Computational Dynamics for Mechanical Systems

two lectures of course CDS 140b: Introduction to Dynamics
Tuesday March 4 and Thursday March 6 2008, 10:30am-11:55am, Steele 214

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1 Numerics of ODEs

1.1 Introduction

P. Deuflhard and F. Bornemann: *Scientific computing with ordinary differential equations.* Springer, 2002.

Consider the planar pendulum as a motivating example. One is interested in the points in space, where the point mass m is located at a certain time, if the pendulum is released at an initial configuration $q(t_0)$ with a certain initial velocity $\dot{q}(t_0)$. Let q denote the angle measured against the vertical as depicted in Figure 1. Then the trajectory $q(t) \in \mathbb{R}^n$ (in this case $n = 1$) yields the evolution of this angle. With the fixed length l, the positions of the point mass in the plane can then be computed.

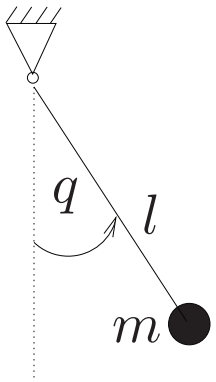

Figure 1: Planar pendulum.

The evolution of the angle $q(t)$ in the time interval $[a, b]$ consists of infinitely many values. Since computers can handle only finite sets of data, the solution is approximated on a time-grid

$$\Delta = \{t_0, \ldots, t_N | a = t_0 < t_1 < \ldots < t_N = b\}$$

Let

$$\tau_k = t_{k+1} - t_k$$

denote the time-step and

$$\tau_\Delta = \max_{0 \le k < N} \tau_k$$

the maximal step-size of the mesh. A time-stepping method yields a sequence of discrete configurations $\{q_k\}_{k=0}^N$ that approximate the real trajectory $q_k \approx q(t_k)$.
Intuitively speaking: if the approximate solution get closer and closer to the real motion for decreasing time-steps as in Figure 2, then the method is converging.

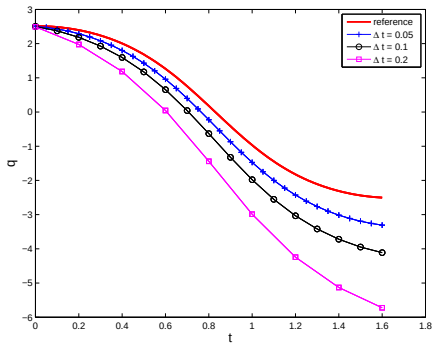

Figure 2: Convergence of approximations to a reference solution for decreasing time-steps.

Two important questions on a numerical scheme:

- Does it converge?
- Does it yield realistic solutions?

Non-converging methods do not make sense. For a converging method, unrealistic behaviour (like artificial energy gain or dissipation) improves for decreasing time-steps. However there are methods, that yield realistic behaviour even for relatively large time-steps, e.g. the mechanical integrators in Section 2 and 3.

1.2 Example of an explicit one-step scheme: forward Euler

Approximate the solution $x \in C^1([a,b],\mathbb{R}^n)$ of the initial value problem

$$x' = f(t,x) \qquad\qquad x(t_0) = x_0 \tag{1}$$

by the recursive iteration

$$x_{k+1} = x_k + \tau_k\, f(t_k, x_k) \tag{2}$$

in this case, the derivative x' has been replaced by a forward difference quotient

$$\frac{x_{k+1} - x_k}{\tau_k} \approx x'(t_k) = f(t_k, x_k)$$

It is called an explicit scheme, since knowing x_k, one can directly compute x_{k+1}. The geometric interpretation of (2) is that during one time-interval, the curve is approximated by the tangent at the beginning of the time-interval, see Figure 3.

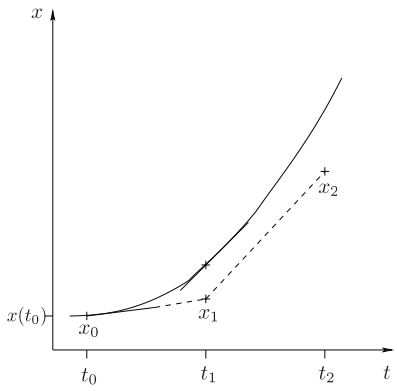

Figure 3: Geometry of forward Euler scheme.

