Contents

1. Hamiltonian Systems and Canonical Equations

In this Section, we will discuss methods for solving canonical equations of the form

$$\frac{dp}{dt} = -\frac{\partial H(p,q)}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial H(p,q)}{\partial p}, \tag{1}$$

where $q(t) = [q_1(t), \ldots, q_d(t)]^T$, $p(t) = [p_1(t), \ldots, p_d(t)]^T$, and $H(p,q)$ is a function $\mathbb{R}^{2d} \to \mathbb{R}$ called the *Hamiltonian*. Its physical sense is the total energy. It is easy to show that the Hamiltonian $H(p,q)$ is constant along the trajectories (i.e., the solutions of Eq. (1)). Indeed, taking its time derivative along any trajectory is zero:

$$\frac{dH}{dt} = \sum_{i=1}^{d} \frac{\partial H}{\partial p_i}\frac{dp_i}{dt} + \frac{\partial H}{\partial q_i}\frac{dq_i}{dt} = \sum_{i=1}^{d} \frac{\partial H}{\partial p_i}\left(-\frac{\partial H}{\partial q_i}\right) + \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} = 0.$$

The need to integrate equations of the form of Eq. (1) for large times arises, for instance, in celestial mechanics and in molecular dynamics. It is of crucial importance to perform numerical integration of Eq. (1) using methods that keep the Hamiltonian as close to a constant as possible. In the next section, we will establish some properties of Hamiltonian systems which will help us to design appropriate methods for their integration.

1.1. Properties of Canonical Equations.

Let us pick some subset $\Omega_0 \subset \mathbb{R}^{2d}$ and evolve it in time according to Eq. (1). In other words, we consider the set of trajectories $(p(t), q(t))$ such that $(p(0), q(0)) \in \Omega_0$. Then, for each moment of time t, set $\Omega_0 \equiv \Omega(0)$ will be mapped to a set $\Omega_t \equiv \Omega(t)$. This map is called the *phase flow*.

Definition 1. *The phase flow ϕ_t associated with Eq. (1) is a one-parameter family of mappings $\phi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$, such that for each t,*

$$\phi_t : \ (p(0), q(0)) \mapsto (p(t), q(t)).$$

Therefore, the phase flow is a differentiable mapping. It is instructive to consider the Jacobian matrix of the phase flow, i.e., the matrix of the derivatives of $(p(t), q(t))$ with respect to the initial conditions $(p(0), q(0))$. Next, we will derive the time evolution equation for the Jacobian matrix of the phase flow. This equation is called the *variational equation.*

Let $p(0) = p^0$ and $q(0) = q^0$. Consider the solution of Eq. (1) as a function of the initial condition:

$$p(t, p^0, q^0) \quad \text{and} \quad q(t, q^0, p^0).$$

Differentiating the canonical equations

$$\frac{dp_i}{dt} = -\frac{\partial H(p,q)}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H(p,q)}{\partial p_i}, \quad 1 \le i \le d, \tag{2}$$

with respect to p_k^0 and q_k^0, $1 \le k \le d$ we obtain the *variational equations*

$$\begin{aligned}
\frac{d}{dt}\frac{\partial p_i}{\partial p_k^0} &= -\sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial q_i \partial p_j}\frac{\partial p_j}{\partial p_k^0} - \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial q_i \partial q_j}\frac{\partial q_j}{\partial p_k^0}, \\
\frac{d}{dt}\frac{\partial p_i}{\partial q_k^0} &= -\sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial q_i \partial p_j}\frac{\partial p_j}{\partial q_k^0} - \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial q_i \partial q_j}\frac{\partial q_j}{\partial q_k^0}, \\
\frac{d}{dt}\frac{\partial q_i}{\partial p_k^0} &= \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial p_i \partial p_j}\frac{\partial p_j}{\partial p_k^0} + \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial p_i \partial q_j}\frac{\partial q_j}{\partial p_k^0}, \\
\frac{d}{dt}\frac{\partial q_i}{\partial q_k^0} &= \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial p_i \partial p_j}\frac{\partial p_j}{\partial q_k^0} + \sum_{j=1}^{d} \frac{\partial^2 H(p,q)}{\partial p_i \partial q_j}\frac{\partial q_j}{\partial q_k^0}.
\end{aligned}$$

Rewriting the variational equations in the matrix form we get

$$\frac{d}{dt}\Psi = \begin{bmatrix} -\frac{\partial^2 H(p,q)}{\partial q \partial p} & -\frac{\partial^2 H(p,q)}{\partial q \partial q} \\ \frac{\partial^2 H(p,q)}{\partial p \partial p} & \frac{\partial^2 H(p,q)}{\partial p \partial q} \end{bmatrix} \Psi, \quad \Psi(0) = I. \tag{3}$$

