Programmierpraktikum

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Numerical Integration of Differential Equations

first vs. second order differential equations

classical dynamics - second order

$$\frac{d^2}{dt^2}\Big(m\,x(t)\Big) \;=\; F(t,x,\dot{x}), \qquad \ddot{x}(t) \;=\; f(t,x,\dot{x})$$

- every higher order differential equation can be transformed into a set of first order differential equations

$$\begin{aligned}\dot{x} &= y \\ \dot{y} &= f(t,x,y)\end{aligned}$$

first order differential equations

- in the following we will consider

$$\boxed{\dot{y} \;=\; f(t,y)}$$

Euler Integration

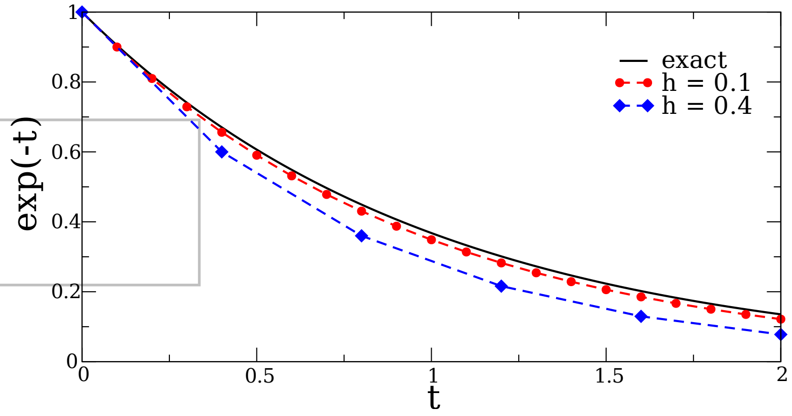
initial condition

$$\dot{y} \;=\; f(t,y), \qquad y(t_0) \;=\; y_0, \qquad t_n \;=\; t_0 + n\,h, \qquad n = 0,\,1,\,2,\,\ldots$$

one step algorithm

$$\frac{y(t+h)-y(t)}{h} \;\approx\; \dot{y} \;=\; f(t,y), \qquad y(t+h) \;\approx\; y(t) \,+\, h\,f(t,y)$$

$$y(t_{n+1}) \;\approx\; y(t_n) \,+\, h\,f(t_n,y_n)$$



- pretty bad

convergence considerations

- the one-step Euler integration converges linearly in the integration step h
- can we find algorithms converging like $O(h^m)$?

Taylor expansion to second order

$$y(t+h) \approx y(t) + h\,\dot{y}(t) + \frac{h^2}{2}\,\ddot{y}(t), \qquad \dot{y} = f(t,y)$$

with

$$\ddot{y} = \frac{d}{dt}\dot{y} = \frac{d}{dt}f(t,y) = f_t + f_y\,\dot{y}$$

and hence

$$y(t+h) - y(t) = \Delta y \approx h\,\dot{y} + \frac{h^2}{2}\left(f_t + f_y\,f\right)$$

accuracy to second order

- goal:

$$\Delta y \;=\; h\,f + \frac{h^2}{2}\,\Big(\,f_t \,+\, f_y\,f\,\Big)$$

- higer derivatives in general unkown
- Runge-Kutta: we need only approximations to the derivates to the desired order

Runge-Kutta Ansatz

$$\Delta y(t) \;=\; a\,f(t,y) \,+\, b\,f\Big(t+\alpha h, y+\beta h f\Big)$$

- free parameters: $a,\ b,\ \alpha,\ \beta$

Runge-Kutta alogrithm - derivation

$$
\begin{aligned}
\Delta y(t) &= a\,f(t,y) \,+\, b\,f\Big(t+\alpha h, y+\beta h f\Big) \\
&= a\,f \,+\, b\,f \,+\, b\Big(f_t\alpha \,+\, f_y f\beta\Big)\,h \\
&:= h\,f \,+\, \frac{h^2}{2}\,\Big(f_t \,+\, f_y\,f\Big)
\end{aligned}
$$

- comparing coefficients

$$
a+b \,=\, h, \qquad \alpha\, b \,=\, \frac{h}{2} \qquad \beta\, b \,=\, \frac{h}{2}
$$

- one free parameter remaining
  (3 conditions, 4 parameters)

Runge-Kutta algorithm

simple Runge-Kutta

$$y_{n+1} \;=\; y_n \;+\; \frac{h}{2}\;\Big[\,f(t_n,y_n)\;+\;f(t_n+h,y_n+hf(t_n,y_n)\,\Big]$$

- converges quadratically with integration step h

classical Runge-Kutta algorithm

- repeat for Taylor expansion to order $O(h^4)$

$$\Delta y \;=\; \frac{h}{6}\;\Big[k_1\;+\;2k_2\;+\;2k_3\;+\;k_4\Big]$$

with

$$k_1 = f(t,y)\,, \qquad k_2 = f\left(t + \frac{h}{2}\,, y + \frac{hk_1}{2}\right)$$

and

$$k_3 = f\left(t + \frac{h}{2}\,, y + \frac{hk_2}{2}\right), \qquad k_4 = f(t+h, y+hk_3)$$