1.3 Example of an implicit one-step scheme: backward Euler

Approximating x' in (1) by a backward difference quotient

$$\frac{x_{k+1} - x_k}{\tau_k} \approx x'(t_{k+1}) = f(t_{k+1}, x_{k+1})$$

yields the backward Euler scheme

$$x_{k+1} = x_k + \tau_k \, f(t_{k+1}, x_{k+1}) \tag{3}$$

which is implicit since due to the presence of the unknown x_{k+1} on the right hand side, the discrete equation of motion (3) has to be solved iteratively.

The term 'one-step scheme' stems from the fact that only one time-interval $[t_k, t_{k+1}]$ is considered in (2) or (3) and x_{k+1} is computed based on the knowledge of x_k. There also exist multi-step methods as e.g. the variational integrator presented in Section 3.

1.4 Consistency, stability and convergence

Definition 1.1 A function $f : [a, b] \times \mathbb{R}^n$ is *globally Lipschitz continuous* in x, if

$$\exists L > 0 \qquad ||f(t, x_1) - f(t, x_2)|| \leq L||x_1 - x_2|| \qquad \forall t \in [a, b] \qquad \forall x_1, x_2 \in \mathbb{R}^n \tag{4}$$

For a globally Lipschitz-continuous right hand side of an initial value problem, the following existence and uniqueness theorem by Picard-Lindelöf holds.

Theorem 1.2 (Picard-Lindelöf) *Let f be globally Lipschitz-continuous in x. Then, for every $x_0 \in \mathbb{R}^n$ and every $t_0 \in [a, b]$, there exists one and only one solution $x \in C^1([a, b], \mathbb{R}^n)$ of the initial value problem (1).*

Remark 1.3 Often, the Lipschitz-condition (4) holds only locally, i.e. for $x_1, x_2 \in \Omega \subset \mathbb{R}^n$. Then it can happen that the solution does not exist on the whole interval $[a, b]$, but only on a smaller time-interval $[\alpha, \beta] \subset [a, b]$, $\alpha \leq t_0 \leq \beta$.

For the initial value problem (1), the following notation is called the evolution of the ODE

$$\phi^{t,t_0} x_0 = x(t) \quad \text{for} \quad x(t_0) = x_0$$

It has the following properties:

- $\phi^{t_0,t_0} x_0 = x_0$
- $\frac{d}{d\tau} \phi^{t+\tau,t} x_{|_{\tau=0}} = f(t,x)$
- $\phi^{t,\sigma} \phi^{\sigma,s} x = \phi^{t,s} x$

Remark 1.4 For autonomous initial value problems

$$x' = f(x) \qquad\qquad x(t_0) = x_0$$

the value of the initial time plays no role and can be assumed to be zero. Here, for $t \in [a,b]$, the one-parameter family $\phi^t : \mathbb{R}^n \to \mathbb{R}^n$ of transformations given by

$$\phi^t x_0 = \phi^{t,0} x_0 = x(t) \quad \text{for} \quad x(0) = x_0$$

is called the phase flow of the autonomous initial value problems while the trajectory or orbit through $x_0 \in \mathbb{R}^n$ reads

$$\gamma(x_0) = \{\phi^t x_0 | t \in [a,b]\}$$

Definition 1.5 The computational process for the approximation $x_\Delta(t_i) = x_i$ is called *one-step scheme* if, for all meshes Δ, it can be described by a two-term relation

- $x_\Delta(t_0) = x_0$
- $x_\Delta(t_{k+1}) = \psi^{t_{k+1},t_k} x_\Delta(t_k), \quad k = 1, \ldots, N-1$

with the *discrete evolution* ψ being independent of the time-grid Δ.