The matrix ψ is the matrix of the derivatives of the solution of Eq. (1) with respect to the initial data, i.e., the Jacobian matrix of the phase flow:

$$\Psi := \begin{bmatrix}
\frac{\partial p_1}{\partial p_1^0} & \dots & \frac{\partial p_1}{\partial p_d^0} & \frac{\partial p_1}{\partial q_1^0} & \dots & \frac{\partial p_1}{\partial q_d^0} \\
 & \dots & & \dots & & \\
\frac{\partial p_d}{\partial p_1^0} & \dots & \frac{\partial p_d}{\partial p_d^0} & \frac{\partial p_d}{\partial q_1^0} & \dots & \frac{\partial p_d}{\partial q_d^0} \\
\frac{\partial q_1}{\partial p_1^0} & \dots & \frac{\partial q_1}{\partial p_d^0} & \frac{\partial q_1}{\partial q_1^0} & \dots & \frac{\partial q_1}{\partial q_d^0} \\
 & \dots & & \dots & & \\
\frac{\partial q_d}{\partial p_1^0} & \dots & \frac{\partial q_d}{\partial p_d^0} & \frac{\partial q_d}{\partial q_1^0} & \dots & \frac{\partial q_d}{\partial q_d^0}
\end{bmatrix}, \tag{4}$$

The first matrix in the right-hand side of Eq. (3) is the Jacobian matrix of the right-hand side of the canonical equations (1) given by

(5)
$$\begin{bmatrix} -\frac{\partial^2 H(p,q)}{\partial q \partial p} & -\frac{\partial^2 H(p,q)}{\partial q \partial q} \\ \frac{\partial^2 H(p,q)}{\partial p \partial p} & \frac{\partial^2 H(p,q)}{\partial p \partial q} \end{bmatrix} := \begin{bmatrix} -\frac{\partial^2 H(p,q)}{\partial q_1 \partial p_1} & \dots & -\frac{\partial^2 H(p,q)}{\partial q_1 \partial p_d} & -\frac{\partial^2 H(p,q)}{\partial q_1 \partial q_1} & \dots & -\frac{\partial^2 H(p,q)}{\partial q_1 \partial q_d} \\ & \dots & & \dots & & \\ -\frac{\partial^2 H(p,q)}{\partial q_d \partial p_1} & \dots & -\frac{\partial^2 H(p,q)}{\partial q_d \partial p_d} & -\frac{\partial^2 H(p,q)}{\partial q_d \partial q_1} & \dots & -\frac{\partial^2 H(p,q)}{\partial q_d \partial q_d} \\ & \dots & & \dots & & \\ \frac{\partial^2 H(p,q)}{\partial p_1 \partial p_1} & \dots & \frac{\partial^2 H(p,q)}{\partial p_1 \partial p_d} & \frac{\partial^2 H(p,q)}{\partial p_1 \partial q_1} & \dots & \frac{\partial^2 H(p,q)}{\partial p_1 \partial q_d} \\ & \dots & & \dots & & \\ \frac{\partial^2 H(p,q)}{\partial p_d \partial p_1} & \dots & \frac{\partial^2 H(p,q)}{\partial p_d \partial p_d} & \frac{\partial^2 H(p,q)}{\partial p_d \partial q_1} & \dots & \frac{\partial^2 H(p,q)}{\partial p_d \partial q_d} \end{bmatrix}.$$

It is easy to see that the upper left block of the matrix (5) is negative transposed of the lower right block. Therefore, the trace of the Jacobian matrix is zero. Then the Theorem of Liouville the corresponding flow is *volume-preserving*, i.e., if we take a region $\Omega = \Omega(0) \subset \mathbb{R}^{2d}$ and evolve it according to Eq. (1), then the volume of $\Omega(t)$ is equal to the volume of $\Omega(0)$ at all times. Indeed, the phase volume is the absolute value of the Wronskian of the fundamental solution matrix. The Liouville theorem states that the Wronskian $W(t) \equiv \det \Psi(t)$ of a linear system

$$\frac{dy}{dt} = M(t)y \ \text{ evolves according to } \frac{dW}{dt} = \text{trace}(M(t))W.$$

Furthermore, the phase flow preserves the oriented area. Consider a two-dimensional manifold $A(0)$ in $\mathbb{R}^{2d}$

$$A(0) := \{(p^0(u,v), q^0(u,v)) \mid (u,v) \in K \subset \mathbb{R}^2\}.$$

Let us denote the projection of A onto the plane (p_i, q_i) by $\pi_i(A(0))$. The oriented area of $\pi_i(A(0))$ is the surface integral

$$\texttt{or.area}(\pi_i(A(0))) = \iint_K \det \begin{bmatrix} \frac{\partial p_i^0}{\partial u} & \frac{\partial p_i^0}{\partial v} \\ \frac{\partial q_i^0}{\partial u} & \frac{\partial q_i^0}{\partial v} \end{bmatrix} du dv. \tag{6}$$

At time t, the manifold $A(0)$ is mapped onto $A(t)$, and its oriented area is given by

$$\texttt{or.area}(\pi_i(A(t))) = \iint_K \det \begin{bmatrix} \frac{\partial p_i(t)}{\partial u} & \frac{\partial p_i(t)}{\partial v} \\ \frac{\partial q_i(t)}{\partial u} & \frac{\partial q_i(t)}{\partial v} \end{bmatrix} du dv. \tag{7}$$

One can show that the sum of the oriented areas is invariant, i.e.

$$\sum_{i=1}^{d} \texttt{or.area}(\pi_i(A(t))) = \sum_{i=1}^{d} \texttt{or.area}(\pi_i(A(0))). \tag{8}$$

To show this, we introduce more compact notations.

