Geometric numerical integration

Lecture notes

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Preface

These lecture notes should serve as a brief introduction to the field of geometric numerical integration, with particular focus on symplectic discretization. Symplectic discretization is concerned with finding numerical methods that are appropriate for canonical Hamiltonian systems. In some sense, symplectic discretization is the most developed field of geometric numerical integration, although recent years have seen a dramatic development of various other types of geometric integrators, such as exactly conservative methods, invariant discretization schemes and variational integrators.

No previous knowledge of geometric numerical integration is assumed. We begin by introducing the fundamentals of Hamiltonian mechanics, with particular focus on the underlying geometric properties of Hamiltonian systems. Following this brief introduction, we will discuss several strategies for discretizing Hamiltonian systems in a manner that respects their geometric at a discrete level.

An extensive body of literature appeared on the subject of geometric numerical integration has appeared over the last 20 years or so. These lecture notes are essentially condensed from the standard reference books on this subject matter, which include [2,4,6,8]. Further important background information on the material presented here can be found in [1,3,5,7].

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1 Introduction

Classical numerical methods such as those based on finite difference were developed to approximate the derivatives arising in systems of differential equations with as high accuracy as possible. This process is inherently local, i.e. to approximate derivatives in a given point only values around that point (the so-called stencil) are included in the approximation. The underlying point of view is generally applicable and can be applied to any local differential operator. Numerical schemes based on this approach (e.g. linear multistep methods or Runge–Kutta methods) have proved to be workhorses that allow tackling essentially any class of differential equations.

The main drawback of this local approach is that several differential equations can possess qualitative properties that can also be of global nature. A classical example for such global properties are conservation laws, which impose certain constraints on a system that are not inherently local. Other examples for these qualitative or geometric properties are Lie symmetries, a symplectic or Hamiltonian structure, variational principles from which the given system of equations were derived, and certain asymptotic properties. Since many of these geometric properties are intimately linked to the differential equations and can impose important restrictions on the form of the admitted solutions, these geometric properties should not be disregarded when deriving a numerical approximation of the differential equations. Numerical schemes preserving on a discrete level these geometric properties are termed *geometric numerical integrators*.

Since geometric properties are by its definition not universal but depend on the concrete differential equation at hand, geometric numerical integrators have to be re-derived for each new class of systems of differential equations encountered. This fact can be regarded as one major obstacle, which can render the process of discretization at times quite challenging. Regardless of this complication, if one is interested in the long term evolution or the correct statistical properties of a given system of differential equations, an accurate preservation of geometric properties is usually essential.

The purpose of these lecture notes is to develop, at a very basic level, some ideas of geometric numerical integration with applications to Hamiltonian systems. The Hamiltonian description of differential equations has proved to be very successful in that many of the systems arising in the mathematical sciences actually have an underlying Hamiltonian representation. This makes the problem of finding suitable discretization methods for such systems a topic of superior interest.

2 Introduction to Hamiltonian mechanics

Hamiltonian mechanics emerged as a reformulation of classical Newtonian mechanics and proved particularly important due to its underlying geometric structure. We provide here a short introduction to continuous Hamiltonian mechanics before we will describe how to derive discretization schemes that are appropriate for Hamiltonian systems.

2.1 Newtonian mechanics

We recall here Newton's equations of motions of a system of n point masses in $\mathbb{R}^3$. Denote by $M \in \mathbb{R}^{3n\times 3n}$ the diagonal mass matrix such that

$$M\boldsymbol{q} = (m_1\boldsymbol{q}_1, \dots, m_N\boldsymbol{q}_n)^{\mathrm{T}},$$

where $\boldsymbol{q}_i \in \mathbb{R}^3$, $i = 1, \dots, n$. The second Newton law states that the evolution of the a system of n particles with position vector $\boldsymbol{q} = (\boldsymbol{q}_1, \dots, \boldsymbol{q}_n)^{\mathrm{T}}$ is governed by the system of second-order

ordinary differential equations of the form

$$M\ddot{\boldsymbol{q}} = \mathbf{F}(\boldsymbol{q}), \tag{1}$$

where the force is given by the negative gradient of a potential function $U = U(\boldsymbol{q})$, i.e. $\mathbf{F}(\boldsymbol{q}) = -\nabla_{\boldsymbol{q}} U(\boldsymbol{q})$.

As always (1) can be expressed as a system of $2n$ first-order equations instead of a system of n second-order equations. To accomplish this, we introduce the vector of linear momenta $\boldsymbol{p} \in \mathbb{R}^{3n}$, which is defined by

$$\boldsymbol{p} = M\dot{\boldsymbol{q}}.$$

The system of first-order equations equivalent to (1) is then

$$\dot{\boldsymbol{q}} = M^{-1}\boldsymbol{p}, \quad \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} U(\boldsymbol{q}). \tag{2}$$

System (2) constitutes a special case of the Hamiltonian form of the equations of motion of a classical mechanical system. It is noteworthy, that system (2) preserves the total energy (kinetic plus potential energy), which is given by

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}^{\mathrm{T}} M^{-1}\boldsymbol{p} + U(\boldsymbol{q}).$$

In other words, it can be verified that $\mathrm{d}H/\mathrm{d}t = 0$. Moreover, it follows directly that system (2) can be written in the form

$$\boxed{\dot{\boldsymbol{q}} = \nabla_{\boldsymbol{p}} H, \quad \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} H.} \tag{3}$$

This is the standard form for a canonical Hamiltonian system. In the following, we will use the equivalent notations $\nabla_{\boldsymbol{q}} = \partial/\partial\boldsymbol{q}$ and $\nabla_{\boldsymbol{p}} = \partial/\partial\boldsymbol{p}$ interchangeably.

2.2 Canonical Hamiltonian dynamics

In the previous subsection we have introduced a special example of a Hamiltonian system. What characterizes a so-called canonical Hamiltonian system is the that the equations of motions are formulated in terms of a pair of position vectors $\boldsymbol{q}$ with the associated, conjugated momenta $\boldsymbol{p}$. Since Hamiltonian systems are applicable also to systems that do not originate from classical mechanics (and for which $\boldsymbol{q}$ and $\boldsymbol{p}$ do not have the meaning of position and momenta), it is conventional to call $\boldsymbol{q}$ the *generalized position* and $\boldsymbol{p}$ the *generalized momenta*. The space spanned by the vectors of generalized positions and generalized momenta is called the *phase space* Ω of the system. The phase space is always of even dimension, $2d \geqslant 2$. In our example from before, $d = 3n$, but here we allow $d \geqslant 1$ to be arbitrary.