Definition 1.6 The difference

$$\epsilon(t,x,\tau) = \phi^{t+\tau,t} x - \psi^{t+\tau,t} x$$

is called *consistency error* of the discrete evolution ψ, and it is called *consistent* if

$$\epsilon(t,x,\tau) = o(\tau) \quad \text{for} \quad \tau \to 0 \tag{5}$$

Remark 1.7 Property (5) is equivalent to ψ having the form

$$\psi^{t+\tau,t} x = x + \tau \psi(t,x,\tau) \quad \text{with} \quad \psi(t,x,0) = f(t,x)$$

By setting $\psi(t,x,\tau) = f(t,x)$ one can see that the forward Euler scheme is consistent.

Remark 1.8 (Landau symbols) Consider the functions $g, h : \mathbb{R} \to \mathbb{R}$. Then $g(x) \in \mathcal{O}(h(x))$, or in slightly abused notation $g(x) = \mathcal{O}(h(x))$, means that h is an asymptotic upper bound on g (up to constant factor), i.e.

$$\exists C > 0 \; \exists x_0 \quad \text{such that} \quad \forall x > x_0 \quad |g(x)| < C|h(x)|$$

On the other hand, $g(x) \in o(h(x))$, or in slightly abused notation $g(x) = o(h(x))$, means that g is dominated by h asymptotically, i.e.

$$\forall C > 0 \; \exists x_0 \quad \text{such that} \quad \forall x > x_0 \quad |g(x)| < C|h(x)|$$

Thus the function $h(x)$ grows much faster than $g(x)$ and $\lim_{x\to\infty} \dfrac{g(x)}{h(x)} = 0$.

Definition 1.9 The discrete evolution ψ has *consistency order p*, if the consistency error satisfies

$$\epsilon(t, x, \tau) = \mathcal{O}(\tau^{p+1}) \quad \text{for} \quad \tau \to 0$$

Thus a discrete evolution with consistency order $p > 0$ is indeed consistent.

Definition 1.10 The vector valued mapping

$$\epsilon_\Delta : \Delta \to \mathbb{R}^n \qquad\qquad \epsilon_\Delta(t) = x(t) - x_\Delta(t)$$

is called the *mesh error* and its norm

$$||\epsilon_\Delta||_\infty = \max_{t\in\Delta} |\epsilon_\Delta(t)|$$

the *discretisation error*.

Definition 1.11 Suppose that for any mesh Δ on $[a, b]$ a mesh function x_Δ is given. Then x_Δ *converges* to the solution $x \in C^1([a, b], \mathbb{R}^n)$ of the initial value problem (1) of the discretisation errors satisfy

$$||\epsilon_\Delta||_\infty \to 0 \quad \text{for} \quad \tau \to 0$$

The *convergence is of order p* if

$$||\epsilon_\Delta||_\infty = \mathcal{O}(\tau_\Delta^p) \quad \text{for} \quad \tau \to 0$$

Remark 1.12 The consistency error ϵ represents the error in just one iteration, while the mesh error ϵ_Δ describes the error of the whole approximation.

Theorem 1.13 *Let $x \in C^1([a, b], \mathbb{R}^n)$ be the solution of the initial value problem (1) whose right hand side f is globally Lipschitz-continuous. Further let the discrete evolution $\psi^{t+\tau,t}$ be consistent of order p and have a globally Lipschitz-continuous increment function $\psi(t, x, \tau)$. Then the discrete mesh function x_Δ converges with order p to the trajectory $x(t)$.*

Remark 1.14 Often Lipschitz-continuity of the increment function $\psi(t, x, \tau)$ is referred to as stability. Then

consistency of order p	+	stability	$\Longrightarrow$	convergence of order p

The forward Euler scheme is convergent with order 1.

2 Simulating Hamiltonian dynamics

B. Leimkuhler and S. Reich: *Simulating Hamiltonian dynamics*. Cambridge, 2004.

The forward and backward Euler schemes are discretisations of the initial value problem in (1), the can be applied to general ODEs of that form. While they are converging time-stepping schemes, they lack the ability to represent certain important properties of real motion correctly.