2. Symplectic mappings

Let $x^0, y^0 \in \mathbb{R}^{2d}$ be the vectors

$$x^t := \begin{bmatrix} \frac{\partial p_1(t)}{\partial u} \\ \cdots \\ \frac{\partial p_d(t)}{\partial u} \\ \frac{\partial q_1(t)}{\partial u} \\ \cdots \\ \frac{\partial q_d(t)}{\partial u} \end{bmatrix}, \quad y^t := \begin{bmatrix} \frac{\partial p_1(0)}{\partial v} \\ \cdots \\ \frac{\partial p_d(t)}{\partial v} \\ \frac{\partial q_1(t)}{\partial v} \\ \cdots \\ \frac{\partial q_d(t)}{\partial v} \end{bmatrix}.$$

Note that x^t and y^t are tangent vectors to the manifold $A(t)$ at the point $(p(u,v)(t), q(u,v)(t))$.

Definition 2. *The $2d \times 2d$ matrix*

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{9}$$

where I is the $d \times d$ identity matrix, is called symplectic*.*

Using it, the canonical equation (1) can be rewritten as

$$\frac{d}{dt}\begin{bmatrix} p \\ q \end{bmatrix} = J^{-1}\nabla H(p,q). \tag{10}$$

Definition 3. *A linear map $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called* symplectic *if for all $x, y \in \mathbb{R}^{2d}$ the 2-form*

$$\omega(x,y) := x^T J y \quad \textit{is conserved, i.e.,} \quad \omega(Ax, Ay) = \omega(x,y). \tag{11}$$

Exercise Show that Eq. (11) is equivalent to

$$A^T J A = J. \tag{12}$$

Note that any symplectic A matrix mush have $\det A = \pm 1$. Indeed,

$$\det(A^T J A) = (\det A)^2 \det J = \det J. \quad \text{Hence} \quad (\det A)^2 = 1.$$

The geometric interpretation of the 2-form is the following. Consider the parallelogram spanned by vectors

$$x = \begin{bmatrix} x_p \\ x_q \end{bmatrix} \text{ and } y = \begin{bmatrix} y_p \\ y_q \end{bmatrix}.$$

If $d = 1$ then

$$\omega(x,y) = [x_p, x_q]\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\begin{bmatrix} y_p \\ y_q \end{bmatrix} = x_p y_q - x_q y_p$$

is the oriented area of the parallelogram spanned by vectors x and y. In higher dimensions,

$$\omega(x,y) = [x_p, x_q]\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}\begin{bmatrix} y_p \\ y_q \end{bmatrix} = \sum_{i=1}^{d} (x_p)_i (y_q)_i - (x_q)_i (y_p)_i$$

is the sum of the oriented areas of the projections of the parallelogram spanned by x and y onto the planes (p_i, q_i), $1 \le i \le d$.

Now we define the differential 2-form

$$\omega(x,y) = x^T J y = [x_p\ x_q]\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}\begin{bmatrix} y_p \\ y_q \end{bmatrix} = x_p y_q - x_q y_p = \sum_{i=1}^d \det\begin{bmatrix} \frac{\partial p_i^0}{\partial u} & \frac{\partial p_i^0}{\partial v} \\ \frac{\partial q_i^0}{\partial u} & \frac{\partial q_i^0}{\partial v} \end{bmatrix}. \tag{13}$$

In terms of the tangent vectors x^0 and y^0 the sum of the oriented areas (7) at time 0 and time t can be rewritten as

$$\sum_{i=1}^d \texttt{or.area}(\pi_i(A(0))) = \iint_K \omega(x^0, y^0)dudv, \quad \sum_{i=1}^d \texttt{or.area}(\pi_i(A(t))) = \iint_K \omega(x^t, y^t)dudv. \tag{14}$$

Definition 4. *A differential map $g : U \to \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is called symplectic if the Jacobian matrix $g'(p,q) := \begin{bmatrix} \frac{\partial g}{\partial p} & \frac{\partial g}{\partial q} \end{bmatrix}$ is everywhere symplectic, i.e., if*

$$g'(p,q)^T J g'(p,q) = J \quad \text{or} \quad \omega(g'(p,q)x, g'(p,q)y) = \omega(x,y). \tag{15}$$

Now we will show that the phase flow $\phi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ conserves the two-form if and only if its Jacobian matrix Ψ which is given by Eq. (4) is symplectic, i.e.

$$\Psi^T J \Psi = J. \tag{16}$$

First, using the chain rule, we get that

$$x^t = \begin{bmatrix} \frac{\partial p(t)}{\partial u} \\ \frac{\partial q(t)}{\partial u} \end{bmatrix} = \begin{bmatrix} \frac{\partial p(t)}{\partial p^0} & \frac{\partial p(t)}{\partial q^0} \\ \frac{\partial q(t)}{\partial p^0} & \frac{\partial q(t)}{\partial q^0} \end{bmatrix}\begin{bmatrix} \frac{\partial p^0}{\partial u} \\ \frac{\partial q^0}{\partial u} \end{bmatrix} = \Psi(t)x^0.$$

Similarly,

$$y^t = \begin{bmatrix} \frac{\partial p(t)}{\partial v} \\ \frac{\partial q(t)}{\partial v} \end{bmatrix} = \begin{bmatrix} \frac{\partial p(t)}{\partial p^0} & \frac{\partial p(t)}{\partial q^0} \\ \frac{\partial q(t)}{\partial p^0} & \frac{\partial q(t)}{\partial q^0} \end{bmatrix}\begin{bmatrix} \frac{\partial p^0}{\partial v} \\ \frac{\partial q^0}{\partial v} \end{bmatrix} = \Psi(t)y^0.$$