Consider now a system with d degrees of freedom, whose phase space variables are $\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p})^{\mathrm{T}} = (q_1, \ldots, q_d, p_1, \ldots, p_d)^{\mathrm{T}}$. The system of Hamiltonian equations on the $2d$-dimensional phase space is given by

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad i = 1, \ldots, d,$$

which is simply the component form of the equivalent system (3) given before. H is the Hamilton function of the given Hamiltonian system, which physically often (but not always) is the total energy of the system. If $H = H(\boldsymbol{q}(t), \boldsymbol{p}(t))$ does not explicitly depend on time, it is always a constant of motion (first integral) of the system, since

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{q}} \cdot \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} + \frac{\partial H}{\partial p} \cdot \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{q}} \cdot \frac{\partial H}{\partial \boldsymbol{p}} - \frac{\partial H}{\partial \boldsymbol{p}} \cdot \frac{\partial H}{\partial \boldsymbol{q}} = 0.$$

Example 1. Consider the case of $d = 1$ (i.e. there is one degree of freedom), and the system with Hamiltonian function

$$H = T(p) + U(q), \qquad T = p^2/(2m), \quad U = kq^2/2,$$

where m is the point mass attached to a weightless spring with spring constant k. Here T is the kinetic energy and U is the potential energy. The Hamiltonian equations of motion are

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = \frac{\partial H}{\partial q} = -kq.$$

These are the governing equations of the classical *harmonic oscillator*, which is seen upon eliminating p from the above system (i.e. differentiate the equation for $\dot{q}$ again and substitute the equation for $\dot{p}$ in the resulting expression):

$$\ddot{q} - \frac{k}{m}q = 0.$$

We can write the canonical Hamiltonian equations

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{p}}, \qquad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \boldsymbol{q}}$$

in matrix–vector form:

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \mathbb{J}_c \frac{\partial H}{\partial \boldsymbol{z}} \qquad \Leftrightarrow \qquad \frac{\mathrm{d}z^i}{\mathrm{d}t} = J_c^{ij} \frac{\partial H}{\partial z^j}.$$

Here, we define $\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p})^{\mathrm{T}}$. The matrix

$$\mathbb{J}_c = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ -\mathbb{I} & \mathbb{O} \end{pmatrix} \tag{4}$$

is referred to as *canonical Poisson tensor*. Here, it is a $2d$-dimensional matrix, where $\mathbb{I}$ is the d-dimensional identity matrix and $\mathbb{O}$ is the d-dimensional zero matrix. Note that $\mathbb{J}_c^2 = -\mathbb{I}$, which is a matrix version of the definition of the imaginary unit, $i^2 = -1$. For this reason, one says the Hamiltonian equations possess a *symplectic structure* (symplectic = Greek for complex).

2.3 Geometric properties of Hamiltonian mechanics

The success story of the Hamiltonian formulation of a system of differential equations is largely owing to the underlying geometric properties of such systems, which we will explore at least partially here.

2.3.1 Flow maps

We first introduce the concept of the *solution operator* (or the *flow map*). Consider the real numbers $t, t_0 \in I \subset \mathbb{R}$, the *solution operator* (or flow map) $\boldsymbol{\Phi}_H(t, t_0)$ of the system (3) is the transformation mapping the phase space Ω to itself such that for all initial conditions $(\boldsymbol{q}(t_0), \boldsymbol{p}(t_0))$ in Ω we have

$$(\boldsymbol{q}, \boldsymbol{p}) = \boldsymbol{\Phi}_H(t, t_0)(\boldsymbol{q}(t_0), \boldsymbol{p}(t_0)),$$

which is the solution to (3) at time t. For fixed t and t_0, the solution operator can seen as a transformation of Ω to itself, since then the point $(\boldsymbol{q}(t_0), \boldsymbol{p}(t_0))$ is mapped to the point $(\boldsymbol{q}, \boldsymbol{p})$. Note that $\boldsymbol{\Phi}_H(t, t_0)(\boldsymbol{q}(t_0), \boldsymbol{p}(t_0))$ is only well-defined for sufficiently small $|t - t_0|$ since for a given initial $(\boldsymbol{q}(t_0), \boldsymbol{p}(t_0))$ the solution might not exist globally on all Ω. In other words, for fixed t and t_0, the domain of the transformation $\boldsymbol{\Phi}_H(t, t_0)$ may be considerably smaller than Ω.

Example 2. The Hamiltonian system with Hamiltonian $H = pq^2$ has the canonical equations of motion

$$\dot{q} = q^2, \quad \dot{p} = -2pq,$$

which can be integrated to obtain the analytical solution explicitly. We find for the solution operator

$$\mathbf{\Phi}_H(t, t_0)(q(t_0), p(t_0)) = \left(\frac{q(t_0)}{1 - (t - t_0)q(t_0)}, p(t_0)(1 - (t - t_0)q(t_0))^2 \right).$$

Thus, the solution operator is only well-defined as long as $q(t_0) < 1/(t - t_0)$, although H itself is a smooth function defined everywhere on $\mathbb{R}^2$.

The flow map $\mathbf{\Phi}_H(t, t_0)$ satisfies the following important property:

$$\mathbf{\Phi}_H(t_2, t_0) = \mathbf{\Phi}_H(t_2, t_1)\mathbf{\Phi}_H(t_1, t_0), \quad t_0, t_1, t_2 \in I. \tag{5}$$

In other words, the flow map of the system from t_0 to t_2 is given as the composition of the flow maps from the system from t_0 to t_1 followed by the flow map from t_1 to t_2. The implication is that the flow map from t_0 to t_2 is defined as long as the flow map from t_0 to t_1 and the flow map from t_1 to t_2 is defined.

In the following we will be mainly concerned with autonomous Hamiltonian systems. For such systems, the flow map depends only on the difference $t - t_0$ and we write $\boldsymbol{\varphi}_{t-t_0,H}$ instead of $\mathbf{\Phi}_H(t, t_0)$. In this case, the above property (5) becomes

$$\boldsymbol{\varphi}_{t+s,H} = \boldsymbol{\varphi}_{t,H}\boldsymbol{\varphi}_{s,H}.$$

which is referred to as *semi-group property*.

2.3.2 Liouville theorem

An important property of Hamiltonian systems is that they preserve the so-called *phase space volume*, which is the volume enclosed by neighboring trajectories in the phase space. This property is formulated through the following theorem.

Theorem 1 (Liouville theorem)**.** *The flow map of an autonomous Hamiltonian system preserves the phase space volume, i.e., for each subset D of the phase space Ω it is true that*

$$\operatorname{Vol}(\boldsymbol{\varphi}_{t,H} D) = \operatorname{Vol} D.$$

Proof. We start with a general system of first-order ODEs and derive a condition on the right-hand side which implies volume conservation, which we then show to hold for Hamiltonian systems.