Let $q \in \mathcal{Q}$ denote the configuration variable in the configuration manifold $\mathcal{Q}$. Then velocity $\dot{q} \in T_q\mathcal{Q}$ belongs to the tangent space $T_q\mathcal{Q}$ which is a linear space attached to $\mathcal{Q}$ at the configuration or base point q. The Hamiltonian $H : T^*\mathcal{Q} \to \mathbb{R}$ of a mechanical system is formulated in terms of the configuration q and the conjugate momentum $p \in T_q^*\mathcal{Q}$ whereby $T_q^*\mathcal{Q}$ represents the dual space of $T_q\mathcal{Q}$. In gneral, the Hamiltonian consists of the sum of kinetic and potential energy, thus $H(q,p) = \frac{1}{2m}p^2 + V(q)$, where m denotes the mass.

First integrals In previous lectures it has been explained that a function f which Poisson-commutes with the Hamiltonian is conserved along the Hamiltonian flow, i.e. $\dfrac{df}{dt} = \{f, H\} = 0$. This can also be phrased in terms of Noether's theorem stating that the invariance of the Hamiltonian with respect to specific manipulations of it's arguments leads to a conserved quantity, a so-called first integral of the motion. Considering the dynamics of mechanical systems, the following first integrals are the most common.

invariance with respect to		conservation of
time reparametrisation	$\Longrightarrow$	Hamiltonian (total energy)
translation in space	$\Longrightarrow$	linear momentum
rotation in space	$\Longrightarrow$	angular momentum

Mechanical integrators are designed to inherit the conservation properties of the real motion to the approximate trajectory. To achieve that, they exploit the structure of the underlying ODEs.

Hamilton's equations Collecting the configuration and momentum in the phase variable $z = (q,p) \in T^*\mathcal{Q}$, Hamilton's equations of motion read

$$\dot{z} = X_H(z) \tag{6}$$

with the Hamiltonian vector field

$$X_H(z) = \mathbb{J} \cdot \nabla H(z) = \begin{pmatrix} \dfrac{\partial H}{\partial p} \\ -\dfrac{\partial H}{\partial q} \end{pmatrix} \tag{7}$$

and the symplectic matrix $\mathbb{J} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$. Here I denotes the $n \times n$ identity matrix.

Energy-momentum scheme The concept of discrete derivatives introduced by Gonzalez in
O. Gonzalez: *Time Integration and Discrete Hamiltonian Systems.* J. Nonlinear Sci., 6, 499-467, 1996.
is based on the discretisation of (6) via

$$z_{k+1} - z_k = \tau_k \mathsf{X}_H(z_k, z_{k+1}) \tag{8}$$

whereby the discrete Hamiltonian vector field X_H can be viewed as an approximation of the exact Hamiltonian vector field X_H at the midpoint $z_{k+\frac{1}{2}} = \frac{1}{2}(z_{k+1} + z_k)$, in particular $\mathsf{X}_H(z_k, z_{k+1}) \approx X_H(z_{k+\frac{1}{2}})$ and (7) becomes

$$\mathsf{X}_H(z_k, z_{k+1}) = \mathbb{J} \cdot \mathsf{D}H(z_k, z_{k+1}) = \begin{pmatrix} \mathsf{D}_p H(z_k, z_{k+1}) \\ -\mathsf{D}_q H(z_k, z_{k+1}) \end{pmatrix}$$

Note that $\mathsf{D}_q H(z_k, z_{k+1})$ denotes the discrete derivative with respect to the configuration while $\mathsf{D}_p H(z_k, z_{k+1})$ denotes the discrete derivative with respect to the conjugate momentum.

Definition 2.1 (Discrete derivative) A discrete derivative for a smooth function $f : T^*\mathcal{Q} \to \mathbb{R}$ is a mapping $\mathsf{D}f : T^*\mathcal{Q} \times T^*\mathcal{Q} \to \mathbb{R}^{2n}$ with the following properties:

(i) Directionality: $\mathsf{D}f(x, y) \cdot (y - x) = f(y) - f(x)$ for all $x, y \in T^*\mathcal{Q}$

(ii) Consistency: $\mathsf{D}f(x, y) = Df(w) + \mathcal{O}\left(\|y - x\|\right)$ for all $x, y \in T^*\mathcal{Q}$
with $\|y - x\|$ sufficiently small

Here $w = \frac{1}{2}(x + y)$ and $\|\cdot\|$ denotes the standard Euclidian norm in $\mathbb{R}^{2n}$.