- recursive function evaluation

example: Kepler problem

Newton's equation of motion

$$m\dot{\vec{v}} \;=\; -\,\frac{GMm}{|\vec{x}|^3}\;\vec{x}, \qquad \dot{\vec{v}} \;=\; -\,\frac{g}{|\vec{x}|^\alpha}\;\vec{x}, \qquad \alpha = 3$$

first order differentional equation

$$\vec{y} \;=\; (\vec{x},\vec{v}) \;=\; (x,y,\dot{x},\dot{y}), \qquad \dot{\vec{y}} \;=\; \vec{f}(\vec{y})$$

- angular momentum conservation $\rightarrow$ planar orbit

$$\vec{f}(\vec{y}) \;=\; \big(\vec{v}, -g\vec{x}/|\vec{x}|^\alpha\big), \qquad |\vec{x}| = \sqrt{x^2+y^2}$$

integration of Kepler problem

Runge-Kutta for vector variables

$$\dot{\vec{y}} \;=\; \vec{f}\,(t,\vec{y})$$

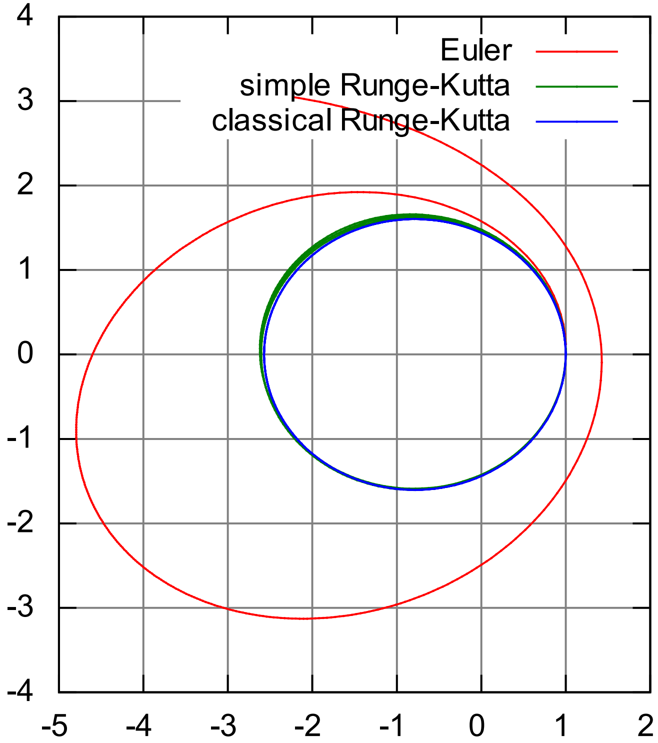
- substitute scalar quantities by vectors
- simple Runge-Kutta

$$\Delta\vec{y} \;=\; \frac{h}{2}\,\Big(\,\vec{f}\,(t,\vec{y}) \,+\, \vec{f}\,(t+h,\vec{y}+h\vec{f}\,(t,\vec{y})\,\Big)$$

- analogous for classical Runge-Kutta

exercise: integration

- write a program for integrating the Kepler problem using
  - *Euler's method*
  - *one-step Runge-Kutta*
  - *classical Runge-Kutta*
- what happens if the potential scales like $V(r) \propto r^{-\alpha}$ and $\alpha \neq 3$?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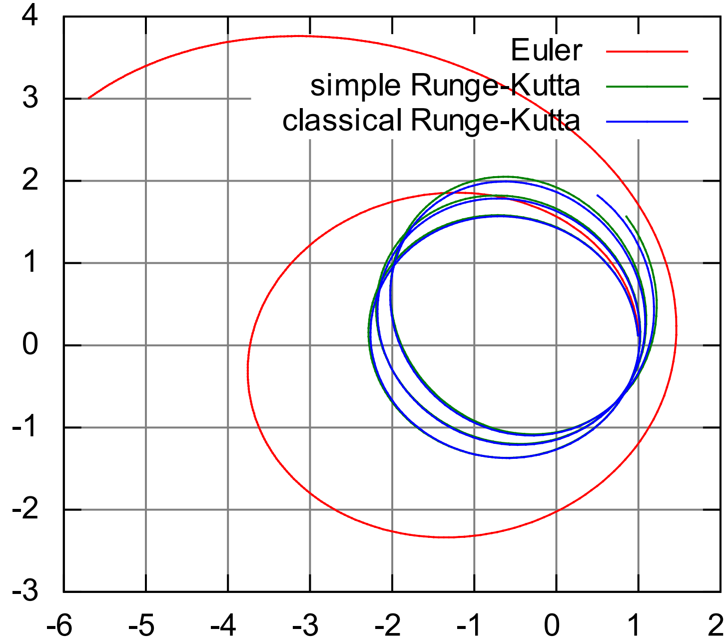
Euler
simple Runge-Kutta
classical Runge-Kutta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