1. Oscillations

Outline

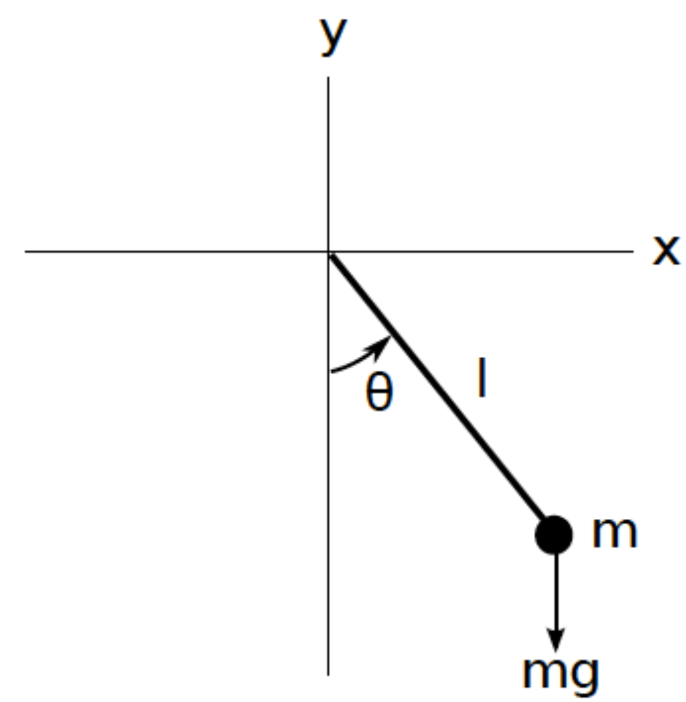
- Linear and nonlinear problems
- The pendulum and the harmonic oscillator
- Symmetries and conservation laws
- Finite difference methods
- Explanation of why some methods conserve energy and others don’t: symplectic methods
- Projects

Linear and nonlinear problems

- General analytical methods to solve differential equations rely on the superposition principle, which applies only for linear equations
- There are no general analytic methods for solving nonlinear problems
- Computer simulation works both for linear and nonlinear problems
- In simulation of a given problem issues of numerical accuracy and stability need to be controlled
- Symmetries are important: is the motion time reversal symmetric?
- Conservation laws are important: is energy conserved?

Simplest nonlinear problem: pendulum

$$\ddot{\theta} = -\frac{g}{l}\sin\theta$$



- This equation is obtained as the tangential component of Newtons law of motion:

$$F_\theta = -mg\sin\theta = ma_\theta = ml\ddot{\theta}$$

- Has no analytic solution
- Time reversal symmetry: if $\theta(t)$ is a solution then $\theta(-t)$ is also a solution
- Conservation of energy: E(t)=E(0)

$$E = \frac{m}{2}l^2\dot{\theta}^2 + mgl(1-\cos\theta)$$

$$\frac{dE}{dt} = ml^2\dot{\theta}\left(\ddot{\theta} + \frac{g}{l}\sin\theta\right) = 0$$

Harmonic oscillator

- For small oscillations the nonlinearity can be linearized: $\sin\theta \to \theta$
- Equation of the motion becomes linear:

$$\ddot{\theta} = -\frac{g}{l}\theta \Rightarrow \theta(t) = A\cos\omega t$$

- Angular frequency $\omega = \sqrt{g/l}$
- Energy $E = \frac{m}{2}l^2\dot{\theta}^2 + \frac{1}{2}mgl\theta^2 = \frac{1}{2}mglA^2$

  conserved as for the pendulum

- Prototype model for any system doing bound motion around a stable equilibrium position since

$$V(x) = V(x_0) + \underbrace{\frac{dV(x_0)}{dx}}_{=-F(x_0)=0}(x - x_0) + \frac{1}{2}\underbrace{\frac{d^2V(x_0)}{dx^2}}_{=k}(x - x_0)^2 + O(x - x_0)^3$$