Example 2.2 (Discrete derivative) A general example of a discrete derivative is given by

$$\mathsf{D}f(z_k, z_{k+1}) = Df\left(z_{k+\frac{1}{2}}\right) + \frac{f(z_{k+1}) - f(z_k) - Df(z_{k+\frac{1}{2}}) \cdot (z_{k+1} - z_k)}{\|z_{k+1} - z_k\|^2} (z_{k+1} - z_k)$$

which is a second-order approximation to the exact derivative at the midpoint $z_{k+\frac{1}{2}} = \frac{1}{2}(z_k + z_{k+1})$.

Proposition 2.3 (Energy conservation) *With this construction, the Hamiltonian H is conserved along a solution sequence $(z_k)_{k\in\mathbb{N}}$ of (8) in the sense that $H(z_{k+1}) - H(z_k) = 0$ for all $k \in \mathbb{N}$.*

3 Geometric numerical integration

E. Hairer, C. Lubich and G. Wanner: *Geometric numerical integration: structure-preserving algorithms for ODEs.* Springer, 2002.

Euler-Lagrange equations The following variational time-stepping scheme exploits the variational structure that leads to a specific set of ODEs, namely the Euler-Lagrange equations of motion.

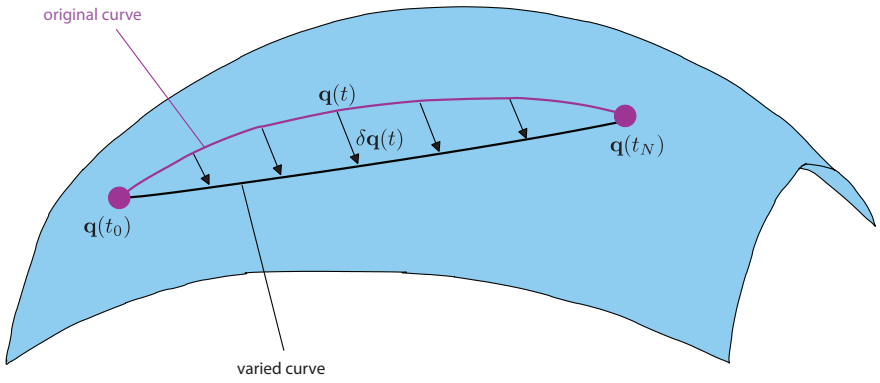

Figure 4: Variation of trajectory.

In general, the Lagrangian $L : T\mathcal{Q} \to \mathbb{R}$ of a mechanical system consists of the difference of the kinetic energy and a potential, thus $L(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$. Then a variational principle, namely Hamilton's principle of stationary action, states that a real trajectory is a stationary point of the action

$$S(q) = \int_a^b L(q,\dot{q})\,dt \tag{9}$$

For all variations $\delta q(t) \in T\mathcal{Q}$ with $\delta q(a) = \delta q(b) = 0$, see Figure 4,

$$\delta S = \delta \int_a^b L(q,\dot{q})\,dt = \int_a^b \frac{\partial L(q,\dot{q})}{\partial q}\delta q + \frac{\partial L(q,\dot{q})}{\partial \dot{q}}\delta\dot{q}\,dt = \int_a^b \left[\frac{\partial L(q,\dot{q})}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q,\dot{q})}{\partial \dot{q}}\right)\right]\delta q\,dt$$

whereby integration by parts and the fact $\delta\dot{q} = \frac{d}{dt}\delta q$ have been used. Thus, a trajectory is a solution of the Euler-Lagrange equations of motion

$$\frac{\partial L(q,\dot{q})}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q,\dot{q})}{\partial \dot{q}}\right) = 0 \tag{10}$$

