Computational Astrophysics I: Introduction and basic concepts

Helge Todt

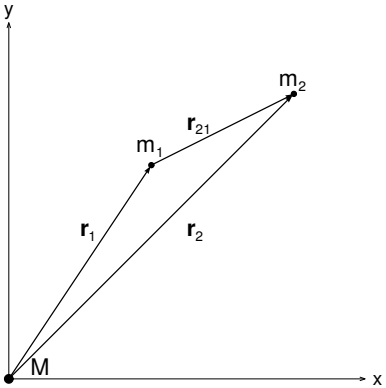
Astrophysics
Institute of Physics and Astronomy
University of Potsdam

SoSe 2024, 22.5.2024

The (special) three-body problem

The (special)† three-body problem I

We will not solve the general case of the three-body problem, but consider only the following configuration ($m_1, m_2 < M$):



$$m_1 \frac{d^2\vec{r}_1}{dt^2} = -\frac{GMm_1}{r_1^3}\vec{r}_1 + \frac{Gm_1m_2}{r_{21}^3}\vec{r}_{21} \qquad (1)$$

$$m_2 \frac{d^2\vec{r}_2}{dt^2} = -\frac{GMm_2}{r_2^3}\vec{r}_2 - \frac{Gm_1m_2}{r_{21}^3}\vec{r}_{21} \qquad (2)$$

†not to confuse with the restricted three-body problem, where $m_1 \approx m_2 \gg m_3$
→ Lagrangian points, e.g, L_1 for SOHO, L_2 for JWST

It is useful to divide the Eqn. (1) & (2) each by m_1 and m_2 respectively:

$$\frac{d^2\vec{r}_1}{dt^2} = -\frac{GM}{r_1^3}\vec{r}_1 + \frac{Gm_2}{r_{21}^3}\vec{r}_{21} \tag{3}$$

$$\frac{d^2\vec{r}_2}{dt^2} = -\frac{GM}{r_2^3}\vec{r}_2 - \frac{Gm_1}{r_{21}^3}\vec{r}_{21} \tag{4}$$

Moreover we can set – using astronomical units – again:

$$GM \equiv 4\pi^2 \tag{5}$$

The terms

$$+\frac{Gm_2}{r_{21}^3}\vec{r}_{21} \quad \& \quad -\frac{Gm_1}{r_{21}^3}\vec{r}_{21} \tag{6}$$

can be written with help of mass ratios

$$\frac{m_2}{M} \quad \& \quad -\frac{m_1}{M} \tag{7}$$

so that

$$\texttt{ratio}[0] = \frac{m_2}{M} GM \quad \& \quad \texttt{ratio}[1] = -\frac{m_1}{M} GM \tag{8}$$

The *accelerations* are then calculated like this (in C/C++):

```
dx = x[1] - x[0]
   ...
dr3 = pow(dx * dx + dy * dy , 3./2. )
   ...
ax = -GM * x[i] / r3 + ratio[i] * dx / dr3
ay = -GM * y[i] / r3 + ratio[i] * dy / dr3
```

Methods for solving the Newtonian equations of motion

Review → Newtonian equations of motion (2nd order ODE → reduction to 1st order)

$$\frac{dv}{dt} = a(t) \quad \& \quad \frac{dx}{dt} = v(t) \tag{9}$$

Numerical solution from Taylor expansion:

$$v_{n+1} = v_n + a_n \Delta t + \mathcal{O}((\Delta t)^2) \tag{10}$$

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2 + \mathcal{O}((\Delta t)^3) \tag{11}$$

Euler method: account only for $\mathcal{O}(\Delta t)$ (for $\Delta t \to 0$):

$$v_{n+1} = v_n + a_n \Delta t \tag{12}$$

$$x_{n+1} = x_n + v_n \Delta t \tag{13}$$

therefore, only having $\mathcal{O}(\Delta t)$:
→ local truncation error in one time step: $\sim (\Delta t)^2$
→ global error over t: $\sim (\Delta t)$, because n steps with $n = \frac{t}{\Delta t} \sim \frac{1}{\Delta t}$,

$\rightarrow$ so order of global error reduced by $\frac{1}{\Delta t}$

A method is of nth order, if the global error is of the order of $(\Delta t)^n$. The Euler method is of of 1st order.

Note, the Euler-Cromer method (semi-implicit Euler method) is also of 1st order, but conserves energy (symplectic integrator):

$$v_{n+1} = v_n + a_n(x_n)\Delta t \tag{14}$$
$$x_{n+1} = x_n + v_{n+1}\Delta t \tag{15}$$

but there is also a 2nd variant of the (semi-implicit) Euler method

$$x_{n+1} = x_n + v_n\Delta t \tag{16}$$
$$v_{n+1} = v_n + a_{n+1}(x_{n+1})\Delta t \tag{17}$$

$\rightarrow$ used for Verlet integration (see below Eqn. (27) & (28))