Euler works poorly

- Apply Euler to the harmonic oscillator:

$$\theta(t+\Delta t) = \theta(t) + \dot{\theta}(t)\Delta t$$
$$\dot{\theta}(t+\Delta t) = \dot{\theta}(t) - \frac{g}{l}\theta(t)\Delta t$$

- Test if the Euler method conserves energy:

$$\begin{gathered}
E(t+\Delta t) - E(t) = \\
= \left(\frac{m}{2}l^2\dot{\theta}(t+\Delta t)^2 + \frac{1}{2}mgl\theta(t+\Delta t)^2\right) - \left(\frac{m}{2}l^2\dot{\theta}(t)^2 + \frac{1}{2}mgl\theta(t)^2\right) = \\
= \left(\frac{m}{2}l^2\left[\dot{\theta}(t) - \frac{g}{l}\theta(t)\Delta t\right]^2 + \frac{1}{2}mgl\left[\theta(t) + \dot{\theta}(t)\Delta t\right]^2\right) - \left(\frac{m}{2}l^2\dot{\theta}(t)^2 + \frac{1}{2}mgl\theta(t)^2\right) = \\
= \frac{mgl}{2}\left[\dot{\theta}(t)^2 + \frac{g}{l}\theta(t)^2\right]\Delta t^2
\end{gathered}$$

- Energy conservation is violated!
- Euler fails a basic requirement of a good integrator: it should conserve energy

Euler-Cromer is much better

$$\dot{\theta}(t+\Delta t) = \dot{\theta}(t) - \frac{g}{l}\theta(t)\Delta t$$
$$\theta(t+\Delta t) = \theta(t) + \dot{\theta}(t+\Delta t)\Delta t$$

- Energy conservation test:

$$E(t+\Delta t) - E(t) =$$
$$= \left(\frac{m}{2}l^2\dot{\theta}(t+\Delta t)^2 + \frac{1}{2}mgl\theta(t+\Delta t)^2\right) - \left(\frac{m}{2}l^2\dot{\theta}(t)^2 + \frac{1}{2}mgl\theta(t)^2\right) =$$
$$= \left(\frac{m}{2}l^2[\dot{\theta}(t) - \frac{g}{l}\theta(t)\Delta t]^2 + \frac{1}{2}mgl[\theta(t) + \underbrace{\dot{\theta}(t+\Delta t)}_{=\theta(t)+\dot{\theta}(t+\Delta t)}\Delta t]^2\right) - \left(\frac{m}{2}l^2\dot{\theta}(t)^2 + \frac{1}{2}mgl\theta(t)^2\right) =$$
$$= \frac{mgl}{2}\left[\dot{\theta}(t)^2 - \frac{g}{l}\theta(t)^2\right]\Delta t^2 - 2\frac{g}{l}\dot{\theta}(t)\theta(t)\Delta t^3 + O(\Delta t)^4$$

- The Δt^2 and Δt^3 terms average to zero over a whole period
- Thus the method is conserves energy to order Δt^4
- Thus Euler-Cromer is much better than Euler

Verlet method

- Forward and backward differences

$$x(t+\Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$$
$$x(t-\Delta t) = x(t) - v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$$

- Add and subtract

$$x(t+\Delta t) + x(t-\Delta t) = 2x(t) + a(t)\Delta t^2 + O(\Delta t)^4$$
$$x(t+\Delta t) - x(t-\Delta t) = 2v(t)\Delta t + O(\Delta t)^3$$

- Rearranging gives the Leapfrog method

$$x(t+\Delta t) = 2x(t) - x(t-\Delta t) + a(t)\Delta t^2 + O(\Delta t)^4$$
$$v(t) = \frac{x(t+\Delta t) - x(t-\Delta t)}{2\Delta t} + O(\Delta t)^2$$