Variational integrators In the context of variational integrators, see

J.E. Marsden and M. West: *Discrete mechanics and variational integrators.* Acta Numerica, 357-514, 2001.

instead of discretising the equation of motion (10), the variational principle is discretised. The Lagrangian is replaced by a discrete Lagrangian $L_d : \mathcal{Q} \times \mathcal{Q} \to \mathbb{R}$ which approximates the integral of the continuous one over one time interval

$$L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q,\dot{q})\,dt$$

Examples of discrete Lagrangians read

- midpoint rule

$$L_d(q_k, q_{k+1}) = \tau_k L\left(\frac{q_k + q_{k+1}}{2}, \frac{q_{k+1} - q_k}{\tau_k}\right) = \tau_k \left[\frac{m}{2}\frac{(q_{k+1} - q_k)^2}{\tau_k^2} - V(q_{k+\frac{1}{2}})\right] \tag{11}$$

- trapezoidal rule: Newmark with $\gamma = \frac{1}{2}$ and $\beta = 0$

$$\begin{aligned} L_d(q_k, q_{k+1}) &= \frac{\tau_k}{2} L\left(q_k, \frac{q_{k+1} - q_k}{\tau_k}\right) + \frac{\tau_k}{2} L\left(q_{k+1}, \frac{q_{k+1} - q_k}{\tau_k}\right) \\ &= \tau_k \left[\frac{m}{2}\frac{(q_{k+1} - q_k)^2}{\tau_k^2} - \frac{1}{2}(V(q_k) + V(q_{k+1}))\right] \end{aligned}$$

- explicit scheme

$$L_d(q_k, q_{k+1}) = \tau_k L\left(q_k, \frac{q_{k+1} - q_k}{\tau_k}\right) = \tau_k \left[\frac{m}{2}\frac{(q_{k+1} - q_k)^2}{\tau_k^2} - V(q_k)\right]$$

The action integral (9) is now approximated by a discrete action sum

$$S_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$$

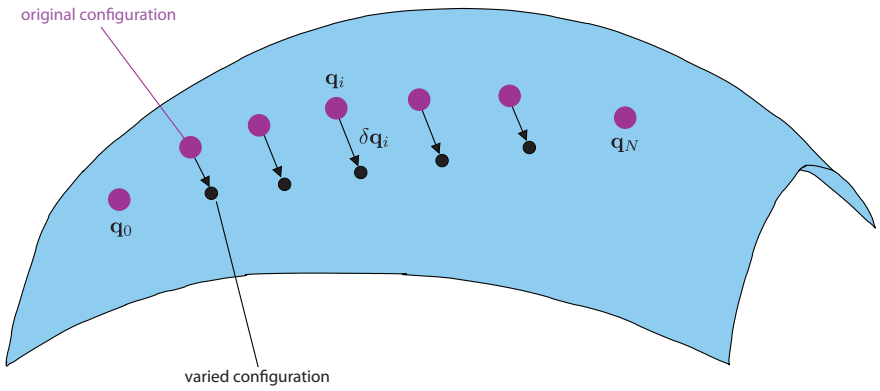

Figure 5: Discrete variation of discrete trajectory.

A discrete variational principle states that for all discrete variation sequences $\{\delta q_k\}_{n=0}^N$ with fixed end points $\delta q_0 = \delta q_N = 0$, see Figure 5, the discrete action must be stationary, i.e.

$$\begin{aligned} \delta S_d &= \sum_{k=0}^{N-1} D_1 L_d(q_k, q_{k+1})\delta q_k + D_2 L_d(q_k, q_{k+1})\delta q_{k+1} \\ &= D_1 L_d(q_0, q_1)\delta q_0 + \sum_{k=1}^{N-1} \left(D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1})\right)\delta q_k + D_2 L_d(q_{N-1}, q_N)\delta q_N \end{aligned}$$