Consider the system of n first-order ODEs

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \mathbf{f}(\boldsymbol{z}). \tag{6}$$

For the special case of a Hamiltonian system $\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p})^{\mathrm{T}}$ and $\mathbf{f}(\boldsymbol{z}) = \mathbf{f}(\boldsymbol{q}, \boldsymbol{p}) = (\partial H/\partial \boldsymbol{p}, -\partial H/\partial \boldsymbol{q})^{\mathrm{T}}$. Suppose the given system occupies the domain D with volume V at some time t_0. Denote

$D(t) = \boldsymbol{\varphi}_t(D)$ and $V(t) = \operatorname{Vol} D(t)$, where $\boldsymbol{\varphi}_t$ is the flow related to the given system of ODEs. Without loss of generality we suppose that $t_0 = 0$. We then have

$$V(0) = \int_{D(0)} \mathrm{d}z_1 \cdots \mathrm{d}z_n =: \int_{D(0)} \mathrm{d}\boldsymbol{z}.$$

Suppose that $\tilde{\mathbf{z}}(t) = \boldsymbol{\varphi}_t(\boldsymbol{z})$, then at time t the volume occupied in phase space is given by

$$V(t) = \int_{D(t)} \mathrm{d}\tilde{\mathbf{z}} = \int_{D(0)} \det\left(\frac{\partial \tilde{\mathbf{z}}}{\partial \boldsymbol{z}}\right) \mathrm{d}\boldsymbol{z} = \int_{D(0)} \det\left(\frac{\partial \boldsymbol{\varphi}_t(\boldsymbol{z})}{\partial \boldsymbol{z}}\right) \mathrm{d}\boldsymbol{z}, \tag{7}$$

where the second equality follows from the transformation rule for integrals and the third equality results from the definition of the flow map. Note that the determinant can always be assumed as positive for a continuous flow. To compute the derivative of the flow map, we expand the flow map in a Taylor series about the time $t = 0$. We then find

$$\tilde{\mathbf{z}} = \boldsymbol{\varphi}_t(\boldsymbol{z}) = \boldsymbol{\varphi}_0(\boldsymbol{z}) + \frac{\mathrm{d}\boldsymbol{\varphi}_t(\boldsymbol{z})}{\mathrm{d}t}\Big|_{t=0} t + \mathcal{O}(t^2) = \boldsymbol{z} + \mathbf{f}(\boldsymbol{z})t + \mathcal{O}(t^2),$$

where we have used (6) in the last step. Taking the derivative with respect to $\boldsymbol{z}$ we obtain

$$\frac{\partial \boldsymbol{\varphi}_t(\boldsymbol{z})}{\partial \boldsymbol{z}} = \mathbb{I} + \frac{\partial \mathbf{f}(\boldsymbol{z})}{\partial \boldsymbol{z}} t + \mathcal{O}(t^2),$$

where $\mathbb{I}$ is the identity matrix. To take the determinant of the right-hand side we need the following identity

$$\det(\mathbb{I} + \mathbb{A}t) = 1 + t \operatorname{tr}\mathbb{A} + \mathcal{O}(t^2).$$

In our case, we thus have to use the trace of $\partial \mathbf{f}(\boldsymbol{z})/\partial \boldsymbol{z}$, which is given by $\sum_i \partial f^i / \partial z^i = \operatorname{div} \mathbf{f}$, i.e. the divergence of $\mathbf{f}$. Substituting into (7) one derives

$$V(t) = \int_{D(0)} \Big(1 + t \operatorname{div} \mathbf{f} + \mathcal{O}(t^2)\Big) \, \mathrm{d}\boldsymbol{z}.$$

Taking the derivative with respect to t at $t = 0$ we obtain

$$\frac{\mathrm{d}V(t)}{\mathrm{d}t}\Big|_{t=0} = \int_{D(0)} \operatorname{div} \mathbf{f} \, \mathrm{d}\boldsymbol{z}.$$

In other words, if the divergence of the right-hand side $\mathbf{f}$ of the ODE system vanishes then the derivative of $V(t)$ is zero at time $t = 0$. Applying the flow $\boldsymbol{\varphi}_t$ we produce that the derivative of $V(t)$ is zero for any point inside of the interval $[0, t]$, which implies that $V(t)$ is constant. Since the point $t = 0$ has been chosen arbitrarily, the same result holds at an arbitrary time $t = t_0$.

For the Hamiltonian equations we have $\mathbf{f}(\boldsymbol{z}) = \mathbf{f}(\boldsymbol{q}, \boldsymbol{p}) = (\partial H/\partial \boldsymbol{p}, -\partial H/\partial \boldsymbol{q})^{\mathrm{T}}$ and thus

$$\operatorname{div} \mathbf{f} = \sum_i \left(\frac{\partial}{\partial q^i} \frac{\partial H}{\partial p^i} + \frac{\partial}{\partial p^i} \left(-\frac{\partial H}{\partial q^i} \right) \right) = 0.$$

This completes the proof of Liouville's theorem. □

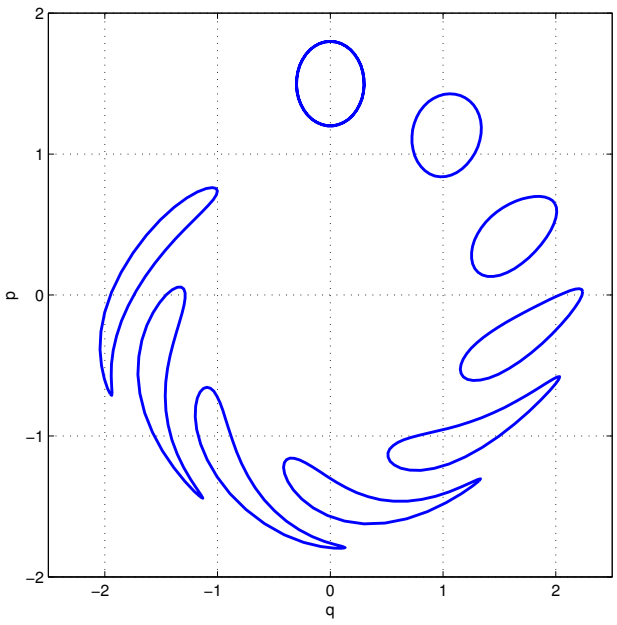

Figure 1: Visualization of the Liouville theorem. Time evolution of a set of initial conditions of the mathematical pendulum (top middle). The system moves clockwise and changes form while at the same time preserving the total area (2d volume).

3 Symplectic integration

This section is devoted to the construction elementary symplectic discretization methods. To do this, we first define the notion of symplecticity in some more detail. We restrict ourselves to canonical Hamiltonian systems.