Therefore, for the 2-form we get

$$\omega(x^t, y^t) = (x^t)^T J y^t = (x^0)^T \Psi^T J \Psi y^0 = \omega(\Psi(t)x^0, \Psi(t)y^0).$$

Theorem 1. *(Poincare, 1899) Let $H(p,q)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed t, the flow ϕ_t is a symplectic transformation wherever it is defined.*

Proof. The derivative of the flow ϕ_t with respect to the initial data is the matrix $\Psi(t)$ defined by Eq. (4). Now take the time derivative of the left-hand side of Eq. (15):

$$\begin{aligned} \frac{d}{dt}\left(\Psi^T J \Psi\right) &= \left(\frac{d}{dt}\Psi\right)^T J\Psi + \Psi^T J\left(\frac{d}{dt}\Psi\right) \\ &= \Psi^T\left(J^{-1}\nabla^2 H\right)^T J\Psi + \Psi^T J J^{-1}\nabla^2 H\Psi = -\Psi^T\nabla^2 H\Psi + \Psi^T\nabla^2 H\Psi = 0. \end{aligned}$$

Here we took into account that $J^T = -J$, $J^{-T} = J$, and $J^{-T}J = -I$. Since $\Psi(0) = I$, at $t = 0$ we have $\Psi(0)^T J\Psi(0) = J$. Therefore, for all t, $\Psi^T(t)J\Psi(t) = J$. □

In summary, we have established that the phase flow ϕ_t associated with the canonical equations (1) conserve the following quantities:

- the Hamiltonian $H(p, q)$,
- the phase volume
$$\int_\Omega \det \Psi(t) dp^0 dq^0,$$
- the 2-form
$$\omega(x^t, y^t) = \omega(\Psi(t)x^0, \Psi(t)y^0).$$

3. Symplectic integrators

In this section, our goal will be to determine which methods for IVPs for ODEs are symplectic, i.e., they perform a symplectic mapping at each time step for every h. The precise definition is the following.

Definition 5. *A one-step method is called symplectic if for every smooth Hamiltonian $H(p, q)$ and for every step size h the mapping*

$$\psi_h : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad \psi_h : \ (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$$

is symplectic. This means that its Jacobian matrix

$$\Psi_h := \left[\begin{array}{cc} \frac{\partial \psi_h(p_n,q_n)}{\partial p_n} & \frac{\partial \psi_h(p_n,q_n)}{\partial q_n} \end{array} \right]$$

is symplectic for all h, i.e. $\Psi_h^T J \Psi_h = J$ for all h.

The following theorem, discovered independently by F. Lasagni (1988), J.M. Sanz-Sena (1988), and Y. B. Suris (1989) characterizes the class of all symplectic Runge-Kutta methods.

Theorem 2. *If the elements of the Butcher array of a Runge-Kutta method satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \ \text{for all } 1 \le i, j \le s, \tag{17}$$

then the Runge-Kutta method is symplectic.

Its proof is found in e.g. [1] and in [4].

Remark It has been proven by F. Lasagni, that for the class of irreducible RK methods [2] Theorem 2 provides also a necessary condition for symplecticity.

Eq. (17) implies that symplectic RK methods must be implicit. Indeed, take $i = j$. For ERK, $a_{ii} = 0$ for all i. then Eq. (17) implies that $b_i = 0$ for all i while for any consistent RK $\sum_i b_i = 1$.

We will consider two families of symplectic methods:

- s-stage Gauss collocation methods of orders $2s$,
- symmetric splitting methods.

3.1. **Example: Simple Harmonic Oscillator.** In this Section, we work out some details on the example of a simple 1D harmonic oscillator with the Hamiltonian given by

$$H(p,q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \tag{18}$$

where ω is the angular frequency of the oscillations. The canonical equation for this system is linear which makes the application of implicit methods easy:

$$\frac{d}{dt}\begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} 0 & -m\omega^2 \\ m^{-1} & 0 \end{bmatrix}\begin{bmatrix} p \\ q \end{bmatrix}. \tag{19}$$

For brevity, we denote the matrix in the right-hand side of Eq. (19) by A:

$$A := \begin{bmatrix} 0 & -m\omega^2 \\ m^{-1} & 0 \end{bmatrix}.$$

We have demonstrated using the matlab program `symplectic_demo.m` that both Forward and Backward Euler methods as well as the 2nd order Runge-trapezoidal method are not appropriate integrators while the implicit midpoint rule preserves the phase volume. In order to understand what is wrong with the first three methods and what is special about the implicit midpoint rule, we will work out each of them.

Forward Euler. Applying the Forward Euler method to Eq. (19) we get

$$u_{n+1} = u_n + hAu_n = (I + hA)u_n, \text{ i.e. } \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} 1 & -hm\omega^2 \\ hm^{-1} & 1 \end{bmatrix}\begin{bmatrix} p_n \\ q_n \end{bmatrix}.$$

Hence for the Forward Euler method, the matrix

$$\Psi_h = \begin{bmatrix} 1 & -hm\omega^2 \\ hm^{-1} & 1 \end{bmatrix}. \quad \det\Psi_h = 1 + h^2\omega^2 > 1.$$

Therefore, Ψ_h is not symplectic. Furthermore, $|\det\Psi_h|$ is the factor by which the phase volume is changing at every step. As we see, the phase volume increases by the factor of $1 + h^2\omega^2$ at each step.