This yields the discrete Euler-Lagrange time-stepping scheme

$$D_2L_d(q_{k-1}, q_k) + D_1L_d(q_k, q_{k+1}) = 0 \tag{12}$$

for $k = 1, \ldots, N-1$, thus one obtains $\{q_k\}_{k=2}^N$. (12) is a two-step scheme. For a given initial configuration q_0 and velocity $\dot{q}_0$, or corresponding initial conjugate momentum $p_0 = m\dot{q}_0$, the first unknown configuration q_1 can be determined using the discrete Legendre transform

$$p_k = -D_1L(q_k, q_{k+1})$$

With regard to (12), it also holds

$$p_k = D_2L(q_{k-1}, q_k)$$

Just as n second-order ODEs can be transformed in $2n$ first-order ODEs, the n-dimensional two-step scheme can be transformed into a $2n$-dimensional one-step scheme reading

$$\begin{aligned} p_k &= -D_1L(q_k, q_{k+1}) \\ p_{k+1} &= D_2L(q_k, q_{k+1}) \end{aligned}$$

that defines $\{(q_k, p_k)\}_{k=1}^N$. However, in terms of computational costs, it is usually less expensive, to solve the n-dimensional system (12) for the configurations and to determine the conjugate momenta afterwards in a post-processing step.

Energy behaviour The discrete trajectory is not exactly energy-conserving, however, it has good energy behaviour in the sense that the energy oscillates with small amplitudes close to the correct value.

Symplecticity Consider two vectors $\xi = (\xi_q, \xi_p), \eta = (\eta_q, \eta_p) \in \mathbb{R}^2$ and the area of a parallelogram spanned by them

$$\omega(\xi, \eta) = \det \begin{pmatrix} \xi_q & \eta_q \\ \xi_p & \eta_p \end{pmatrix} = \xi_q\eta_p - \xi_p\eta_q = \xi^T \cdot \mathbb{J} \cdot \eta$$

A linear map $A : \mathbb{R}^2 \to \mathbb{R}^2$ is called symplectic (area preserving, see Figure 6) if

$$\omega(\xi, \eta) = \omega(A \cdot \xi, A \cdot \eta) \qquad \Longleftrightarrow \qquad A^T \cdot \mathbb{J} \cdot A = \mathbb{J}$$

A nonlinear map, as e.g. the discrete evolution $\psi : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$ corresponding to the discrete Euler-Lagrange equations (12), is called symplectic, if its Jacobian $D\psi$ is symplectic, i.e.

$$D\psi^T \cdot \mathbb{J} \cdot D\psi = \left(\frac{\partial(q_{k+1}, p_{k+1})}{\partial(q_k, p_k)}\right)^T \cdot \mathbb{J} \cdot \frac{\partial(q_{k+1}, p_{k+1})}{\partial(q_k, p_k)} = \mathbb{J}$$

Details can be found in the mentioned literature, however, a necessary condition for symplecticity of an integrator is that the Jacobi-determinant of the discrete flow ψ is equal to one along the trajectory, i.e.

$$\det D\psi = \det \frac{\partial(q_{k+1}, p_{k+1})}{\partial(q_k, p_k)} = 1 \tag{13}$$

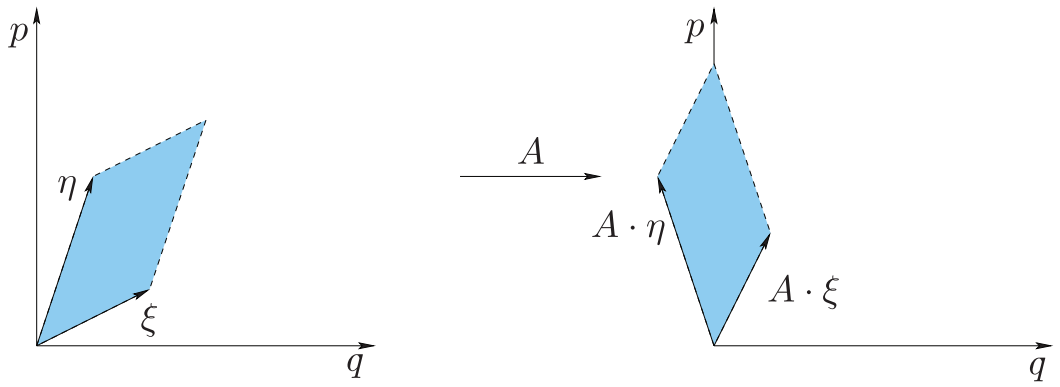

Figure 6: Symplecticity (area preservation) of a linear map.