Definition 1. Let

$$\mathbb{J} = \begin{pmatrix} \mathbb{O} & \mathbb{I} \\ -\mathbb{I} & \mathbb{O} \end{pmatrix},$$

be the $2d \times 2d$-dimensional canonical Poisson tensor. A map $\boldsymbol{\varphi}\colon \Omega \to \mathbb{R}^{2d}$ with $\Omega \subseteq \mathbb{R}^{2d}$ is called *symplectic* if

$$\Phi^{\mathrm{T}}(\boldsymbol{z})\, \mathbb{J}^{-1}\, \Phi(\boldsymbol{z}) = \mathbb{J}^{-1},$$

for all $\boldsymbol{z} \in \Omega$, where $\Phi(\boldsymbol{z}) = \partial\boldsymbol{\varphi}/\partial\boldsymbol{z}$ denotes the Jacobian matrix of $\boldsymbol{\varphi}$.

In other words, a map is symplectic if and only if it preserves the form of the canonical Poisson tensor.

Theorem 2 (Poincaré Theorem)**.** *If the Hamiltonian function H is twice continuously differentiable then the flow map $\boldsymbol{\varphi}_t$ of the associated Hamiltonian system is symplectic.*

Proof. Write the system of Hamiltonian equations in matrix–vector form:

$$\frac{\mathrm{d}\boldsymbol{\varphi}_t(\boldsymbol{z})}{\mathrm{d}t} = \mathbb{J}\nabla H(\boldsymbol{\varphi}_t(\boldsymbol{z})).$$

Differentiating this expression with respect to $\mathbf{z}$ and denoting by $\Phi_t(\boldsymbol{z})$ the Jacobian matrix of $\boldsymbol{\varphi}_t$ yields

$$\frac{\mathrm{d}\Phi_t(\boldsymbol{z})}{\mathrm{d}t} = \mathbb{J}H_{\boldsymbol{zz}}(\boldsymbol{\varphi}_t(\boldsymbol{z}))\Phi_t(\boldsymbol{z}).$$

This implies that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\Phi_t^{\mathrm{T}}(\boldsymbol{z})\mathbb{J}^{-1}\Phi_t(\boldsymbol{z})) &= \left(\frac{\mathrm{d}\Phi_t}{\mathrm{d}t}\right)^{\mathrm{T}}\mathbb{J}^{-1}\Phi_t + \Phi_t^{\mathrm{T}}\mathbb{J}^{-1}\left(\frac{\mathrm{d}\Phi_t}{\mathrm{d}t}\right)\\ &= (\Phi_t^{\mathrm{T}}H_{\boldsymbol{zz}}(\boldsymbol{\varphi}_t)\mathbb{J}^{\mathrm{T}})\mathbb{J}^{-1}\Phi_t + \Phi_t^{\mathrm{T}}\mathbb{J}^{-1}(\mathbb{J}H_{\boldsymbol{zz}}(\boldsymbol{\varphi}_t)\Phi_t)\\ &= -\Phi_t^{\mathrm{T}}H_{\boldsymbol{zz}}(\boldsymbol{\varphi}_t)\Phi_t + \Phi_t^{\mathrm{T}}H_{\boldsymbol{zz}}(\boldsymbol{\varphi}_t)\Phi_t = 0,\end{aligned}$$

where we have used that $\mathbb{J}^T\mathbb{J}^{-1} = -\mathbb{J}\mathbb{J}^{-1} = -\mathbb{I}$. From these computations it follows that

$$\Phi_t^{\mathrm{T}}\mathbb{J}^{-1}\Phi_t = \Phi_0^{\mathrm{T}}\mathbb{J}^{-1}\Phi_0$$

and since $\Phi_0 = \partial\boldsymbol{\varphi}_t/\partial\boldsymbol{z}|_{t=0} = \partial\boldsymbol{z}/\partial\boldsymbol{z} = \mathbb{I}$ we obtain

$$\Phi_t^{\mathrm{T}}\mathbb{J}^{-1}\Phi_t = \mathbb{J}^{-1},$$

which is the definition of a symplectic map. □

Remark 1. If $\boldsymbol{\varphi}_t$ is a symplectic flow map one can show that it is also the flow map of a Hamiltonian system. In other words, symplecticity is the main ingredient of a Hamiltonian system.

Having introduced the notion of a symplectic map we now introduce the notion of a symplectic numerical schemes. To do this, we first recall the definition of the local truncation error, of the consistency as well as the order of a numerical scheme.

Definition 2. Let there be given a system of ordinary differential equations $\boldsymbol{z}' = \mathbf{f}(\boldsymbol{z})$ and a numerical one-step method of the form $\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \Delta t\mathbf{F}(\boldsymbol{z}^n, \boldsymbol{z}^{n+1})$. The *local truncation error* $\boldsymbol{\tau}^n$ at step t^n is obtained by substituting the exact solution $\boldsymbol{z}(t)$ into the numerical scheme,

$$\boldsymbol{\tau}^n = \boldsymbol{z}(t^{n+1}) - \boldsymbol{z}(t^n) - \Delta t\mathbf{F}(\boldsymbol{z}(t^n), \boldsymbol{z}(t^{n+1})).$$

The one-step method is of order p, if $\boldsymbol{\tau}^n = \mathcal{O}((\Delta t)^{p+1})$.

A numerical method is called *consistent*, if $\boldsymbol{\tau}^n \to 0$ in the limit of $\Delta t \to 0$. For a numerical scheme to be consistent, it has to be at least of first order.

Definition 3. A numerical one-step method is symplectic if the map

$$\boldsymbol{z}^{n+1} = \boldsymbol{\varphi}_{\Delta t}(\boldsymbol{z}^n)$$

is symplectic provided it will be used for a Hamiltonian system.

The most elementary class of symplectic discretization schemes is given by the so-called symplectic Euler methods.

Theorem 3 (Symplectic Euler methods)**.** *The Euler methods of the following form*

$$\boxed{\boldsymbol{q}^{n+1} = \boldsymbol{q}^n + \Delta t H_{\boldsymbol{p}}(\boldsymbol{q}^n, \boldsymbol{p}^{n+1}), \qquad \boldsymbol{p}^{n+1} = \boldsymbol{p}^n - \Delta t H_{\boldsymbol{q}}(\boldsymbol{q}^n, \boldsymbol{p}^{n+1}),} \tag{8a}$$

and

$$\boxed{\boldsymbol{q}^{n+1} = \boldsymbol{q}^n + \Delta t H_{\boldsymbol{p}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^n), \qquad \boldsymbol{p}^{n+1} = \boldsymbol{p}^n - \Delta t H_{\boldsymbol{q}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^n),} \tag{8b}$$

are symplectic.

Proof. We give an idea for the proof of this theorem for the first of the two schemes in the case of $d = 1$. Generalizing to $d > 1$ and the second scheme are analogous.

