2}\Delta t^2 \left(\sum_{i=0}^{n-1} F_i^2 + 2\sum_{i=0}^{n-1}\sum_{j=0}^{i-1} F_i F_j + F_n \sum_{j=0}^{i-1} F_j \right) \tag{69}$$

$$= -\frac{1}{2} S_{n-1}^2 - \frac{1}{2}\Delta t\, F_n S_{n-1} \tag{70}$$

Hence the total energy changes as

$$\Delta E_n = \Delta K_n + \Delta U_n = \frac{1}{2} S_{n-1}^2 - \frac{1}{2} S_{n-1}^2 - \frac{1}{2}\Delta t\, F_n S_{n-1} \tag{71}$$

$$= -\frac{1}{2}\Delta t\, F_n S_{n-1} = -\frac{1}{2}\Delta t\, F_n v_n \tag{72}$$

For oscillatory motion: $v_n = 0$ at turning points, $F_n = 0$ at equilibrium points
$\rightarrow \Delta E_n = -\frac{1}{2}\Delta t\, F_n v_n$ is 0 four times of each cycle $\rightarrow \Delta E_n$ oscillates with $T/2$.
As F_n and v_n are bound $\rightarrow \Delta E_n$ is bound, more important: average of ΔE_n over half a cycle (T)

$$\langle \Delta E_n \rangle = \frac{\Delta t^2}{T} \sum_{n=0}^{\frac{1}{2}T/\Delta t} F_n v_n \simeq \frac{\Delta t}{T} \int_0^{\frac{T}{2}} F\, v\, dt = \frac{\Delta t}{T} \int_{x(0)}^{x(\frac{T}{2})} F\, dx \tag{73}$$

$$= -\frac{\Delta t}{T} \left(U(T/2) - U(0) \right) = 0 \tag{74}$$

as U has same value at each turning point
$\rightarrow$ energy conserved on average with Euler-Cromer for oscillatory motion

□

For comparison: with explicit Euler method ΔE_n contains term $\sum_{i=0}^{n-1} F_i^2$ which increases monotonically with n and

$$\Delta E_n = -\frac{1}{8}\Delta t^2 \left(F_0^2 - F_n^2\right) \tag{75}$$

with $v_0 = 0 \rightarrow F_0^2 \geq F_n^2 \rightarrow \Delta E_n$ oscillates between 0 and $-\frac{1}{8}\Delta t^2 F_0^2$ per cylce.
Energy is bounded as for Euler-Cromer, but $\langle \Delta E_n \rangle \neq 0$

Consider the following ODE

$$\frac{dx}{dt} = -cx \tag{76}$$

with $c > 0$ and $x(t=0) = x_0$. Analytic solution is $x(t) = x_0 \exp(-ct)$. The explicit Euler method gives:

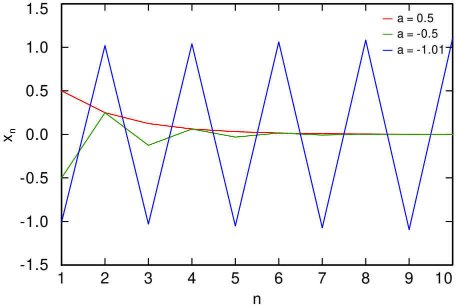
$$x_{n+1} = x_n + \dot{x}_n \Delta t = x_n - c x_n \Delta t = x_n(1 - c\Delta t) \tag{77}$$

So, every step will give $(1 - c\Delta t)$ and after n steps:

$$x_n = (1 - c\Delta t)^n x_0 = (a)^n x_0 \tag{78}$$

But, with $a = 1 - c\Delta t$:

$$\begin{aligned} 0 < a < 1 \quad &\Rightarrow \Delta t < 1/c \quad && \text{monotonic decline of } x_n \text{ (correct)} \\ -1 < a < 0 \quad &\Rightarrow 1/c < \Delta t < 2/c \quad && \text{oscillating decline of } x_n \\ a < -1 \quad &\Rightarrow \Delta t > 2/c \quad && \text{oscillating increase of } x_n\,! \end{aligned} \tag{79}$$



Stability of the explicit Euler method for different $a = 1 - c\Delta t$

In contrast, consider implicit Euler method (Euler-Cromer):

$$x_{n+1} = x_n + \dot{x}_{n+1}\Delta t = x_n - c x_{n+1}\Delta t \tag{80}$$

$$\Rightarrow x_{n+1} = \frac{x_n}{1 + c\Delta t} \tag{81}$$

declines for all Δt (!)