Symmetry – reversibility in time Let $\rho : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ be an invertible linear transformation, e.g. $\rho = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ which is for $n = 1$ the reflection at the q-axis. The evolution of an initial value problem is reversible if it fulfills the property

$$\rho \circ \phi^{t+\tau,t} x = \phi^{t-\tau,t} \rho \circ x$$

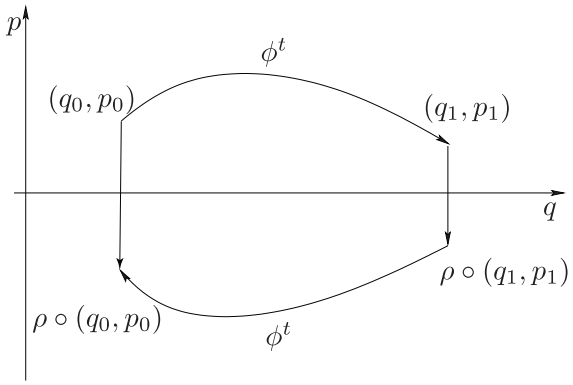

Figure 7: Reversible evolution.

The Hamiltonian $H(q,p) = \frac{1}{2m}p^2 + V(q)$ as well as the Lagrangian $L(q,\dot{q}) = \frac{m}{2}\dot{q}^q - V(q)$ are obviously invariant with respect to that transformation, $H(q,p) = H(q,-p)$ and $L(q,\dot{q}) = L(q,-\dot{q})$. Therefore, they have reversible flows.
An analogous property of a one-step method is that the discrete evolution is symmetric or reversibile in time. It reads

$$\psi^{t_k+\tau_k,t_k} \circ \psi^{t_{k+1}-\tau_k,t_{k+1}} = I \tag{14}$$

and means that the system travels backward on exactly the same discrete trajectory if the time-step τ is replaced by $-\tau$.

4 Constrained dynamics

So far, the planar pendulum has been formulated in terms of a 1-dimensional configuration variable, the angle relative to the vertical, see Figure 1. Such a formulation, in which the number of unknowns and therefore the dimension of the equations of motion is minimal is called a formulation in generalised coordinates. The number of generalised coordinates equals the number of degrees of freedom of the system. However, the pendulum could also be formulated in terms of the Cartesian coordinates of the point mass in the plane, see Figure 8.

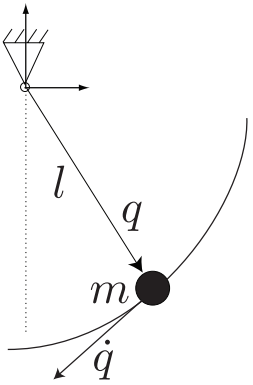

Figure 8: Planar pendulum in constrained coordinates.

Then the configuration $q \in \mathbb{R}^2$ is constrained by $m = 1$ condition

$$g(q) = \frac{1}{2}(||q||^2 - l^2) = 0$$

Thus the configuration is constrained to the circle S^1_l of radius l. This circle is called the constraint manifold for the pendulum. It is generally defined as

$$\mathcal{C} = \{q \in \mathbb{R}^n | g(q) = 0\}$$

which is $n - m$-dimensional. Thus for the planar pendulum in Cartesian coordinates, the constraint manifold is the circle $\mathcal{C} = S^1_l$ which is $n - m = 2 - 1 = 1$-dimensional. Likewise, velocities are constrained to the tangent space of the constraint manifold.

$$T\mathcal{C} = \{(q, \dot{q}) \in T\mathcal{Q} | g(q) = 0, Dg(q) \cdot \dot{q} = 0\}$$