Compute the derivative of (8a) with respect to q^n and p^n:

$$\begin{aligned} \frac{\partial q^{n+1}}{\partial q^n} &= 1 + \Delta t H_{pp} \frac{\partial p^{n+1}}{\partial q^n} + \Delta t H_{pq}, & \frac{\partial q^{n+1}}{\partial p^n} &= \Delta t H_{pp} \frac{\partial p^{n+1}}{\partial p^n} \\ \frac{\partial p^{n+1}}{\partial q^n} &= -\Delta t H_{qp} \frac{\partial p^{n+1}}{\partial q^n} - \Delta t H_{qq}, & \frac{\partial p^{n+1}}{\partial p^n} &= 1 - \Delta t H_{qp} \frac{\partial p^{n+1}}{\partial p^n}. \end{aligned}$$

Note that all derivatives of H are evaluated at point (p^{n+1}, q^n). The above system can be written in matrix form

$$\begin{pmatrix} 1 & -\Delta t H_{pp} \\ 0 & 1 + \Delta t H_{qp} \end{pmatrix} \begin{pmatrix} \dfrac{\partial q^{n+1}}{\partial q^n} & \dfrac{\partial q^{n+1}}{\partial p^n} \\ \dfrac{\partial p^{n+1}}{\partial q^n} & \dfrac{\partial p^{n+1}}{\partial p^n} \end{pmatrix} = \begin{pmatrix} 1 + \Delta t H_{qp} & 0 \\ -\Delta t H_{qq} & 1 \end{pmatrix}.$$

This last equation defines the Jacobi matrix $\Phi_{\Delta t}(q^n, p^n)$ of the methods. Direct computations verify that indeed

$$\Phi_{\Delta t}^{\mathrm{T}} \mathbb{J}^{-1} \Phi_{\Delta t} = \mathbb{J}^{-1}$$

and thus the method is symplectic. □

The symplectic Euler methods (8) are in general implicit numerical schemes. However, for the important class of separable Hamiltonian systems with the Hamiltonian function given by $H(\boldsymbol{q}, \boldsymbol{p}) = T(\boldsymbol{p}) + U(\boldsymbol{q})$ both schemes are explicit. This will be demonstrated in the following subsection.

3.1 Construction of some simple symplectic methods

A simple way for deriving symplectic discretizaton methods rests on the idea of *splittings*. In this case we assume that H can be written as the sum of $N \geqslant 2$ additional Hamiltonians H_i, $i = 1, \ldots, N$, i.e.

$$H(\boldsymbol{z}) = \sum_{i=1}^{N} H_i(\boldsymbol{z}).$$

The main underlying assumption is that each Hamiltonian system of the form

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \mathbb{J} \nabla H_i$$

is explicitly integrable. Although this assumption appears to be overly restrictive, an explicit integration of a split Hamiltonian system is indeed often possible for those systems arising in classical mechanics. For example, consider the Hamiltonian function of the form

$$H(\boldsymbol{q},\boldsymbol{p}) = T(\boldsymbol{p}) + U(\boldsymbol{q}).$$

We have seen above that this is the standard form of the Hamiltonian for almost all systems of classical mechanics. We now set $H_1(\boldsymbol{p}) = T(\boldsymbol{p})$ for the kinetic energy and $H_2(\boldsymbol{q}) = U(\boldsymbol{q})$ for the potential energy. The Hamiltonian system corresponding to H_1 ist then

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \boldsymbol{0}, \quad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\nabla_{\boldsymbol{q}} U(\boldsymbol{q}).$$

This system of equations is readily solved since $\boldsymbol{q}$ does not depend on time and therefore $\boldsymbol{p}$ has to be linear in t. The associated flow map is therefore

$$\boldsymbol{\varphi}_{t,V}(\boldsymbol{q},\boldsymbol{p}) = \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} - t\nabla_{\boldsymbol{q}} U(\boldsymbol{q}) \end{pmatrix}.$$

In a similar vein we can se that the flow map associated with the kinetic energy is

$$\boldsymbol{\varphi}_{t,T}(\boldsymbol{q},\boldsymbol{p}) = \begin{pmatrix} \boldsymbol{q} + \tau\nabla_{\boldsymbol{p}} T(\boldsymbol{p}) \\ \boldsymbol{p} \end{pmatrix}.$$

Since both flow maps are symplectic (since they belong to a Hamiltonian system), also the composition of the two flow maps is symplectic. Setting $t = \Delta t$ we find that

$$\boldsymbol{\psi}_{\Delta t} := \boldsymbol{\varphi}_{\Delta t,T} \circ \boldsymbol{\varphi}_{\Delta t,U}. \tag{9}$$

This yields the following numerical method: Integrate first the Hamiltonian system associated to $H_2 = U(\boldsymbol{q})$ over the time step Δt and use the result, denoted by $(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})$, as initial condition for the Hamiltonian system corresponding to $H_1 = T(\boldsymbol{p})$.

For this method to be consistent it has to be at least of first order. This is indeed the case since we have:

Theorem 4. *Let there be given $H = H_1 + H_2 + \cdots + H_N$, such that each term is at least twice continuously differentiable. The composition method*

$$\boldsymbol{\psi}_{\Delta t} = \boldsymbol{\varphi}_{\Delta t,H_1} \circ \boldsymbol{\varphi}_{\Delta t,H_2} \circ \cdots \circ \boldsymbol{\varphi}_{\Delta t,H_N}$$

is a symplectic method of at least first order.

Proof. We carry out the proof for the case of $N = 2$. We have to show that the difference between the flow map of the full Hamiltonian system, denoted with $\boldsymbol{\varphi}_{\Delta t,H}$ and the flow map of the composition method, $\boldsymbol{\psi}_{\Delta t}$, is at least $\mathcal{O}((\Delta t)^2)$. To show this we expand $\boldsymbol{\varphi}_{\Delta t,H}$ in a Taylor series about $\boldsymbol{z}^0$:

$$\boldsymbol{\varphi}_{\Delta t,H}(\boldsymbol{z}^0) = \boldsymbol{z}^0 + \Delta t\dot{\boldsymbol{z}}(0) + \mathcal{O}((\Delta t)^2) = \boldsymbol{z}^0 + \Delta t\mathbb{J}\nabla H(\boldsymbol{z}^0) + \mathcal{O}((\Delta t)^2).$$

Similarly, we have that

$$\boldsymbol{\varphi}_{\Delta t,H_i}(\boldsymbol{z}^0) = \boldsymbol{z}^0 + \Delta t\mathbb{J}\nabla H_i(\boldsymbol{z}^0) + \mathcal{O}((\Delta t)^2), \quad i = 1,2.$$

For the flow map of the composition method we find

$$\begin{aligned}\psi_{\Delta t}(\boldsymbol{z}^0) &= \varphi_{\Delta t,H_1}(\varphi_{\Delta t,H_2}(\boldsymbol{z}^0)) = \varphi_{\Delta t,H_1}(\boldsymbol{z}^0 + \Delta t\mathbb{J}\nabla H_2(\boldsymbol{z}^0)) + \mathcal{O}((\Delta t)^2)\\ &= \boldsymbol{z}^0 + \Delta t\mathbb{J}\nabla H_2(\boldsymbol{z}^0) + \Delta t\mathbb{J}\nabla H_1(\boldsymbol{z}^0) + \mathcal{O}((\Delta t)^2) = \boldsymbol{z}^0 + \Delta t\mathbb{J}\nabla H(\boldsymbol{z}^0) + \mathcal{O}((\Delta t)^2)\\ &= \varphi_{\Delta t,H}(\boldsymbol{z}^0) + \mathcal{O}((\Delta t)^2)).\end{aligned}$$