Backward Euler. Applying the Backward Euler method to Eq. (19) we get

$$u_{n+1} = u_n + hAu_{n+1}. \text{ Hence} u_{n+1} = (I - hA)^{-1}u_n.$$

Writing this explicitly, we get

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = \begin{bmatrix} 1 & hm\omega^2 \\ -hm^{-1} & 1 \end{bmatrix}^{-1}\begin{bmatrix} p_n \\ q_n \end{bmatrix} = \frac{1}{1+h^2\omega^2}\begin{bmatrix} 1 & -hm\omega^2 \\ hm^{-1} & 1 \end{bmatrix}\begin{bmatrix} p_n \\ q_n \end{bmatrix}.$$

Hence for the Backward Euler method, the matrix

$$\Psi_h = \frac{1}{1+h^2\omega^2}\begin{bmatrix} 1 & -hm\omega^2 \\ hm^{-1} & 1 \end{bmatrix}. \quad \det\Psi_h = \frac{1}{1+h^2\omega^2} < 1.$$

Therefore, Ψ_h is not symplectic and the phase volume decreases by the factor of $1 + h^2\omega^2$ at each step.

Runge-Trapezoidal. Applying the Runge-trapezoidal method

$$
\begin{aligned}
k_1 &= f(t_n, u_n), \\
k_2 &= f(t_n + h, u_u + hk_1), \qquad (20)\\
u_{n+1} &= u_n + \tfrac{1}{2}h(k_1 + k_2),
\end{aligned}
$$

to Eq. (19) we get

$$u_{n+1} = u_n + \tfrac{1}{2}h(A + A(I + hA))u_n = (I + hA + \tfrac{1}{2}h^2A^2)u_n.$$

Hence for the Backward Euler method, the matrix

$$\Psi_h = (I + hA + \tfrac{1}{2}h^2A^2) = \begin{bmatrix} 1 & -hm\omega^2 \\ hm^{-1} & 1 \end{bmatrix} - \frac{\omega^2h^2}{2}I = \begin{bmatrix} 1 - \frac{1}{2}h^2\omega^2 & -hm\omega^2 \\ hm^{-1} & 1 - \frac{1}{2}h^2\omega^2 \end{bmatrix}.$$

Calculating its determinant we get:

$$\det \Psi_h = 1 - h^2\omega^2 + \tfrac{1}{4}h^4\omega^4 + h^2\omega^2 = \left(1 + \frac{h^2\omega^2}{2}\right)^2 > 1.$$

Therefore, Ψ_h is not symplectic and the phase volume increases by the factor of $1 + h^2\omega^2 + \frac{1}{4}h^4\omega^4$ at each step. Note that the Runge-trapezoidal method leads to ever faster growth of the phase volume than the Forward Euler with the same step size.

Implicit Midpoint Rule. The implicit trapezoidal rule is given by

$$
\begin{aligned}
k_1 &= f(t_n + \tfrac{1}{2}h, u_n + \tfrac{1}{2}hk_1), \qquad (21)\\
u_{n+1} &= u_n + hk_1,
\end{aligned}
$$

Applying it to Eq. (19) we get

$$k_1 = A(u_n + \tfrac{1}{2}hk_1).$$

Hence,

$$k_1 = (I - \tfrac{1}{2}hA)^{-1}Au_n, \quad \text{and} \quad u_{n+1} = (I + h((I - \tfrac{1}{2}hA)^{-1}A))u_n.$$

Therefore, the matrix Ψ_h is

$$
\begin{aligned}
\Psi_h &= (I + h((I - \tfrac{1}{2}hA)^{-1}A)) \\
&= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{h}{1 + \frac{h^2\omega^2}{4}} \begin{bmatrix} 1 & -\frac{1}{2}mh\omega^2 \\ \frac{1}{2}hm^{-1} & 1 \end{bmatrix} \begin{bmatrix} 0 & -m\omega^2 \\ m^{-1} & 0 \end{bmatrix} \\
&= \frac{1}{1 + \frac{h^2\omega^2}{4}} \begin{bmatrix} 1 - \frac{1}{4}h^2\omega^2 & -hm\omega^2 \\ hm^{-1} & 1 - \frac{1}{4}h^2\omega^2 \end{bmatrix}.
\end{aligned}
$$

Calculating its determinant we get:

$$\det \Psi_h = \frac{1}{\left(1 + \frac{h^2\omega^2}{4}\right)^2} \left(1 - \frac{h^2\omega^2}{2} + \frac{h^4\omega^4}{16} + h^2\omega^2\right) = 1.$$

Therefore, the necessary symplecticity condition holds. Now we verify that Ψ_h is symplectic:

$$\Psi_h^T J \Psi_h = \left(1+\frac{h^2\omega^2}{4}\right)^{-2} \begin{bmatrix} 1-\frac{1}{4}h^2\omega^2 & hm^{-1} \\ -hm\omega^2 & 1-\frac{1}{4}h^2\omega^2 \end{bmatrix} \begin{bmatrix} hm^{-1} & 1-\frac{1}{4}h^2\omega^2 \\ \frac{1}{4}h^2\omega^2-1 & hm\omega^2 \end{bmatrix} = J.$$