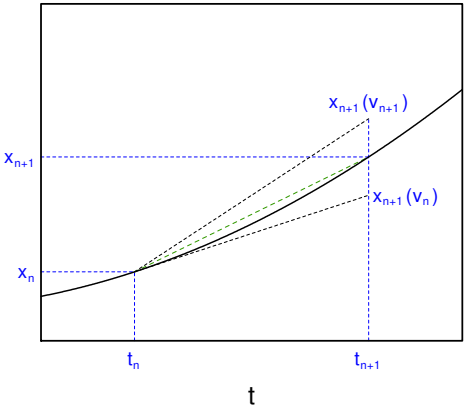
Possible improvement: use velocity from the *midpoint* of the interval

cf. Heun's method (Karl Heun, 1859-1929)

$$v_{n+1} = v_n + a_n \Delta t \quad \text{(as for Euler)} \tag{18}$$

$$x_{n+1} = x_n + \frac{1}{2}(v_n + v_{n+1})\Delta t \tag{19}$$

$$= x_n + v_n \Delta t + \frac{1}{2} a_n \Delta t^2 \tag{20}$$



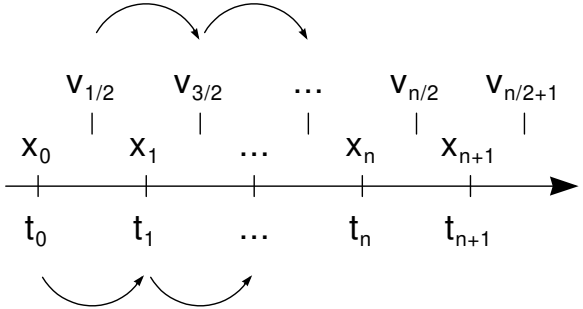
→ accuracy of position is of 2nd order and velocity is of 1st order (only good for constant acceleration, not more accurate than Euler, as error increases with each time step)

Better (stable for oscillatory motions with const. $\Delta t \leq 2/\omega$, therefore common, error bounded):

Halfstep method / Leapfrog integration

$$v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + a_n \Delta t \tag{21}$$

$$x_{n+1} = x_n + v_{n+\frac{1}{2}} \Delta t \tag{22}$$



$\rightarrow$ 2nd order with same number of steps as Euler (1st order), time-reversable, exact conservation of momenta, energy conserved up to 3rd order

But: not self starting, i.e. from Eq. (21) $\nrightarrow v_{\frac{1}{2}}$
therefore Euler method for the first half step:

$$v_{\frac{1}{2}} = v_0 + \frac{1}{2} a_0 \Delta t \tag{23}$$

Moreover, velocity steps can be eliminated by using Eq. (21) & (22):

$$(x_{n+1} - x_n) - (x_n - x_{n-1}) = (v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}})\Delta t \tag{24}$$

$$x_{n+1} - 2x_n + x_{n-1} = a_n \Delta t \tag{25}$$

$$\rightarrow \; x_{n+1} = 2x_n - x_{n-1} + a_n \Delta t^2 \quad \text{(Størmer's method}^{\dagger}\text{)} \tag{26}$$

with start values $x_0, x_1 = x_0 + v_0 + \frac{1}{2} a_0(x_0)\Delta t^2$ (so v_0 is still required!)

† Carl Størmer (1874-1957), Norwegian physicist, theoretical description of aurora borealis $\rightarrow$ trajectories of charged particles in magnetic field

Or, by interpolation of intermediate values as combination of symplectic, semi-implicit Euler methods (Eq. (14)-(17))

$$\left.\begin{aligned} v_{n+\frac{1}{2}} &= v_n + a_n \tfrac{1}{2}\Delta t \\ x_{n+\frac{1}{2}} &= x_n + v_{n+\frac{1}{2}} \tfrac{1}{2}\Delta t \end{aligned}\right\} \quad (27) \qquad \left.\begin{aligned} x_{n+1} &= x_{n+\frac{1}{2}} + v_{n+\frac{1}{2}} \tfrac{1}{2}\Delta t \\ v_{n+1} &= v_{n+\frac{1}{2}} + a_{n+1} \tfrac{1}{2}\Delta t \end{aligned}\right\} \quad (28)$$

by substituting system (27) into system (28) one obtains Leapfrog with integer steps:

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n \Delta t^2 \quad (29)$$

$$v_{n+1} = v_n + \frac{1}{2}(a_n + a_{n+1})\Delta t \quad (30)$$

$\rightarrow$ so-called Verlet integration[†] (see next slides)

[†]Loup Verlet (1931-2019), french physicist, pioneered computer simulations

Higher order methods

for that purpose: Taylor expansion of x_{n-1} (negative time step):

$$x_{n-1} = x_n - v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2 - \mathcal{O}((\Delta t)^3) \tag{31}$$

$$+ \quad x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2 + \mathcal{O}((\Delta t)^3) \tag{32}$$

$$= \quad x_{n+1} + x_{n-1} = 2x_n + a_n (\Delta t)^2 + \mathcal{O}((\Delta t)^4) \tag{33}$$

$$\Rightarrow \quad x_{n+1} = 2x_n - x_{n-1} + a_n (\Delta t)^2 \tag{34}$$

Analogously:

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2 + \mathcal{O}((\Delta t)^3) \tag{35}$$

$$- \quad (x_{n-1} = x_n - v_n \Delta t + \frac{1}{2} a_n (\Delta t)^2 - \mathcal{O}((\Delta t)^3)) \tag{36}$$

$$= \quad x_{n+1} - x_{n-1} = 2 v_n \Delta t + \mathcal{O}((\Delta t)^3) \tag{37}$$

$$\Rightarrow \quad v_n = \frac{x_{n+1} - x_{n-1}}{2\Delta t} \qquad \text{(Verlet)} \tag{38}$$

$\rightarrow$ method of 2nd order in v and 3rd order in x

But:

- not self starting (needs start values $x_0, x_1 = x_0 + v_0 + \frac{1}{2}a_0\Delta t^2$, see above)
- Eq. (38) contains differences of two values of same order of magnitude and expected $\Delta x \ll x \rightarrow$ round-off errors possible (subtractive cancelation)

Therefore, from Eq. (37)

$$x_{n-1} = x_{n+1} - 2v_n\Delta t \qquad \text{insert in Eq. (34):} \tag{39}$$

$$x_{n+1} = 2x_n - x_{n+1} + 2v_n\Delta t + a_n(\Delta t)^2 \tag{40}$$

Solve for x_{n+1}, yields:

Velocity Verlet

$$x_{n+1} = x_n + v_n\Delta t + \frac{1}{2}a_n(\Delta t)^2 \tag{41}$$

$$v_{n+1} = v_n + \frac{1}{2}(a_{n+1} + a_n)\Delta t \qquad \text{(see below for derivation)} \tag{42}$$

$\rightarrow$ self-starting
$\rightarrow$ minimizes round-off errors (no differences)
$\rightarrow$ 4th order in x (why? $\rightarrow$ Eq. (35) & (36))
Eq. (42) results from Eq. (38) for v_{n+1}:

$$v_{n+1} = \frac{x_{n+2} - x_n}{2\Delta t} \tag{43}$$

$$\text{and} \quad x_{n+2} = 2x_{n+1} - x_n + a_{n+1}(\Delta t)^2 \quad \text{from Eq. (34)} \tag{44}$$

$$\Rightarrow \quad v_{n+1} = \frac{2x_{n+1} - x_n + a_{n+1}(\Delta t)^2 - x_n}{2\Delta t} \tag{45}$$

$$= \frac{x_{n+1} - x_n}{\Delta t} + \frac{1}{2}a_{n+1}(\Delta t)^2 \quad \& \; x_{n+1} \text{ from Eq. (41)}$$

$$= \frac{x_n + v_n\Delta t + \frac{1}{2}a_n(\Delta t)^2 - x_n}{\Delta t} + \frac{1}{2}a_{n+1}\Delta t \tag{46}$$

$$= v_n + \frac{1}{2}(a_{n+1} + a_n)\Delta t \tag{47}$$

Alternatively:
(developed for liquid particles in a Lennard-Jones potential)

Beeman method (Schofield 1973; Beeman 1976)

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{6}(4a_n - a_{n-1})(\Delta t)^2 \quad (48)$$

$$v_{n+1} = v_n + \frac{1}{6}(2a_{n+1} + 5a_n - a_{n-1})\Delta t \quad (49)$$

$\rightarrow$ not self-starting
$\rightarrow$ locally: $\mathcal{O}(\Delta t)^4$ in x and $\mathcal{O}(\Delta t)^3$ in v, globally $\mathcal{O}(\Delta t)^3$
$\rightarrow$ better energy conservation than for Verlet, but more calculation steps

even better: $\rightarrow$ Runge-Kutta method of 4th order

The Runge-Kutta method

Runge-Kutta method of 4th order I

Remember:

Euler-Richardson method (Euler-halfstep method)

$$a_n = F(x_n, v_n, t_n)/m \tag{50}$$

$$v_M = v_n + a_n \frac{1}{2}\Delta t \tag{51}$$

$$x_M = x_n + v_n \frac{1}{2}\Delta t \tag{52}$$

$$a_M = F\left(x_M, v_M, t_n + \frac{1}{2}\Delta t\right)/m \tag{53}$$

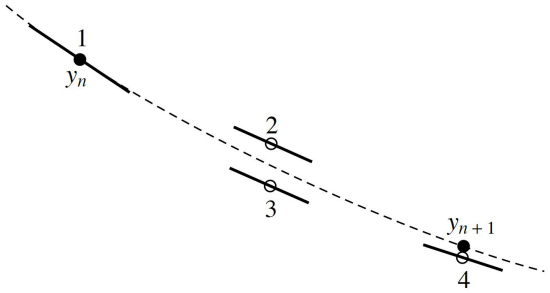
$$v_{n+1} = v_n + a_M \Delta t \tag{54}$$

$$x_{n+1} = x_n + v_M \Delta t \tag{55}$$

$\rightarrow$ calculation of F or a, respectively, for the whole step at the "midpoint" of the interval, instead of using the values from the beginning

$\equiv$ Runge-Kutta method *2nd order*

We will refine the halfstep method by using more supporting points:



With the Runge-Kutta method[†] the initial value problem

$$dy/dx = y' = f(x, y), \quad y(x_0) = y_0 \tag{56}$$

is solved by calculating approximate values y_i at selected supporting points x_i to obtain the wanted $y(x)$. These y_i are calculated with help of the following scheme (cf. Bronstein), where also only linear terms are calculated, but in form of a "polygonal line":

- supporting point at the beginning and at the end of the interval
- two additional supporting points in the middle of the interval with doubled weight

Derivation: include higher order terms in Taylor expansion, replace partial derivatives with coefficients to be determined ...

[†]Carl Runge (1856-1927), Wilhelm Kutta (1867-1944)

Move from x_0 to $x_i = x_0 + ih$ (step size h, $i = 0, 1, 2, \ldots$) $\rightarrow$ single step method

x	y	$k = h \cdot f(x, y) = h \cdot dy/dx$
x_0	y_0	k_1
$x_0 + h/2$	$y_0 + k_1/2$	k_2
$x_0 + h/2$	$y_0 + k_2/2$	k_3
$x_0 + h$	$y_0 + k_3$	k_4
$x_1 = x_0 + h$	$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$	

Cf.: Simpson's rule[†] (actually Kepler's rule , "Keplersche Fassregel", 1615) for integration of $y'(x)$ via a parabola:

$$\int_a^b y'(x)dx \approx \frac{b-a}{6}\left(y'(a) + 4\,y'\left(\frac{a+b}{2}\right) + y'(b)\right) \tag{57}$$

[†]Thomas Simpson (1710-1761)