This result show that the composition method is at least a first order approximation of the exact flow map. □

With this result we can now complete our composition method (9). We start with the point $(\boldsymbol{q}^n, \boldsymbol{p}^n)$ and use the flow map $\varphi_{\Delta t,U}$. This yields the intermediate point

$$\bar{\boldsymbol{q}} = \boldsymbol{q}^n, \quad \bar{\boldsymbol{p}} = \boldsymbol{p}^n - \Delta t\nabla_{\boldsymbol{q}} U(\boldsymbol{q}^n).$$

Now using the flow map $\varphi_{\Delta t,T}$ we obtain

$$\boldsymbol{q}^{n+1} = \bar{\boldsymbol{q}} + \Delta t\nabla_{\boldsymbol{p}} T(\bar{\boldsymbol{p}}), \quad \boldsymbol{p}^{n+1} = \bar{\boldsymbol{p}}.$$

Eliminating the intermediate point $(\bar{\boldsymbol{q}}^n, \bar{\boldsymbol{p}}^n)$ we find

$$\boldsymbol{q}^{n+1} = \boldsymbol{q}^n + \Delta t\nabla_{\boldsymbol{p}} T(\boldsymbol{p}^{n+1}), \quad \boldsymbol{p}^{n+1} = \boldsymbol{p}^n - \Delta t\nabla_{\boldsymbol{q}} U(\boldsymbol{q}^n).$$

This is nothing but a special case for the first symplectic Euler method (8a). Had we used the composition $\varphi_{\Delta t,U} \circ \varphi_{\Delta t,T}$ we would have found the second sympectic Euler method (8b). Both methods are explicit numerical schemes for the Hamiltonian of the form $H = H_1(\boldsymbol{p}) + H_2(\boldsymbol{q})$.

What remains to be discussed is the case of how to use the idea of splitting if the individual Hamiltonian subsystems are not explicitly integrable. Indeed, it is often the case that a Hamiltonian can be partitioned into Hamiltonian functions corresponding to subsystems, but not always can these subsystems be integrated explicitly. In this case, it is still possible to decompose the flow map of the full system into the composition of flow maps of the subsystems, but now the non-integrable flow maps have to be approximated using a numerical method (e.g. using the symplectic Euler methods or other suitable symplectic methods). This technique makes splitting methods universally applicable and in addition provides an efficient method for the integration of Hamiltonian systems by decomposing a complicated model into easier to handle subproblems.

3.2 Symmetric composition methods

Let there be given a numerical one-step method, $\varphi_{\Delta t}$. The associated *adjoint method* $\varphi^*_{\Delta t}$ is defined through

$$\varphi^*_{\Delta t} = (\varphi_{-\Delta t})^{-1}.$$

In other words, it is true that

$$\boldsymbol{z}^n = \varphi_{-\Delta t}(\boldsymbol{z}^{n+1})$$

and thus the adjoint method is defined by

$$\varphi^*_{\Delta t}(\boldsymbol{z}^n) = \boldsymbol{z}^{n+1}.$$

It follows from this definition that $\varphi_{\Delta t} = (\varphi^*_{\Delta t})^*$, i.e. the adjoint of the adjoint yields again the initial method. A method $\varphi_{\Delta t}$ is called *symmetric* if it is self-adjoint, i.e. $\varphi^*_{\Delta t} = \varphi_{\Delta t}$ holds.

Example 3. The symplectic Euler method (8a) is not symmetric. We start with $\boldsymbol{z}^{n+1} = \boldsymbol{\varphi}_{\Delta t}(\boldsymbol{z}^n)$ implicitly defined by

$$\boldsymbol{q}^{n+1} = \boldsymbol{q}^n + \Delta t H_{\boldsymbol{p}}(\boldsymbol{q}^n, \boldsymbol{p}^{n+1}), \qquad \boldsymbol{p}^{n+1} = \boldsymbol{p}^n - \Delta t H_{\boldsymbol{q}}(\boldsymbol{q}^n, \boldsymbol{p}^{n+1}),$$

and compute the inverse $(\boldsymbol{\varphi}_{\Delta t})^{-1}$ by exchanging $\boldsymbol{z}^n$ and $\boldsymbol{z}^{n+1}$. This yields

$$\boldsymbol{q}^{n} = \boldsymbol{q}^{n+1} + \Delta t H_{\boldsymbol{p}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n}), \qquad \boldsymbol{p}^{n} = \boldsymbol{p}^{n+1} - \Delta t H_{\boldsymbol{q}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n}).$$

Replacing Δt by $-\Delta t$ we can write

$$\boldsymbol{q}^{n+1} = \boldsymbol{q}^n + \Delta t H_{\boldsymbol{p}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^n), \qquad \boldsymbol{p}^{n+1} = \boldsymbol{p}^n - \Delta t H_{\boldsymbol{q}}(\boldsymbol{q}^{n+1}, \boldsymbol{p}^n).$$

This implies that the adjoint of the symplectic Euler method (8a) is the symplectic Euler method (8b). Hence, none of the symplectic Euler methods is symmetric.

A symmetric method can be constructed systematically by composing a numerical method with its adjoint.

Theorem 5. *Let there be given the numerical method $\boldsymbol{\varphi}_{\Delta t}$ as well as its adjoint $\boldsymbol{\varphi}^*_{\Delta t}$. The method*

$$\boldsymbol{\psi}_{\Delta t} := \boldsymbol{\varphi}^*_{\Delta t/2} \circ \boldsymbol{\varphi}_{\Delta t/2}$$

is symmetric.