Now we will check whether the implicit midpoint rule conserves the Hamiltonian. The Hamiltonian given by Eq. (29) can be rewritten as a quadratic form:

$$H(p,q) = \frac{1}{2}[p\ q] \begin{bmatrix} m^{-1} & 0 \\ 0 & m\omega^2 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix}. \tag{22}$$

We will devise a bit more general procedure. We look for a diagonal matrix such that the corresponding quadratic form is conserved by the implicit midpoint rule applied to Eq. (19), i.e.

$$[p_{n+1}\ q_{n+1}] \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = [p_n\ q_n]\psi_h^T \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \Psi_h \begin{bmatrix} p_n \\ q_n \end{bmatrix} = [p_n\ q_n] \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} p_n \\ q_n \end{bmatrix}.$$

Therefore, we need to find a and b such that

(23)

$$\left(1+\frac{h^2\omega^2}{4}\right)^{-2} \begin{bmatrix} 1-\frac{1}{4}h^2\omega^2 & -hm\omega^2 \\ hm^{-1} & 1-\frac{1}{4}h^2\omega^2 \end{bmatrix} \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} 1-\frac{1}{4}h^2\omega^2 & hm^{-1} \\ -hm\omega^2 & 1-\frac{1}{4}h^2\omega^2 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}.$$

We calculate the left hand side of Eq. (23)

(24)

$$\left(1+\frac{h^2\omega^2}{4}\right)^{-2} \begin{bmatrix} a\left(1-\frac{h^2\omega^2}{4}\right)^2 + bh^2m^{-2} & \left(1-\frac{h^2\omega^2}{4}\right)(-ahm\omega^2+bhm^{-1}) \\ \left(1-\frac{h^2\omega^2}{4}\right)(-ahm\omega^2+bhm^{-1}) & ah^2m^2\omega^4 + b\left(1-\frac{h^2\omega^2}{4}\right)^2 \end{bmatrix}$$

Setting the off-diagonal entries of the left-hand side of the matrix (24) to zero we get that a and b are related via

$$am\omega^2 = bm^{-1}. \quad \text{Hence} \quad am^2\omega^2 = b \text{ and } b2m^{-2} = a\omega^2. \tag{25}$$

Assuming this relationship between a and b holds we plug it in Eq. (24) and get:

$$\left(1+\frac{h^2\omega^2}{4}\right)^{-2} \begin{bmatrix} a\left(1+\frac{h^2\omega^2}{4}\right) & 0 \\ 0 & b\left(1+\frac{h^2\omega^2}{4}\right) \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}.$$

Noting that the coefficients of the matrix in Eq. (22) satisfy Eq. (25) we conclude that the implicit midpoint rule preserves the Hamiltonian.

Exercise (1) The Stoermer-Verlet method for integration of Hamiltonian systems of the form

$$\frac{dp}{dt} = -\nabla_q H(p,q), \quad \frac{dq}{dt} = \nabla_p H(p,q) \text{ or, equivalently, } \frac{d}{dt}\begin{bmatrix} p \\ q \end{bmatrix} = J^{-1}\nabla H(p,q)$$

is given by

$$p_{n+1/2} = p_n - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_n), \tag{26}$$

$$q_{n+1} = q_n + \frac{h}{2}\left(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1})\right), \tag{27}$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_{n+1}). \tag{28}$$

Rewrite this scheme for the case of a separable Hamiltonian, i.e., a Hamiltonian of the form $H(p, q) = T(p) + U(q)$. Show that it is an explicit scheme in this case. This scheme is also known as *velocity Verlet*. Apply the obtained scheme to the simple harmonic oscillator in 1D with the Hamiltonian

$$H(p, q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}. \tag{29}$$

Rewrite the resulting equations in the form

$$\begin{bmatrix} p_{n+1} \\ q_{n+1} \end{bmatrix} = A \begin{bmatrix} p_n \\ q_n \end{bmatrix},$$

where A is a 2×2 matrix that you need to find.

(2) Show that the linear map given by the found matrix A is symplectic, i.e., $A^T J A = J$.

(3) The velocity Verlet scheme does not conserve the Hamiltonian given by Eq. (29). Prove that it conserves the so called *shadow Hamiltonian* given by

$$H^* = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \left(1 - \left(\frac{\omega h}{2}\right)^2\right). \tag{30}$$

This problem was inspired by [5], see slides 16 - 24.