- Disadvantage: not self starting
- The last eq gives

$$x(t-\Delta t) = x(t+\Delta t) - 2v(t)\Delta t$$

- Using this in Leapfrog gives

$$x(t+\Delta t) = x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$$

- Next write Leapfrog one more timestep forward

$$x(t+2\Delta t) = 2x(t+\Delta t) - x(t) + a(t+\Delta t)\Delta t^2$$
$$v(t+\Delta t) = \frac{x(t+2\Delta t) - x(t)}{2\Delta t}$$

$$\Rightarrow v(t+\Delta t) = \frac{x(t+\Delta t) - x(t)}{\Delta t} + \frac{1}{2}a(t+\Delta t)\Delta t = v(t) + \frac{1}{2}[a(t+\Delta t) + a(t)]\Delta t$$

- Putting it all together gives the Verlet method:

$$\boxed{\begin{aligned} x(t+\Delta t) &= x(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + O(\Delta t)^4 \\ v(t+\Delta t) &= v(t) + \frac{1}{2}[a(t+\Delta t) + a(t)]\Delta t + O(\Delta t)^2 \end{aligned}}$$

Both time reversal symmetric and conserves energy

Runge-Kutta

- A commonly used higher order method is obtained by averaging increments over four points in the time interval:

$$a_1 = a(x(t), v(t), t)\Delta t, b_1 = v(t)\Delta t$$
$$a_2 = a(x(t) + b_1/2, v(t) + a_1/2, t + \Delta t/2)\Delta t, b_2 = (v(t) + a_1/2)\Delta t$$
$$a_3 = a(x(t) + b_2/2, v(t) + a_2/2, t + \Delta t/2)\Delta t, b_3 = (v(t) + a_2/2)\Delta t$$
$$a_4 = a(x(t) + b_3, v(t) + a_3, t + \Delta t)\Delta t, b_4 = (v(t) + a_3)\Delta t$$
$$v(t + \Delta t) = v(t) + \frac{1}{6}(a_1 + 2a_2 + 2a_3 + a_4)$$
$$x(t + \Delta t) = x(t) + \frac{1}{6}(b_1 + 2b_2 + 2b_3 + b_4)$$

- Here a(x(t),v(t),t) is the acceleration at position x(t), velocity v(t), and time t

Adaptive time steps

- In problems where the acceleration is velocity dependent the above methods become less efficient
- An example of this is the double pendulum where energy exchanges between two arms to produce intervals of high speed
- In these cases adaptive time steps or predictor-corrector methods can improve performance
- Adaptive time steps means that short time steps are taken where the increments are big, and larger time steps are used when the increments are small
- The required time step can be determined on the fly in the simulation

Why do some methods conserve energy?

- The Hamiltonian formulation of classical mechanics is based on the observation that

$$F = ma \ , \ p = mv \Rightarrow \dot{p} = -\frac{\partial H}{\partial x} \ , \ \dot{x} = \frac{\partial H}{\partial p}$$

  where $H = \frac{p^2}{2m} + V(x)$ is called the Hamilton function and gives the total energy

- Symplectic means "area preserving", so that the area element $dA = |dxdp|$ is unchanged under the map $(x, p) \to (x', p')$ which gives

$$dA' = \left| \left(\frac{\partial x'}{\partial x}\hat{x} + \frac{\partial p'}{\partial x}\hat{p} \right) dx \times \left(\frac{\partial x'}{\partial p}\hat{x} + \frac{\partial p'}{\partial p}\hat{p} \right) dp \right| = |J|\, dA \ \Rightarrow \ dA' = dA \ \text{ if the Jacobian } J = \begin{pmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{pmatrix} = 1$$

- This prevents the coordinates and momenta from running away, and as a consequence it is possible to show that a slightly perturbed energy is conserved