For the equations of motion this means therefore:

$$\vec{k}_{1v} = \vec{a}(\vec{x}_n, \vec{v}_n, t)\,\Delta t \quad (= \vec{a}_{\text{grav.}}(\vec{x}_n)\,\Delta t \quad \text{in our case}) \tag{58}$$

$$\vec{k}_{1x} = \vec{v}_n\,\Delta t \tag{59}$$

$$\vec{k}_{2v} = \vec{a}\left(\vec{x}_n + \frac{\vec{k}_{1x}}{2}, \vec{v}_n + \frac{\vec{k}_{1v}}{2}, t_n + \frac{\Delta t}{2}\right)\Delta t \tag{60}$$

$$\vec{k}_{2x} = \left(\vec{v}_n + \frac{\vec{k}_{1v}}{2}\right)\Delta t \tag{61}$$

$$\vec{k}_{3v} = \vec{a}\left(\vec{x}_n + \frac{\vec{k}_{2x}}{2}, \vec{v}_n + \frac{\vec{k}_{2v}}{2}, t_n + \frac{\Delta t}{2}\right)\Delta t \tag{62}$$

$$\vec{k}_{3x} = \left(\vec{v}_n + \frac{\vec{k}_{2v}}{2}\right)\Delta t \tag{63}$$

$$\vec{k}_{4v} = \vec{a}(\vec{x}_n + \vec{k}_{3x}, \vec{v}_n + \vec{k}_{3v}, t + \Delta t)\,\Delta t \tag{64}$$

$$\vec{k}_{4x} = (\vec{v}_n + \vec{k}_{3v})\,\Delta t \tag{65}$$

So, finally

$$v_{n+1} = v_n + \frac{1}{6}(k_{1v} + 2k_{2v} + 2k_{3v} + k_{4v}) \quad (66)$$

$$x_{n+1} = x_n + \frac{1}{6}(k_{1x} + 2k_{2x} + 2k_{3x} + k_{4x}) \quad (67)$$

$\rightarrow$ Runge-Kutta methods are self-starting

Adaptive stepsize: step doubling

1. calculate new coordinates $(\vec{x}, \vec{v})$ via *two* Runge-Kutta steps each with Δt
2. calculate new coordinates $(\vec{x}, \vec{v})'$ via *one* Runge-Kutta step with $2\Delta t$

$\rightarrow$ calculation overhead increases only by 11/8, because of same derivatives on the beginning of the interval

Now, if

$$\frac{|(x,v) - (x,v)'|}{|(x,v)|} \geq \epsilon_{\max} \tag{68}$$

with an accuracy criterion $\epsilon_{\max}$ $\rightarrow$ decrease stepsize Δt
If

$$\frac{|(x,v) - (x,v)'|}{|(x,v)|} \leq \epsilon_{\min} \quad \text{mit} \quad \epsilon_{\min} < \epsilon_{\max} \tag{69}$$

$\rightarrow$ increase Δt

Predictor-corrector method

First *prediction* of the new position, e.g.:

$$x_{\mathrm{p}} = x_{n-1} + 2v_n\Delta t \tag{70}$$

$\rightarrow$ yields accleration a_{p} $\rightarrow$ *corrected* position by trapezoidal rule:

$$v^0_{n+1} = v_n + \frac{1}{2}(a_{\mathrm{p}} + a_n)\Delta t \tag{71}$$

$$x^0_{n+1} = x_n + \frac{1}{2}(v_{n+1} + v_n)\Delta t \tag{72}$$

$\rightarrow$ yields better value for a_{n+1} and hence

$$v^1_{n+1} = v_n + a_{n+1}\Delta t \tag{73}$$

$$x^1_{n+1} = x_n + v_{n+1}\Delta t \tag{74}$$

repeated iteration until $|x^{k+1}_{n+1} - x^k_{n+1}| < \epsilon$ with intended accuracy ϵ

Bulirsch-Stoer method I

Especially interesting for interactions of several bodys (*few-body problem*):

- resonances in planetary systems
- influence by one-time passage of a star
- influence of the galactic gravitational potential

→ Requires:

- high numerical accuracy
- flexibility
- high computation rate

Idea: combination of

- modified midpoint method
- Richardson extrapolation
- extrapolation via rational functions

→ Bulirsch-Stoer method (Stoer & Bulirsch 1980)[†]
cf. Numerical Recipes

[†]Roland Bulirsch (1932-2022), Josef Stoer (*1934)

Modified midpoint method

For an ODE $dx/dt = f(t, x)$ over a time step $H = Nh$ with N equidistant sub-steps

$$
\begin{aligned}
x_0 &= x(t) && (75)\\
x_1 &= x_0 + hf(t, x_0) && (76)\\
&\dots && (77)\\
x_n &= x_{n-2} + 2hf(t + [n-1]h, x_{n-1}) \quad n = 2, \dots, N && (78)\\
x(t+H) \approx \tilde{x} &= \frac{1}{2}[x_N + x_{N-1} + hf(t + H, x_N)] && (79)
\end{aligned}
$$

$\rightarrow$ 2nd order method, but with only one derivative per h-(sub)step
(where 2nd order Runge-Kutta has two derivatives per step)

Gragg† (1965): error in Eq. (79) $\rightarrow$ even power series:

$$\tilde{x} - x(t+H) = \sum_{i=1}^{\infty} \alpha_i h^{2i} \tag{80}$$

$\rightarrow$ for even N (so, $N = 2, 4, 6, \ldots$) all odd error terms cancel out $\rightarrow$ accuracy increases two orders at a time when combining two crossings of interval H with increasing N:

Let $x_{N/2}$ the result for $x(t+H)$ with half the number of steps:

$$x(t+H) \approx \frac{4\tilde{x}_N - \tilde{x}_{N/2}}{3} \tag{81}$$

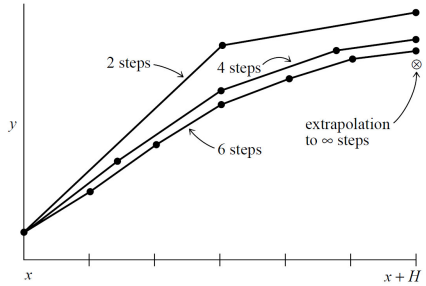
$\rightarrow$ 4th order accuracy (as for RK4), but only with 1.5 derivatives (RK4: 4)

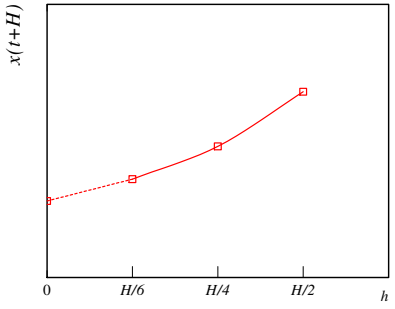
†William B. Gragg (1936-2016)

Richardson extrapolation

Idea: result $x(t + H)$ is an analytic function of h with $h = H/N$:

1. calculate $x_{t+H}(h = 2, 4, 6, \ldots)$
2. fit function $x_{t+H}(h)$ to $x_{t+H}(N = 2)$, $x_{t+H}(N = 4)$, ...
3. extrapolate $x_{t+H}(h \to 0)$, corresponding to $N \to \infty$





Extrapolation via polynomial

Compute k-times x_{t+H} with $N = 2, 4, 6, \ldots$:

$$x_{t+H}(h) = a_0 + a_1 h + a_2 h^2 + \ldots + a_k h^{k-1} \tag{82}$$

where following Lagrange

$$x_{t+H}(h) = \frac{(h-h_2)(h-h_3)\ldots(h-h_k)}{(h_1-h_2)(h_1-h_3)\ldots(h_1-h_k)} x_{t+H}(h_1) \tag{83}$$

$$+\frac{(h-h_1)(h-h_3)\ldots(h-h_k)}{(h_2-h_1)(h_2-h_3)\ldots(h_2-h_k)} x_{t+H}(h_2) \tag{84}$$

$$+\ldots+\frac{(h-h_1)(h-h_2)\ldots(h-h_{k-1})}{h_k-h_1)(h_k-h_2)\ldots(h_k-h_{k-1})} x_{t+H}(h_k) \tag{85}$$

In the original Bulirsch-Stoer method: rational function ($P(h)/Q(h)$) instead of Lagrange polynomial $\rightarrow$ much better approximation for functions with poles

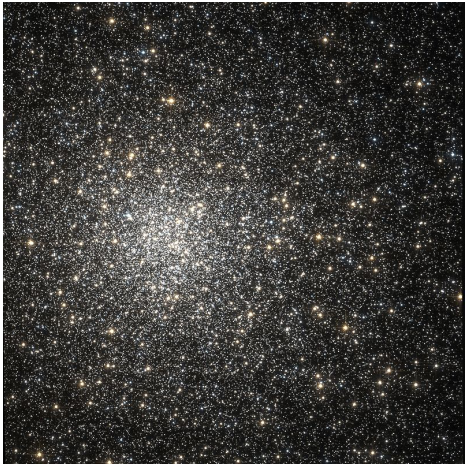
Consider an N-body system with

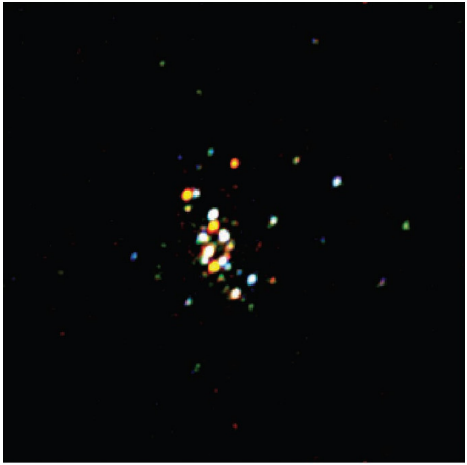
$$\frac{d^2\vec{x}_i}{dt^2} = -\sum_{j=1;j\neq i}^{N} \frac{Gm_j(\vec{x}_i - \vec{x}_j)}{|\vec{x}_i - \vec{x}_j|^3} \tag{86}$$

problem: $a_{ij} \propto \frac{1}{r_{ij}^2}$ for very small distances r_{ij} (close encounters)
$\rightarrow$ small distances $\rightarrow$ large accelerations $\rightarrow$ requires small Δt
$\rightarrow$ slows down calculations & increases numerical accumulation error

possibly uncomplicated for *one time* encounters

But in star clusters:
$\rightarrow$ formation of close binaries $\rightarrow$ *periodic*
so-called "binary hardening": transfer of the energy of the binary system to the cluster by consecutive close encounters





M 62 (NGC 6266). *Left:* optical HST. *Right:* X-ray CHANDRA

$\rightarrow$ above-average rate of close binary systems (e.g., low-mass X-ray binaries) in globular clusters (Pooley et al. 2003)

obvious (and inaccurate) idea: "softening" term in Eq. (86):

$$\vec{F}_{ij} = \frac{G\, m_i\, m_j (\vec{r}_j - \vec{r}_i)}{(\epsilon^2 + |\vec{r}_i - \vec{r}_j|^2)^{3/2}} \tag{87}$$

such that (88)

$$\max |\vec{a}_j| = \frac{2G\, m_i}{3^{3/2}\, \epsilon^2} \quad \text{at } r = \frac{1}{\sqrt{2}}\epsilon \tag{89}$$

$\rightarrow$ adaptive Δt not arbitrarily small; but: close binary orbits and passages not resolvable

When is "softening" applicable?