3.2. **Gauss Collocation Methods.**

3.2.1. *Gauss-Legendre Quadrature.* Gauss collocation methods are Runge-Kutta methods with s-stages of order $2s$ where the numbers c_1, ..., c_s are chosen to be the roots of the shifted Legendre polynomial of degree s to the interval $[0, 1]$. These roots a choice of weights w_1, ..., w_s such that the quadrature rule

$$I(f) := \int_0^1 f(t)dt \approx Q(f) := \sum_{i=1}^{s} w_i f(c_i) \tag{31}$$

is exact if $f(t)$ is a polynomial of degree less or equal to $2s-1$. Indeed, the shifted Legendre polynomials are orthogonal with respect to the inner product

$$(f, g) = \int_0^1 f(t)g(t)dt.$$

The first five polynomials and their roots are

$$p_0(t) = 1, \tag{32}$$

$$p_1(t) = 2t - 1, \quad \text{roots}: \quad c_1 = \tfrac{1}{2} \tag{33}$$

$$p_2(t) = 6t^2 - 6t + 1, \quad \text{roots}: \quad c_1 = \tfrac{1}{2} - \tfrac{\sqrt{3}}{6},\ c_2 = \tfrac{1}{2} + \tfrac{\sqrt{3}}{6} \tag{34}$$

$$p_3(t) = 20t^3 - 30t^2 + 12t - 1, \tag{35}$$

$$\text{roots}: \quad c_1 = \tfrac{1}{2} - \tfrac{\sqrt{15}}{10},\ c_2 = \tfrac{1}{2},\ c_3 = \tfrac{1}{2} + \tfrac{\sqrt{15}}{10},$$

$$p_4(t) = 70t^4 - 140t^3 + 90t^2 - 20t + 1, \tag{36}$$

$$\text{roots}: \quad c_1 = \frac{1}{2}\left(1 - \sqrt{\frac{15 + 2\sqrt{30}}{35}}\right),\ c_2 = \frac{1}{2}\left(1 - \sqrt{\frac{15 - 2\sqrt{30}}{35}}\right),$$

$$c_3 = \frac{1}{2}\left(1 + \sqrt{\frac{15 - 2\sqrt{30}}{35}}\right),\ c_4 = \frac{1}{2}\left(1 + \sqrt{\frac{15 + 2\sqrt{30}}{35}}\right). \tag{37}$$

The weights of the quadrature rule (31) are defined so that the rule is exact on all polynomials of degree $\leq s-1$. Let $f(t)$ be a polynomial of degree $\leq s-1$. Then it coincides with the interpolating polynomial at the points c_1, ..., c_s. Hence $f(t)$ can be written in the form of Lagrange's interpolant

$$f(t) = \sum_{i=1}^{s} f(c_i) l_i(t), \quad \text{where} \quad l_i(t) := \prod_{k \neq i} \frac{(t - c_k)}{(c_i - c_k)}.$$

Integrating $f(t)$ we get

$$\int_0^1 f(t)dt = \sum_{i=1}^{s} f(c_i) w_i, \quad \text{where} \quad w_i := \int_0^1 l_i(t)dt.$$

Now we show that this quadrature rule is exact on all polynomials of degree $\leq 2s-1$.

Theorem 3. *If c_i, $i = 1, \ldots, s$ are the roots of the shifted Legendre polynomial $p_s(t)$ and the weights $w_i = \int_0^1 \prod_{k \neq i} \frac{(t-c_k)}{(c_i-c_k)} dt$, then for all polynomials $f(t)$ of degree $\leq 2s-1$, the Gaussian quadrature is exact, i.e.,*

$$I(f) = \int_0^1 f(t)dt = Q(t) = \sum_{i=1}^{s} f(c_i) w_i.$$

Proof. The key idea in the proof of this fact is division of the polynomial $f(t)$ by the polynomial $p_s(t)$. Let $f(t)$ be a polynomial of degree $\leq 2s-1$. Then

$$f(t) = p_s(t)q(t) + r(t), \quad \text{where} \quad q(t), r(t) \in \mathbb{P}_{s-1},$$

i.e, $q(t)$ and $r(t)$ are polynomials of degree $\leq\ s-1$. By construction, the quadrature rule $Q(f)$ is exact for $r(t)$. Then we have

$$I(f) = I(qp_s + r) = \int_0^1 q(t)p_s(t)dt + \int_0^1 r(t)dt = \int_0^1 r(t)dt = I(r) = Q(r).$$

Here we have used the fact that the polynomial $p_s(t)$ is orthogonal to all polynomials of degree $\leq\ s-1$. We continue:

$$I(f) = Q(r) = \sum_{i=1}^{s} w_i r(c_j) = \sum_{i=1}^{s} w_s(p_s(c_i)q(c_i) + r(c_i)) = Q(f).$$

Here we have used the fact that c_i's are the zeros of $p_s(t)$.

It remains to prove that the quadrature rule is not exact for all polynomials of degree $2s$. Let us make the polynomial $p_s(t)$ of norm 1. Let $f(t)$ be a polynomial of degree $2s$. Then $q(t)$ is of degree n and $r(t)$ is of degree $\leq\ s-1$. On one hand,

$$I(f) = I(qp_s + r) = \int_0^1 q(t)p_n(t)dt + \int_0^1 r(t)dt = Q(r) + (q, p_s).$$

Note that $(q, p_s) \neq 0$. On the other hand,

$$Q(f) = Q(p_s q + r) = Q(r),$$

as c_i's are the zeros of $p_s(t)$. Hence $I(f) \neq Q(f)$ for all polynomials f of degree $2s$. ☐