Proof. We have to show that $\boldsymbol{\psi}^*_{\Delta t} = \boldsymbol{\psi}_{\Delta t}$ holds. We start with

$$\boldsymbol{\psi}_{-\Delta t} = \boldsymbol{\varphi}^*_{-\Delta t/2} \circ \boldsymbol{\varphi}_{-\Delta t/2} = (\boldsymbol{\varphi}_{\Delta t/2})^{-1} \circ (\boldsymbol{\varphi}^*_{\Delta t/2})^{-1} = (\boldsymbol{\varphi}^*_{\Delta t/2} \circ \boldsymbol{\varphi}_{\Delta t/2})^{-1} = (\boldsymbol{\psi}_{\Delta t})^{-1}.$$

This implies that $\boldsymbol{\psi}_{-\Delta t} = (\boldsymbol{\psi}_{\Delta t})^{-1}$ and hence $\boldsymbol{\psi}_{\Delta t} = (\boldsymbol{\psi}_{-\Delta t})^{-1} = \boldsymbol{\psi}^*_{\Delta t}$. □

We now demonstrate the construction of a symmetric symplectic method by combining the two symplectic Euler methods (8) with a half time step. This yields

$$\begin{aligned}
\boldsymbol{q}^{n+1/2} &= \boldsymbol{q}^n + \frac{1}{2}\Delta t \nabla_{\boldsymbol{p}} H(\boldsymbol{q}^n, \boldsymbol{p}^{n+1/2}), \quad \boldsymbol{p}^{n+1/2} = \boldsymbol{p}^n - \frac{1}{2}\Delta t \nabla_{\boldsymbol{q}} H(\boldsymbol{q}^n, \boldsymbol{p}^{n+1/2}),\\
\boldsymbol{q}^{n+1} &= \boldsymbol{q}^{n+1/2} + \frac{1}{2}\Delta t \nabla_{\boldsymbol{p}} H(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n+1/2}), \quad \boldsymbol{p}^{n+1} = \boldsymbol{p}^{n+1/2} - \frac{1}{2}\Delta t \nabla_{\boldsymbol{q}} H(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n+1/2}).
\end{aligned}$$

This expression can be simplified if the half step $\boldsymbol{q}^{n+1/2}$ is eliminated. The resulting method is the so-called *Störmer–Verlet method*

$$\boxed{\begin{aligned}
\boldsymbol{p}^{n+1/2} &= \boldsymbol{p}^n - \frac{1}{2}\Delta t \nabla_{\boldsymbol{q}} H(\boldsymbol{q}^n, \boldsymbol{p}^{n+1/2}),\\
\boldsymbol{q}^{n+1} &= \boldsymbol{q}^n + \frac{1}{2}\Delta t \left(\nabla_{\boldsymbol{p}} H(\boldsymbol{q}^n, \boldsymbol{p}^{n+1/2}) + \nabla_{\boldsymbol{p}} H(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n+1/2})\right),\\
\boldsymbol{p}^{n+1} &= \boldsymbol{p}^{n+1/2} - \frac{1}{2}\Delta t \nabla_{\boldsymbol{q}} H(\boldsymbol{q}^{n+1}, \boldsymbol{p}^{n+1/2}).
\end{aligned}} \tag{10}$$

This method is important in the numerical integration of many body problems and as such plays a central role in molecular dynamics. Since we derived the Störmer–Verlet method by composition of two symplectic methods, the resulting method is indeed symplectic too.

Taylor series expansion reveals that the Störmer–Verlet method is a method of *second order*. This is interesting since both symplectic Euler methods are only first order. However, that the Störmer–Verlet method is second order is indeed a special case of the following theorem.

Theorem 6. *A symmetric numerical method is always of even order.*

Proof. The proof of this statement can be found in the book by Leimkuhler und Reich [6, pp. 86]. □

This theorem implies that the symmetric composition of a first-order method with its adjoint is always a method of second order.

Example 4. The forward Euler method for the Hamiltonian system

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \mathbb{J}\nabla H(\boldsymbol{z})$$

is $\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \Delta t \mathbb{J}\nabla H(\boldsymbol{z}^n)$. This method is neither symmetric nor symplectic. The inverse of the numerical phase flow $\boldsymbol{\varphi}_{\Delta t}$ ist given by exchanging $\boldsymbol{z}^n$ and $\boldsymbol{z}^{n+1}$, i.e. $\boldsymbol{z}^n = \boldsymbol{z}^{n+1} + \Delta t \mathbb{J}\nabla H(\boldsymbol{z}^{n+1})$. Replacing Δt by $-\Delta t$ yields the adjoint method, which after rearranging can be written as $\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \Delta t \mathbb{J}\nabla H(\boldsymbol{z}^{n+1})$. The adjoint $\boldsymbol{\varphi}^*_{\Delta t}$ of the forward Euler method is hence the backward Euler method (and vice versa).

We now construct a symmetric method based on the backward Euler method. Thus $\boldsymbol{\psi}_{\Delta t}$ is the composition of the backward Euler with the forward Euler method. This gives

$$\boldsymbol{z}^{n+1/2} = \boldsymbol{z}^n + \frac{\Delta t}{2}\mathbb{J}\nabla H(\boldsymbol{z}^{n+1/2}), \quad \boldsymbol{z}^{n+1} = \boldsymbol{z}^{n+1/2} + \frac{\Delta t}{2}\mathbb{J}\nabla H(\boldsymbol{z}^{n+1/2}).$$

Adding both equations yields

$$\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \Delta t \mathbb{J}\nabla H(\boldsymbol{z}^{n+1/2})$$

which is the so-called *implicit midpoint method*, $\boldsymbol{z}^{n+1/2} = (\boldsymbol{z}^n + \boldsymbol{z}^{n+1})/2$. This method is symmetric (per construction), second order, and it is also symplectic! Indeed, it is one of the most important symplectic methods there is.

3.3 Symplectic Runge–Kutta methods

Runge–Kutta methods are amongst the most popular numerical schemes for initial value problems. They allows constructing higher order numerical methods by introducing multiple intermediate stages between the initial time step t^n and the next time step t^{n+1}. Runge–Kutta methods are still one-step methods in contrast to linear multistep methods which achieve higher order by using the previously computed numerical solution at steps t^n, t^{n-1}, etc.

Definition 4. Let there be given a system of ordinary differential equations

$$\frac{\mathrm{d}\boldsymbol{z}}{\mathrm{d}t} = \mathbf{f}(t, \boldsymbol{z}),$$

with initial conditions $\boldsymbol{z}(0) = \boldsymbol{z}^0$. An *s-stage Runge–Kutta method* for this initial value problem is of the form

$$\begin{aligned} \mathbf{Z}_i &= \boldsymbol{z}^n + \Delta t \sum_{j=1}^{s} a_{ij} \mathbf{f}(t^n + c_j \Delta t, \mathbf{Z}_j), \quad 1 \le i \le s, \\ \boldsymbol{z}^{n+1} &= \boldsymbol{z}^n + \Delta t \sum_{i=1}^{s} b_i \mathbf{f}(t^n + c_i \Delta t, \mathbf{Z}_i). \end{aligned} \tag{11}$$

In the above definition of the Runge–Kutta method, we denote by $\mathbf{Z}_i$ the s stages, c_i are the nodes, b_i are the weights of the quadrature rule and a_{ij} is the Runge–Kutta array. Consistency of the method requires that

$$\sum_{j=1}^{s} b_j = 1, \quad c_i = \sum_{j=1}^{s} a_{ij}, \quad i = 1, \dots, s.$$

The Runge–Kutta methods (11) is *explicit* if $a_{ij} = 0$, $\forall i \leq j$, otherwise it is *implicit*. Implicit Runge–Kutta methods require the solution of an implicit system of algebraic equations to obtain the stages $\mathbf{Z}_i$ (e.g. using Newton's method). Runge–Kutta methods are often displayed using a so-called *Butcher tableau*:

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

Both explicit and implicit Runge–Kutta methods play an important role in practical applications. While explicit Runge–Kutta methods have the advantage that no implicit system of algebraic equations has to be solved in each time step, their stability properties are in general not en par with implicit Runge–Kutta methods. Moreover, it can be shown that there is no explicit Runge–Kutta method of order $p \geq 5$ that does not need at least $s > p$ stages. No such restriction exists for implicit Runge–Kutta methods. Moreover, for implicit Runge–Kutta methods it can be shown that using carefully choses nodes c_i it is possible to construct methods of order $2s$ using only s stages. In other words, it is possible to construct second order and fourth order implicit Runge–Kutta methods that only require one and two stages, respectively. These are the so-called *Gauss–Legendre Runge–Kutta methods*, which are important examples of geometric numerical integrators.