$\rightarrow$ if close encounters are irrelevant
$\rightarrow$ collisionless systems, e.g., galaxy

Illustration: distances in a galaxy

Galaxy: $\varnothing \approx 10^{23}$ cm with 10^{11} stars with $R_* \approx 10^{11}$ cm $\rightarrow d \approx 10^{19}$ cm

10^{11} sand grains

$\rightarrow$ $100\times$ width of

$\rightarrow$ average distance between sand grains ≈ 10 km

$\rightarrow t_{*,\mathrm{coll}} \gg t_{\mathrm{Hubble}} \rightarrow$ collisionless

stars perceive only the average gravitational potential of the galaxy

Regularization V

Better: regularization (technique in physics to avoid ∞) with help of transformation of spacetime coordinates.
Consider vector $\vec{R}$ between two particles (center of mass frame):

$$\frac{d^2\vec{R}}{dt^2} = -G(m_1+m_2)\frac{\vec{R}}{|\vec{R}|^3} + \vec{F}_{12} \tag{90}$$

with external force $\vec{F}_{12} = \vec{F}_1 - \vec{F}_2$ per mass, by other particles
1. regularized time τ

$$dt = R^n d\tau \tag{91}$$

$$\frac{d^2}{dt^2} = \frac{1}{R^{2n}}\frac{d^2}{d\tau^2} - \frac{n}{R^{2n+1}}\frac{dR}{d\tau}\frac{d}{d\tau} \tag{92}$$

$$\frac{d^2\vec{R}}{d\tau^2} = \frac{n}{R}\frac{dR}{d\tau}\frac{d\vec{R}}{d\tau} - G(m_1+m_2)\frac{\vec{R}}{R^{3-2n}} + R^{2n}\vec{F}_{12} \tag{93}$$

for $n = 1 \to R \propto dt/d\tau$ and without R^{-2}- singularity,
but with $\vec{R}/R$ term (indefinite for $R \to 0$)

therefore:

2. regularized distance u, initially only for 1 dimension (already known by Euler), without external force (see Aarseth 2003):

$$\frac{d^2R}{d\tau^2} = \frac{1}{R}\left(\frac{dR}{d\tau}\right)^2 - G(m_1+m_2) \tag{94}$$

$$\tag{95}$$

and with *conservation of energy*, total energy h per reduced mass $\mu = m_1 m_2/(m_1+m_2)$:

$$h = \frac{1}{2}\left(\frac{dR}{dt}\right)^2 - \frac{G}{R}(m_1+m_2) \tag{96}$$

$\rightarrow h$ is fixed without external force, and with

$$\frac{dR}{dt} = \frac{1}{R}\frac{dR}{d\tau} \tag{97}$$

$$\Rightarrow \quad \frac{d^2R}{d\tau^2} = 2hR + G(m_1+m_2) \tag{98}$$

$\rightarrow$ no more singularities. With $u^2 = R$:

$$\frac{d^2u}{d\tau^2} = \frac{1}{2}hu \tag{99}$$

$\rightarrow$ harmonic oscilator (h is const.)
$\rightarrow$ easy to integrate
$\rightarrow$ method: change from (x, t) to (u, τ) below some distinct distance (for 1d collision!)

in 2 dimensions (Levi-Civita 1904)[†]:

$$x = u_1^2 - u_2^2 \tag{100}$$
$$y = 2u_1 u_2 \tag{101}$$
$$\text{or} \quad \vec{R} = \mathcal{L}\vec{u} \tag{102}$$
$$\text{where } \mathcal{L} = \mathcal{L}(\vec{u}) = \begin{pmatrix} u_1 & -u_2 \\ u_2 & u_1 \end{pmatrix} \tag{103}$$

With the following properties:

$$\mathcal{L}(\vec{u})^T \mathcal{L}(\vec{u}) = R\mathcal{I} \tag{104}$$
$$\frac{d}{dt}\mathcal{L}(\vec{u}) = \mathcal{L}\left(\frac{d\vec{u}}{dt}\right) \tag{105}$$
$$\mathcal{L}(\vec{u})\vec{v} = \mathcal{L}(\vec{v})\vec{u} \tag{106}$$
$$\vec{u}\cdot\vec{u}\mathcal{L}(\vec{v})\vec{v} - 2\vec{u}\cdot\vec{v}\mathcal{L}(\vec{u})\vec{v} + \vec{v}\cdot\vec{v}\mathcal{L}(\vec{u})\vec{u} = 0 \tag{107}$$

[†] Tullio Levi-Civita (1873-1941), Italian mathematician and physicist

With help of Eqn. (105 & 106) coordinates change to

$$\frac{d\vec{R}}{d\tau} = 2\mathcal{L}(\vec{u})\frac{d\vec{u}}{d\tau} \tag{108}$$

$$\frac{d^2\vec{R}}{d\tau^2} = 2\mathcal{L}(\vec{u})\frac{d^2\vec{u}}{d\tau^2} + 2\mathcal{L}\left(\frac{d\vec{u}}{d\tau}\right)\frac{d\vec{u}}{d\tau} \tag{109}$$

Hence in Eq. (93) with $n = 1$ and with Eq. (107) and some transformations:

$$2\vec{u}\cdot\vec{u}\mathcal{L}(\vec{u})\frac{d^2\vec{u}}{d\tau^2} - 2\frac{d\vec{u}}{d\tau}\cdot\frac{d\vec{u}}{d\tau}\mathcal{L}(\vec{u})\vec{u} + G(m_1+m_2)\mathcal{L}(\vec{u})\vec{u} = (\vec{u}\cdot\vec{u})^3\vec{F}_{12} \tag{110}$$

further transformations lead to a form without singularities and indefinitenesses:

$$\frac{d^2\vec{u}}{d\tau^2} = \frac{1}{2}h\vec{u} + \frac{1}{2}R\mathcal{L}^T(\vec{u})\vec{F}_{12} \tag{111}$$