In Taylor approximation Eq. (51) for $x' = f(x,t)$ we neglected terms of $\mathcal{O}(\Delta t^2)$:

$$x(t_0 + \Delta t) = x(t_0) + \Delta t\, x'(t_0) + \frac{\Delta t^2}{2!} x''(t_0) + \frac{\Delta t^3}{3!} x^{(3)}(t_0) + \frac{\Delta t^4}{4!} x^{(4)}(\zeta_0) \tag{82}$$

with $t_0 < \zeta_0 < t_1$, nectlect this term, then difference equation:

$$\rightarrow\ x(t_0 + \Delta t) = x(t_0) + \Delta t\, f(x_0, t_0) + \frac{\Delta t^2}{2} f'(x_0, t_0) + \frac{\Delta t^3}{6} f''(x_0, t_0) \tag{83}$$

Using chain rule for f' with partial derivatives f_t etc.:

$$x' = f(x,t) \tag{84}$$

$$x'' = f' = f_t \frac{dt}{dt} + f_x\, x' = f_t + f_x f \tag{85}$$

$$x^{(3)} = f'' = f_{tt} + 2f_{tx} f + f_{xx} f^2 + f_t f_x + f_x^2 f \tag{86}$$

$\rightarrow$ replace f', f'' in Eq. (83) $\rightarrow$ third-order Taylor's method
problem: compute and find partial derivatives of f (for Newton: $\partial_{x,v,t} F(x,v,t)$)

Hence: replace $\sum_j^p \frac{\Delta t^j}{j!} f^{(j-1)}(t_n, x_n)$ with some function $ak_1 + bk_2$:

$$x_{n+1} = x_n + ak_1 + bk_2 \quad (87)$$
$$k_1 = \Delta t\, f(t_n, x_n) \quad (88)$$
$$k_2 = \Delta t\, f(t_n + \alpha\Delta t, x_n + \beta k_1) \quad (89)$$

and determine constants a, b, α, β so that error in Eq. (87) is minimum
$\rightarrow$ Eq. (87) $\hat{=}$ Taylor series:

$$x_{n+1} = x_n + \Delta t\, f(t_n, x_n) + \frac{\Delta t^2}{2} f'(t_n, x_n) + \ldots \quad (90)$$
$$\text{with } f' = f_t + f_x f : \quad (91)$$
$$x_{n+1} = x_n + \Delta t\, f + \frac{\Delta t^2}{2}(f_t + f_x f) + \mathcal{O}(\Delta t^3) \quad (92)$$

Now, Taylor expansion of $f(t_n + \alpha\Delta t, x_n + \beta k_1)$:

$$f(t_n + \alpha\Delta t, x_n + \beta k_1) = f(t_n, x_n) + \alpha\Delta t\, f_t + \beta k_1 f_x + \mathcal{O}(\Delta t^2) \quad (93)$$

Higher-Order Taylor series method III

→ combine Eq. (93) with Eqn. (87 - 89)

$$x_{n+1} = x_n + ak_1 + bk_2 = a\Delta t\, f(t_n, x_n) + b\Delta t\, f(t_n + \alpha\Delta t, x_n + \beta k_1) \quad (94)$$

$$= x_n + \Delta t(a+b)f + b\Delta t^2(\alpha f_t + \beta f_x\, f) \quad (95)$$

$$\stackrel{!}{=} x_n + \Delta t\, f + \frac{\Delta t^2}{2}(f_t + f_x f) \quad (\rightarrow \text{Eq. } (51)) \quad (96)$$

$$\Rightarrow \quad a + b = 1 \quad \& \quad \alpha = \beta = \frac{1}{2b} \quad (97)$$

→ 3 equations for 4 unknowns → one variable can be chosen arbitrarily, e.g.,

$$a = b = \frac{1}{2} \quad \& \quad \alpha = \beta = 1 \quad (98)$$

→ modified Euler method (so-called Runge-Kutta method of order 2)

$$x_{n+1} = x_n + \frac{1}{2}(k_1 + k_2) = x_n + \frac{1}{2}(\Delta t\, f(t_n, x_n) + \Delta t\, f(t_n + \Delta t, x_n + \Delta t\, k_1)) \quad (99)$$

$$x_{n+1} = x_n + \frac{\Delta t}{2}(f(t_n, x_n) + f(t_n + \Delta t, x_n + \Delta t\, f(t_n, x_n))) \quad (100)$$

(analogously: construct RK4-method → see later)

Higher-Order Taylor series method IV

Alternative choice: $\alpha = \beta = 1/2, a = 0, b = 1 \rightarrow$ midpoint method

$$x_{n+1} = x_n + ak_1 + bk_2 \tag{101}$$

$$= x_n + k_2 = x_n + \Delta t\, f\left(t_n + \frac{1}{2}\Delta t, x_n + \frac{1}{2}k_1\right) \tag{102}$$

$$x_{n+1} = x_n + \Delta t\, f\left(t_n + \frac{\Delta t}{2}, x_n + \frac{\Delta t}{2} f(t_n, x_n)\right) \tag{103}$$

$\rightarrow$ also known as Euler-Richardson method

The Euler-Richardson method

Sometimes it is better, to calculate the velocity for the midpoint of the interval:

Euler-Richardson method ("Euler half step method")

$$a_n = F(x_n, v_n, t_n)/m \tag{104}$$

$$v_M = v_n + a_n \frac{1}{2}\Delta t \tag{105}$$

$$x_M = x_n + v_n \frac{1}{2}\Delta t \tag{106}$$

$$a_M = F\left(x_M, v_M, t_n + \frac{1}{2}\Delta t\right)/m \tag{107}$$

$$v_{n+1} = v_n + a_M \Delta t \tag{108}$$

$$x_{n+1} = x_n + v_M \Delta t \tag{109}$$

We need twice the number of steps of calculation, but may be more efficient, as we might choose a larger step size as for the Euler method.

Cromer, A. 1981, American Journal of Physics, 49, 455