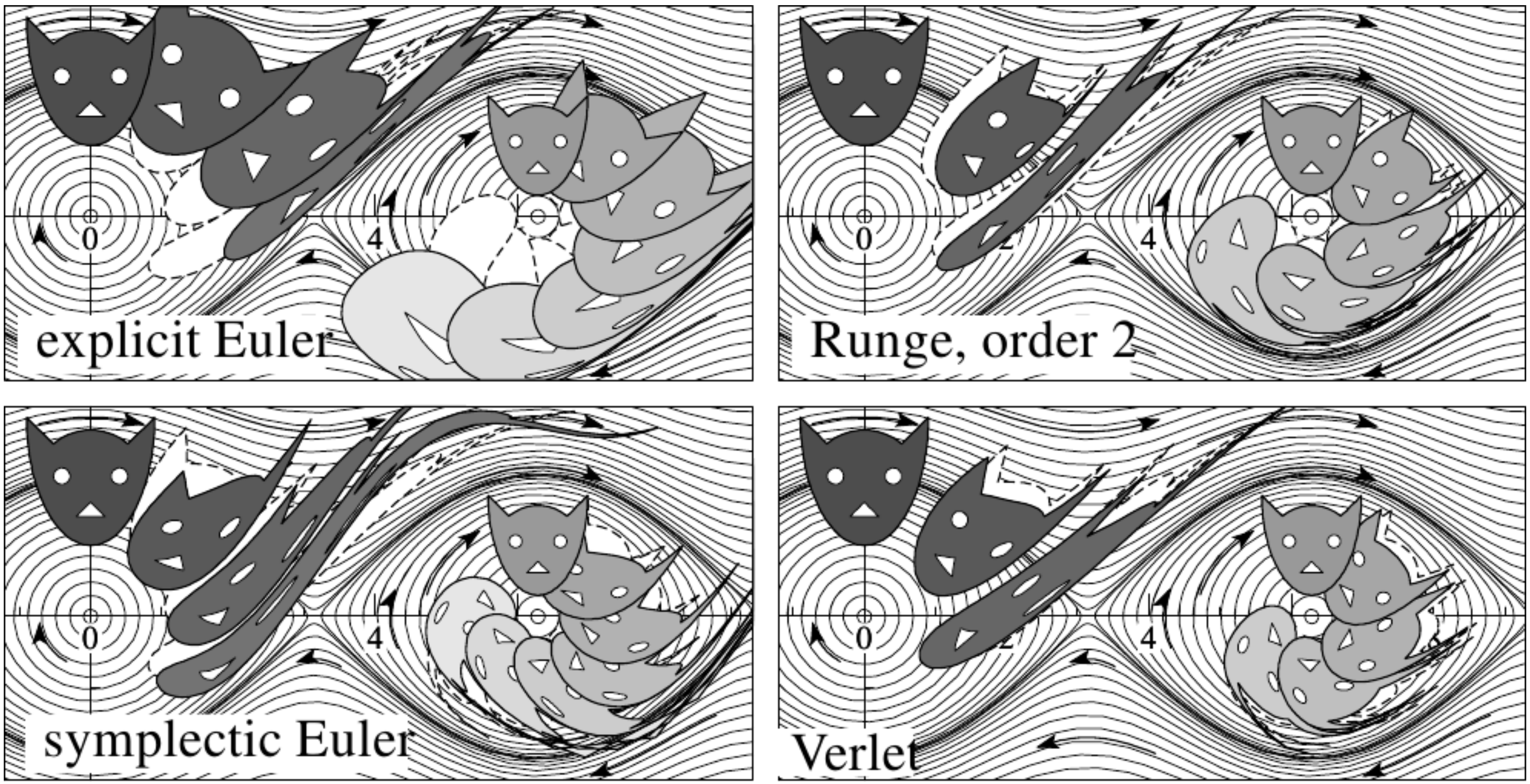
- Example: Euler-Cromer is symplectic since $J = \begin{pmatrix} 1 & 0 \\ \frac{\partial F}{\partial x}\Delta t & 1 \end{pmatrix} = 1$

- Verlet and leapfrog are also symplectic

- Euler and Runge-Kutta are not symplectic

- Higher order symplectic methods can be constructed systematically

Symplectic integrators: area preserving



integration of pendulum motion

References

- Symplectic integration is discussed, with references, in the course book, linked is on the course page