Binary star without external forces $\vec{F}_{12} \rightarrow$ energy h conserved
Binary star with external forces:

$$h = \left[2\frac{d\vec{u}}{d\tau} \cdot \frac{d\vec{u}}{d\tau} - G(m_1 + m_2) \right] \Big/ R \tag{112}$$

The time evolution in usual coordinates

$$\frac{d}{dt}\left[\frac{1}{2}\left(\frac{dR}{dt} \right)^2 - \frac{G}{R}(m_1 + m_2) \right] = \frac{d\vec{R}}{dt} \cdot \vec{F}_{12} \tag{113}$$

after transformation

$$\frac{dh}{d\tau} = 2\frac{d\vec{u}}{d\tau} \cdot \mathcal{L}(\vec{u})\vec{F}_{12} \tag{114}$$

can be solved continuously for $R = 0$ simultaneously with Eq. (111)

Application of the 2d solution to the so-called Pythagoraian three-body problem ($\vec{L} = 0$) in Szebehely & Peters (1967):

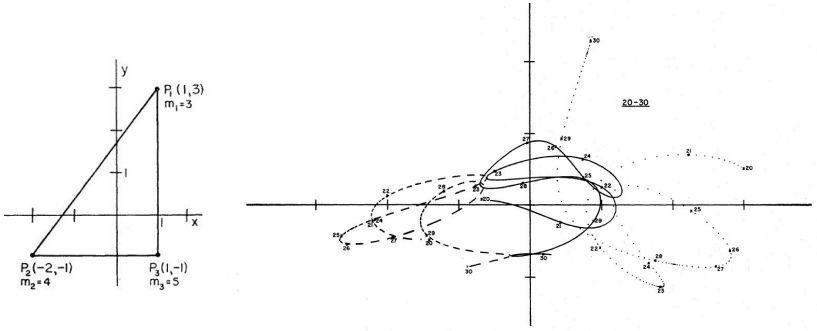


FIG. 4. Orbits between $t=20$ and $t=30$.

because of $\vec{L} = 0$ three-body collision possible $\rightarrow$ does not occur (3rd body gives perturbation $\vec{F}_{12}$)

Regularization for 3 dimensions (Kustaanheimo & Stiefel 1965) requires transformation to 4d coordinates:

$$R_1 = u_1^2 - u_2^2 - u_3^2 + u_4^2 \quad (115)$$
$$R_2 = 2(u_1 u_2 - u_3 u_4) \quad (116)$$
$$R_3 = 2(u_1 u_3 + u_2 u_4) \quad (117)$$
$$R_4 = 0 \quad (118)$$

and $\vec{R} = \mathcal{L}(\vec{u})\vec{u}$, such that

$$\mathcal{L} = \begin{bmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{bmatrix} \quad (119)$$

$\rightarrow$ yields again equations similar to (111) & (114)

see Bodenheimer et al. (2007) and Aarseth (2003)

Problems:

1. number of interactions is $N(N-1)/2 \propto \mathcal{O}(N^2)$
2. multiple timescales for adaptive time steps for each particle i:

$$\Delta t_i \simeq k\sqrt{\frac{1}{|\vec{a}_i|}} \tag{120}$$

with acceleration $\vec{a}_i$ and small factor k

N-body simulations for large N II

possible solutions:

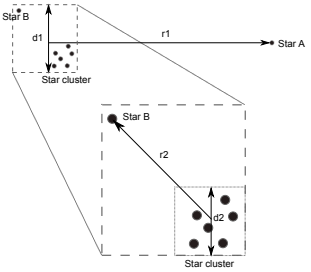
1. Tree method (Barnes & Hut 1986, 1989)
   $\rightarrow$ hierarchical structure and calculation of multipoles of the potential $\rightarrow \mathcal{O}(N \log N)$

   Holmberg (Lund, 1941) even $\mathcal{O}(N)$ with help of light bulbs on 2d grid (flux $\propto 1/r^2$)
2. Fourier transformation: compute potential $\Phi(\vec{x})$ with FFT $\rightarrow$ CA 2
3. Leapfrog method (2nd order integ.):

$$\vec{r}_i^{\,n+1/2} = \vec{r}_i^{\,n-1/2} + \Delta t_i \vec{v}_i^{\,n} \quad (121)$$

$$\vec{v}_i^{\,n+1} = \vec{v}_i^{\,n} + \Delta t_i \vec{a}_i^{\,n+1/2} \quad (122)$$

with time step doubling $\Delta t_i = \Delta t_{\max}/2^{n_i}$ for each particle i



The gravitational effect excerted by the star cluster and the single star B on star A can be approximated by a point mass. (from Barnes-Hut Galaxy Simulator)

Example: time step doubling with → leapfrog method

particle A: time step $\Delta t/2$, particle B: time step Δt
starting via

$$\vec{r}_i{}^{\,n+1/2} = \vec{r}_i{}^{\,n} + \frac{1}{2}\Delta t_i \vec{v}_i{}^{\,n} + \frac{1}{8}\Delta t_i^2 \vec{a}_i{}^{\,n} \quad \text{for } i = A, B. \tag{123}$$

