Summary: Chapter 1

- Let $D \subset \mathbb{R}^n$ be an open set and $f : D \to \mathbb{R}^n$ sufficiently differentiable. For $t_0 \in \mathbb{R}$ and $y_0 \in D$, we consider the *ordinary differential equation (ODE)*

  $$\begin{aligned} \dot{y} &= f(y), \\ y(t_0) &= y_0, \end{aligned}$$

  where $y := y(t)$ and $\dot{y}(t) := \frac{\mathrm{d}}{\mathrm{d}t} y(t)$.

  The *flow* $\varphi_t : y_0 \mapsto y(t, 0, y_0)$ of this ODE is a 1-parameter group.

- Let $h = t_{n+1} - t_n$ be the step size, we consider the *numerical flow* $\Phi_h : y_n \mapsto y_{n+1}$ given by, for example, a one-step numerical scheme.

  Expl: *Explicit Euler method; Implicit Euler method; Midpoint rule; Symplectic Euler method for partitioned system; Störmer-Verlet scheme.*

- A *Hamiltonian problem* reads

  $$\begin{aligned} \dot{p} &= -\nabla_q H(p, q), \\ \dot{q} &= \nabla_p H(p, q), \end{aligned}$$

  where the given function $H : D \subset \mathbb{R}^{2d} \to \mathbb{R}$ is called *Hamiltonian function* or *energy*, and $\nabla_p H(p, q) := \left(\frac{\partial H}{\partial p}(p, q)\right)^T$. We have *energy conservation*: $H(p(t), q(t)) = H(p(0), q(0))$ along the exact solution $(p(t), q(t))$ of our problem for all times $t > 0$.

  Expl: Kepler problem; Outer solar system; Molecular dynamics; etc.

- We have seen that the Störmer-Verlet scheme and the symplectic Euler scheme have good geometric properties. The "classical" numerical schemes not.

  Goal of this lecture: try to find an explanation ...