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Solutions of Exercise Sheet 3: Verlet Integration

Exercise 2 *(Verlet Integration)*

The equivalence of the first- and second-order schemes easily follows by calculation.

After interchanging $n \leftrightarrow n+1$ and $\Delta t \leftrightarrow -\Delta t$ we end up with the initial scheme which shows time-reversibility.

We determine the Jacobian of the mapping $\Phi_{\Delta t} : \mathbb{R}^2 \to \mathbb{R}^2$, $(q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$ defined by

$$\begin{pmatrix} q_{n+1} \\ v_{n+1} \end{pmatrix} := \begin{pmatrix} q_n + v_n \Delta t \\ v_n \end{pmatrix} + \frac{1}{2} \begin{pmatrix} a_n \Delta t^2 \\ (a_n + a_{n+1}) \Delta t \end{pmatrix}$$

and obtain

$$\Phi'_{\Delta t} = \left(\partial_{x_n} \Phi_{\Delta t}, \, \partial_{v_n} \Phi_{\Delta t} \right) = \begin{pmatrix} 1 & \Delta t \\ 0 & 1 \end{pmatrix}$$

which fulfills the relation $\Phi'^{\mathsf{T}}_{\Delta t} \mathsf{adiag}(1,-1) \Phi'_{\Delta t} = \mathsf{adiag}(1,-1)$.

We determine the Taylor expansions for $q_{n+1} = q(t_n + \Delta t)$ and $q_{n-1} = q(t_n - \Delta t)$ around t_n and obtain

$$\begin{aligned} q_{n+1} &= q_n + v_n \Delta t + \frac{a_n}{2} \Delta t^2 + \frac{\dot{a}_n}{6} \Delta t^3 + \mathcal{O}(\Delta t^4), \\ q_{n-1} &= q_n - v_n \Delta t + \frac{a_n}{2} \Delta t^2 - \frac{\dot{a}_n}{6} \Delta t^3 + \mathcal{O}(\Delta t^4). \end{aligned}$$

Addition of these two series leads to

$$q_{n+1} := 2q_n - q_{n-1} + a_n \Delta t^2 + \mathcal{O}(\Delta t^4),$$

for which reason the error of the Verlet integrator is of order 4.