1) Hence, we get $\vec{r}_A(\Delta t/4)$ and $\vec{r}_B(\Delta t/2)$ and from that
2) $\vec{a}_A(A[\Delta t/4], B[\Delta t/2])$ and analogously $\vec{a}_B \rightarrow$ time asymmetry
3) $\vec{a}_A \rightarrow \vec{v}_A(\Delta t/2) \rightarrow \vec{r}_A(3/4\Delta t)$
4) $\vec{a}_A(A[3/4\Delta t], B[\Delta t/2]) \rightarrow \vec{v}_A(\Delta t) \rightarrow$ reversed time asymmetry
5) Averaging of $\vec{r}_A(\Delta t/4), \vec{r}_A(3/4\Delta t)$ to $\vec{r}_A(\Delta t/2)$, then
6) $\rightarrow \vec{a}_B(A[\Delta t/2], B[\Delta t/2]) \rightarrow \vec{v}_B(\Delta t)$
7) from $\vec{v}_A(\Delta t), \vec{v}_B(\Delta t) \rightarrow \vec{r}_A(5/4\Delta t)$

i.e. next cycle starts, cf. 1) $\vec{r}_A(\Delta t/4)$ & $\vec{r}_B(\Delta t/2)$)

Summary

Methods to solve N-body interactions:

- Runge-Kutta (RK4): standard for any ODE
- 2nd order leapfrog: reasonable accuracy for extremely large number of particles, integration only over a few dynamical times (e.g., Sun orbiting Galactic center)
- Bulirsch-Stoer[†]: highly accurate, for few-body systems
- predictor-corrector: reasonable accuracy for moderate up to *large* number of particles
- for close encounters: softening (collisionless) or accurate regularization (collisions)

[†]alternatively for long-term evolution of few-body systems, e.g., over lifetime of Sun and whithout close encounters: symplectic map $\rightarrow$ split Hamiltonian $H = H_{\text{Kepler}} + H_{\text{interaction}}$, where analytic solution (ellipse) is used for H_{Kepler}, requires transformation to Jacobi coordinates

Outlook: Interacting galaxies I

Arp 271 (Gemini South)

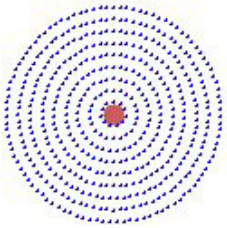
Outlook: Interacting galaxies II

NGC 4676 “Mice” (HST / NASA)

Galactic "Bridges" and "Tails" I

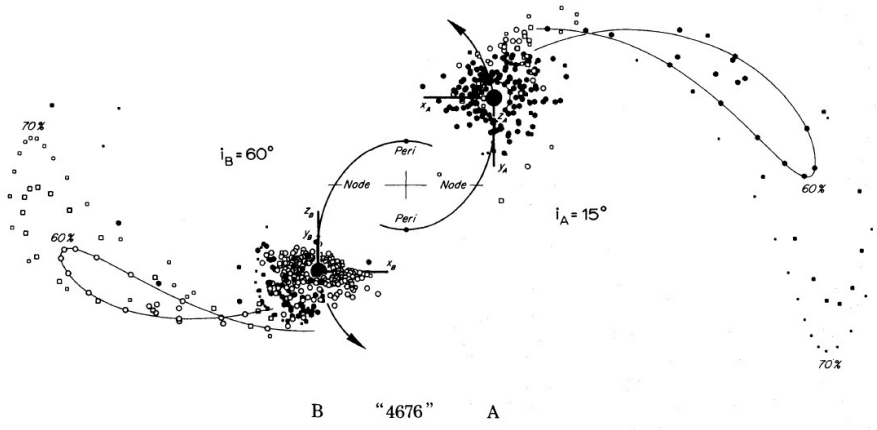
Toomre & Toomre (1972):

- *bridges* (connections between galaxies) and *tails* (structures on the opposite site of the interaction point) as the result of tidal forces between galaxies
- simplified model:
  - encounter of only two galaxies, parabolic (unbound)
  - galaxies as disks of non-interacting "test particles", initially on circular orbits around a central point mass



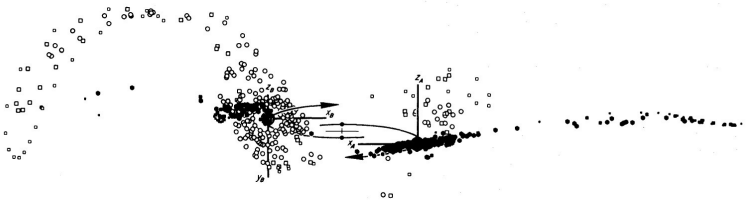
- result: mutual distortion of the galaxies just by gravitation, kinematic evolution to narrow, elongated structures

Galactic "Bridges" and "Tails" II



simulation of NGC 4676 from Toomre & Toomre (1972)
$\rightarrow$ two identical galaxies

Galactic "Bridges" and "Tails" III



NGC 4676 as before, but now seen *edge-on*

Literature I

Aarseth, S. J. 2003, Gravitational N-Body Simulations (Johns Hopkins University Press)

Barnes, J. & Hut, P. 1986, Nature, 324, 446

Barnes, J. E. & Hut, P. 1989, ApJS, 70, 389

Beeman, D. 1976, Journal of Computational Physics, 20, 130

Bodenheimer, P., Laughlin, G. P., Rózyczka, M., & Yorke, H. W., eds. 2007, Numerical Methods in Astrophysics: An Introduction (CRC Press)

Pooley, D., Lewin, W. H. G., Anderson, S. F., et al. 2003, ApJ, 591, L131

Schofield, P. 1973, Computer Physics Communications, 5, 17

Szebehely, V. & Peters, C. F. 1967, AJ, 72, 876

Toomre, A. & Toomre, J. 1972, ApJ, 178, 623