Example 5. *Heun's method* (sometimes also called *explicit trapezoidal rule*) has the Butcher tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Explicitly, this method can be written as

$$\boxed{\begin{aligned} &\mathbf{Z}_1 = \boldsymbol{z}^n \\ &\mathbf{Z}_2 = \boldsymbol{z}^n + \Delta t \mathbf{f}(t^n, \boldsymbol{z}^n) \\ &\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \frac{\Delta t}{2} \left(\mathbf{f}(t^n, \mathbf{Z}_1) + \mathbf{f}(t^{n+1}, \mathbf{Z}_2) \right). \end{aligned}}$$

Heun's method is hence an example for an explicit Runge–Kutta method.

Example 6. The *implicit midpoint method* has the Butcher tableau

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

Explicitly, it reads

$$\boxed{\boldsymbol{z}^{n+1} = \boldsymbol{z}^n + \Delta t \mathbf{f}\left(t^n + \frac{1}{2}\Delta t, \frac{1}{2}(\boldsymbol{z}^n + \boldsymbol{z}^{n+1})\right).}$$

This method uses only one stage, $s = 1$, but is of order $p = 2s = 2$. The implicit midpoint method is the Gauss–Legendre Runge–Kutta method of lowest order.

A further important method is the Gauss–Legendre Runge–Kutta method for $s = 2$ with the Butcher tableau:

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

This method uses two stages but is of fourth order.

After this short introduction to Runge–Kutta method we now aim to establish whether such methods can be symplectic and are thus suitable for Hamiltonian systems.

Theorem 7. *A Runge–Kutta method is symplectic if and only if*

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i, j = 1, \ldots, s.$$

Proof. For the proof of this theorem, see the book by Leimkuhler and Reich (pp. 152) or the book by Iserles (pp. 91). □

A direct consequence of this theorem is that both the implicit midpoint rule and the Gauss–Legendre Runge–Kutta method with $s = 2$ stages is symplectic (indeed one can show that all Gauss–Legendre Runge–Kutta methods are symplectic). Moreover, there is no explicit Runge–Kutta method that is symplectic (this follows directly from the symmetry with respect to i and j in the above equation)! In other words, in designing suitable geometric numerical schemes for Hamiltonian systems, only specific implicit Runge–Kutta methods can be used.

3.4 Conservation properties of symplectic integrators

Conserved quantities, so-called *first integrals* in the case of ODEs, are of central importance in physics and other mathematical sciences.

Definition 5. A non-constant function $I(\boldsymbol{z})$ is called a first integral of the system of ODEs $\dot{\boldsymbol{z}} = f(\boldsymbol{z})$ if

$$\frac{\mathrm{d}I}{\mathrm{d}t} = I'(\boldsymbol{z})\dot{\boldsymbol{z}} = I'(\boldsymbol{z})f(\boldsymbol{z}) = 0$$

for all $\boldsymbol{z}$. Thus, we have for every solution of the ODE system that $I(\boldsymbol{z}(t)) = I(\boldsymbol{z}(t_0)) = \text{const}$ and thus I remains constant under the evolution of the ODE.

We have already seen that the Hamiltonian of an autonomous system is always a first integral. We now collect a few important information about the conservation properties of symplectic integrators. For more details and the proofs of the following theorems, consult the books by Leimkuhler and Reich [6], as well as by Hairer, Lubich and Wanner [4].

Theorem 8. *All explicit and implicit Runge–Kutta methods conserve linear invariants of the form* $I(\boldsymbol{z}) = \mathbf{d}^{\mathrm{T}}\boldsymbol{z}$*, where* $\mathbf{d}$ *is a constant vector.*

Theorem 9. *The Gauss–Legendre Runge–Kutta methods conserve quadratic invariants of the form* $I(\boldsymbol{z}) = \boldsymbol{z}^{\mathrm{T}}C\boldsymbol{z}$*, where* C *is a symmetric square matrix.*

Theorem 10. *For* $n \geqslant 3$*, no Runge–Kutta method can conserve all polynomial invariants of degree* n*.*

While several important first integrals in physics are either linear or quadratic functions (e.g. linear momentum or angular momentum), there are numerous systems of differential equations that admit polynomial invariants of higher order (e.g. the Laplace–Runge–Lenz vector) or even non-polynomial invariants (e.g. conserved quantities involving a logarithm as in the case of the point vortex equations or the Lotka–Volterra systems from population dynamics). The above theorems state that in general Runge–Kutta methods, even Gauss–Legendre Runge–Kutta methods, cannot preserve all of these invariants. If one is thus specifically interested in preserving particular conserved quantities of more complicated form, different geometric numerical methods have to be used, such as projection methods [4] or the multiplier method [9].

Lastly, we are interested in the preservation of the Hamiltonian function by a symplectic method. One would intuitively believe that if a numerical method preserves the symplectic structure of the underlying Hamiltonian systems that it should also preserve its Hamiltonian. This is however not true. In particular, one can show the following theorem to hold (Ge and Marsden, 1988).

Theorem 11. *Let there be given a Hamiltonian system which possesses no further conserved quantity besides the Hamiltonian function* H*. A symplectic numerical method which preserves* H *exactly also preserves the flow map of the original Hamiltonian system exactly (up to a possible reparameterization of times).*

To require that a symplectic method preserves the Hamiltonian function exactly is thus the same as to require that the method yields the exact solution of the original Hamiltonian system. Since this is in general impossible, a symplectic method cannot preserve the Hamiltonian function; symplecticity and preservation of the Hamiltonian function are thus not mutually compatible! Still, the relative change in the Hamiltonian function is typically oscillating and quite small (in fact bounded over exponentially long time periods) and thus symplectic methods can be used for stable long time integrations. Moreover, as we have seen in the other theorems above, symplectic methods can without problem preserve other specific conserved quantities provided they are of the special form compatible with the particular scheme used.

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