3.2.2. *Construction of Gauss collocation methods.* Let u be the numerical solution. We define the *collocation* (or interpolation) polynomial $p(t)$ on the interval $[0, 1]$ so that

$$p(0) = u_n,$$

$$p'(c_i) = hf(t_n + c_i h, p(c_i)), \tag{38}$$

$$p(1) = u_{n+1}. \tag{39}$$

Now let us define the coefficients of the implicit Runge-Kutta method by

$$a_{ij} = \int_0^{c_i} l_j(t)dt, \quad b_i = \int_0^1 l_i(t)dt, \quad 1 \leq i, j \leq s. \tag{40}$$

The equivalence of the methods defined by Eqs. (38) and (40) was shown by Guillou& Soule, 1969, and by Wright, 1970. Let us show it. Set

$$hk_i := p'(c_i).$$

Then the polynomial $p'(t)$ is given by the Lagrange interpolant

$$p'(t) = h\sum_{j=1}^{s} k_j l_j(t). \tag{41}$$

Integrating Eq. (41) we get

$$\int_0^{c_i} p'(t)dt = p(c_i) - p(0) = h\sum_{j=1}^{s} k_j \int_0^{c_i} l_j(t)dt,$$

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

Table 1. Hammer-Hollingsworth, IRK, order 4

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9}+\frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Table 2. Kunzmann-Butcher, IRK, order 6

and

$$\int_0^1 p'(t)dt = p(1) - p(0) = h\sum_{j=1}^{s} k_j \int_0^1 l_j(t)dt.$$

Therefore, the polynomial $p(t)$ satisfies

$$p(c_i) = p(0) + h\sum_{j=1}^{s} a_{ij}k_j, \quad p(1) = p(0) + h\sum_{i=1}^{s} k_i b_i.$$

Therefore, we have

$$k_i = f(t_n + c_i h, u_n + h\sum_{j=1}^{s} a_{ij}k_j), \quad u_{n+1} = u_n + \sum_{i=1}^{s} b_i k_i,$$

i.e., the collocation conditions (38) imply an implicit Runge-Kutta method with coefficients (40) and vice versa.

One can show that Gauss collocation methods with s stages have order $2s$. For $s = 1$, the corresponding method is the implicit trapezoidal rule. For $s = 2$, the corresponding method is the Hammer-Hollingsworth method of order 4 with the Butcher array

For $s = 3$ and 4, the corresponding methods are Kunzmann and Butcher methods of orders 6 and 8 respectively. Here we will write out only the Butcher array for $s = 3$

3.2.3. *Symplectic properties of Gauss collocation methods.* It is shown in [4] that the Gauss collocation methods are symplectic for all s. Furthermore, they preserve quadratic forms, i.e., for any symmetric $2d \times 2d$ matrix M, we have:

$$u_n := \begin{bmatrix} p_n \\ q_n \end{bmatrix}, \quad u_n^T M u_n = u_{n+1}^T M u_{n+1}.$$

Therefore, if the Hamiltonian is quadratic as it is for the simple harmonic oscillator, it is preserved by the Gauss collocation methods. We have shown this explicitly for the implicit midpoint rule.

3.3. **Symmetric Splitting Methods.** It is easy to see that the phase flow ϕ_t of an autonomous equation $\frac{dy}{dt} = f(y)$ satisfies

$$\phi_{-t}^{-1} = \phi_t.$$

This means that if we evolve a region Ω_0 of the phase space according to $\frac{dy}{dt} = f(y)$ for time t and obtain the region Ω_t and then evolve it for time t according to $\frac{dy}{dt} = -f(y)$, we end up with the initial region Ω_0.

However, the mapping Ψ_h done by the numerical method does not necessarily have the same property. This motivates the following definition.

Definition 6. *The adjoint method Ψ_h^* of a method Ψ_h is the inverse map of the original method with reversed time step $-h$, i.e.,*

$$\Psi_h^* := \Psi_{-h}^{-1}.$$

In other words, $u_1 = \Psi_h^*(u_0)$ is implicitly defined by $\Psi_{-h}(u_1) = u_0$. A method for which $\Psi_h^* = \Psi_h$ is called symmetric.

The adjoint method satisfies usual properties:

$$(\Psi_h^*)^* = \Psi_h \quad \text{and} \quad (\Psi_h \circ \Phi_h)^* = \Phi_h^* \circ \Psi_h^*.$$

Exercise (i) Show that the Forward and Backward Euler methods are mutually adjoint. (ii) Show that the implicit midpoint rule is symmetric.

Now we will design symmetric methods using the splitting idea. We split the phase flow ϕ_t of the canonical equations (1) with a separable Hamiltonian

$$H(p, q) = T(p) + U(q)$$

into the"kick" flow ϕ_t^{kick} where q is frozen while p is changed, and the "drift" flow ϕ_t^{drift} where p is frozen and q is changing. The corresponding split of the canonical equations is given by:

$$\text{Drift}: \begin{cases} \frac{dp}{dt} = 0 \\ \frac{dq}{dt} = \nabla_p T(p), \end{cases} \qquad \text{Kick}: \begin{cases} \frac{dp}{dt} = -\nabla_q U(q), \\ \frac{dq}{dt} = 0. \end{cases}$$

Then the symplectic Euler (see [4], Eq. (1)) is composed as

$$\phi_h^{drift} \circ \phi_h^{kick},$$

while the Stoermer-Verlet (see [4], Eq. (2)) is composed as

$$\phi_{h/2}^{kick} \circ \phi_h^{drift} \circ \phi_{h/2}^{kick}.$$

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