- Thorough numerical analysis book:
  Springer Series in Computational Mathematics, Volume 31 2006
  Geometric Numerical Integration
  Structure-Preserving Algorithms for Ordinary Differential Equations
  Authors: Ernst Hairer, Gerhard Wanner, Christian Lubich ISBN: 978-3-540-30663-4 (Print) 978-3-540-30666-5 (Online)
  KTH online link:
  http://link.springer.com.focus.lib.kth.se/book/10.1007/3-540-30666-8/page/1

- Simple course on galactic dynamics with different integrators:
  http://www.artcompsci.org/vol_1/v1_web/v1_web.html

Project 1.1

Study a pendulum and a harmonic oscillator using Euler-Cromer, velocity Verlet and Runge-Kutta. Assume $\sqrt{g/l} = 3\ \mathrm{s}^{-1}$ and $m = 1$ kg. Compare the different methods with each other and with the exact solution of the harmonic oscillator. Plot $\theta(t)$, $\dot{\theta}(t)$ and E. Study the dependence on the time step. Consider initial conditions $\theta(0)/\pi = 0.1$, 0.3 and 0.5; $\dot{\theta}(0) = 0$.

Project 1.2

Determine the period time T as a function of the initial position $\theta(0)$. Which system (harmonic osc./pendulum) has a larger period? Explain! Compare the harmonic oscillator with the perturbation series:

$$T = 2\pi\sqrt{\frac{l}{g}}\left(1 + \frac{1}{16}\theta^2(0) + \frac{11}{3072}\theta^4(0) + \frac{173}{737280}\theta^6(0) + \ldots\right)$$

Project 1.3

Study the damped harmonic oscillator equation:

$$F/m = \ddot{x} = -\omega_0^2\, x - \gamma\, \dot{x}$$

Take $\omega_0 = 3$, $\gamma = 0.5, 1, 2, 3$, $x(0) = 1$, $\dot{x}(0) = 0$. Plot $x(t)$, $v(t)$, $E(t)$. Discuss the features of these plots. Estimate the relaxation time τ, i.e. the time for the amplitude to be reduced to $1/e \approx 0.37$ of the initial amplitude (note that you should look at the "envelope", rather than at the exact value of the solution). Study the dependence of τ on γ. Find the smallest γ such that the pendulum does not pass $x = 0$. This is called the critical damping, γ_c and for $\gamma > \gamma_c$ the systems is called overdamped.

Project 1.4

Consider a damped pendulum with damping given by $-\gamma\,\dot{\theta}$. Take $\gamma = 1$, $\sqrt{g/l} = 3$, $\theta(0) = \pi/2$, $\dot{\theta}(0) = 0$. Determine the phase space portrait, i.e. plot $\dot{\theta}$ vs θ. Discuss.

Project 1.5

A more difficult question. The leap-frog integrator is usually formulated as:

$$v(t + \Delta t/2) = v(t - \Delta t/2) + a(t)\Delta t$$

$$x(t + \Delta t) = x(t) + v(t + \Delta t/2)\Delta t$$

As you can see, the coordinates and velocities leap-frog (hoppa bock) each other. The coordinate trajectory can be identical to velocity verlet. This is achieved by integrating v with half time steps or setting $v(t) = (v(t - \Delta t/2) + v(t + \Delta t/2))/2$.

Take a harmonic oscillator and integrate it with leap-frog and velocity verlet. Take a large time step (such that you get large errors). Compute the average kinetic and potential energy by averaging over very many oscillations and compare the averages with the analytical answer. What do you observe? Can you explain the difference between the integrators?

Before the next meeting

- Upload your report and presentation to canvas, deadline: November 7th 20:00
- Presentation meetings November 8th FD41:
  - group 1: 8:15 - 9:00
  - group 2: 9:15 - 10:00
  - group 3: 10:15 - 11:00
  - group 4: 11:15 - 12:00
- Start in time with the assignments, it might be take more time than you initially think!
- There is an, optional, räknestuga Tuesday 6 November 8:00 - 10:00 to ask question about the assignments, python, etc.