Chapter 16

Symplectic Flows and Maps and Volume Preservation

Main concepts: Liouville's equation, cat wash cycles, volume preservation, symplectic maps, symplectic RK methods, symplectic splitting methods

16.1 Hamiltonian Systems

Hamiltonian systems are pervasive in chemical and physical simulation. These systems arise at very large scales (celestial mechanics, cosmology) and at small scales (atomic and molecular simulation).

Suppose that the *configuration* of some (mechanical) system with d degrees of freedom can be represented by a set of d real numbers $q = (q_1, \ldots, q_d)^T$. (Think of the positions of all nine planets and the sun in our solar system. In some reference frame, the positions are specified by three real numbers for each body, so $d = 3 \times 10 = 30$.)

The motion of the system is given by $q(t)$, a curve in $\mathbb{R}^d$.

Lagrange's theory of mechanical systems is based on two real (scalar) valued functions, the kinetic and potential energies

$$T(q(t), \dot{q}(t)), \quad U(q(t)).$$

The Lagrangian L is the difference of these

$$L(q, \dot{q}) = T - U,$$

and Lagrange's equations of motion are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right) = \frac{\partial L}{\partial q}(q, \dot{q}).$$

Hamilton's equations of motion are derived from Lagrange's equations by introducing a new variable

$$p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}), \quad \text{i.e.,} \quad p_i = \frac{\partial L}{\partial \dot{q}_i}$$

and the *Hamiltonian*

$$H(q, p) = p^T \dot{q} - L(q, \dot{q}), \tag{16.1}$$

where it is implied that the defining relation for p above is invertible for $\dot{q}$ for every q, so that we can express

$$\dot{q} = \dot{q}(q, p).$$

Hamilton's equations of motion have the antisymmetric form

$$\dot{q}_i = \frac{\partial H(q,p)}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H(q,p)}{\partial q_i}, \tag{16.2}$$

or simply

$$\dot{q} = \frac{\partial H(q,p)}{\partial p}, \quad \dot{p} = -\frac{\partial H(q,p)}{\partial q}.$$

We can check that these equations are consistent with Lagrange's equations by differentiating (16.1)

$$\frac{\partial H}{\partial p} = \dot{q} + p^T \frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial p} = \dot{q}, \qquad \frac{\partial H}{\partial q} = p \frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} = -\frac{\partial L}{\partial q} = -\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = -\dot{p}$$

Example. The equation for the mathematical pendulum is $\ddot{q} = -\sin(q)$. The kinetic energy is given by $T(\dot{q}) = \frac{\dot{q}^2}{2}$ and the potential energy by $U(q) = -\cos q$. The Lagrangian is $L(q,\dot{q}) = \frac{\dot{q}^2}{2} + \cos q$, and Lagrange's equation is

$$\frac{d}{dt}\dot{q} = -\sin q.$$

For Hamilton's formulation we find

$$p = \dot{q}, \qquad H = p\dot{q} - L = p^2 - (\frac{p^2}{2} + \cos q) = \frac{p^2}{2} - \cos q$$

with equations of motion

$$\dot{q} = \frac{\partial H}{\partial p} = p, \qquad \dot{p} = -\frac{\partial H}{\partial q} = -\sin q.$$

Example. A particularly important class of Hamiltonians is the *N-body problem* (here formulated with $q_i \in \mathbb{R}^d$, i.e. the full configuration space is of dimension Nd):

$$H(q,p) = \sum_{i=1}^{N} \frac{\|p_i\|^2}{2m_i} + V(q_1, q_2, \ldots, q_N).$$

$m_1, m_2, \ldots, m_N$ are the masses of the N bodies, and V is a potential energy function that describes their interactions. This type of model is routinely used in drug design and materials modelling.

The Hamiltonian is a first integral of (16.2). This is easily checked

$$\frac{dH}{dt} = \sum_i \frac{\partial H}{\partial q_i}\dot{q}_i + \frac{\partial H}{\partial p_i}\dot{p}_i = \sum_i \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i}(-\frac{\partial H}{\partial q_i}) = 0.$$

In most cases, this first integral can be identified with the energy of the system, so that its invariance corresponds to the physical principle of conservation of total energy. Indeed, one often finds $H = T(q,p) + U(q)$.

Sometimes we write (16.2) in the form (1.13) by defining $y = (q_1, \ldots, q_d, p_1, \ldots p_d)^T \in \mathbb{R}^{2d}$, whence

$$\frac{dy}{dt} = J\nabla H(y),$$

with the skew-symmetric matrix J defined by

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{16.3}$$

where I is the identity matrix of dimension d. Here, the conservation of H is immediate from the skew-gradient form introduced in Chapter 14.

16.2 Divergence-Free Vector Fields

Another category of vector field with interesting dynamical features are those with zero divergence. Let $f = f(y)$, $f : \mathbf{R}^d \to \mathbf{R}^d$ be a vector field. Recall that the divergence of f is

$$\mathrm{div} f = \frac{\partial}{\partial y_1} f_1 + \frac{\partial}{\partial y_2} f_2 + \ldots + \frac{\partial}{\partial y_d} f_d.$$

It happens in certain situations that $\mathrm{div} f \equiv 0$. As an illustration, the vector field of the system

$$\begin{aligned} \frac{dx}{dt} &= h_1(y) \\ \frac{dy}{dt} &= h_2(x) \end{aligned}$$

is clearly divergence free, as is the following one:

$$\begin{aligned} \frac{dx}{dt} &= x + h_1(y) \\ \frac{dy}{dt} &= h_2(x) - y \end{aligned}$$

A very important special case of divergence-free vector fields are those associated to Hamiltonian systems, since, from (16.2), we find

$$\mathrm{div} f = \frac{\partial}{\partial q_1}\frac{\partial H}{\partial p_1} + \frac{\partial}{\partial q_2}\frac{\partial H}{\partial p_2} + \ldots + \frac{\partial}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial}{\partial p_1}\frac{\partial H}{\partial q_1} - \frac{\partial}{\partial p_2}\frac{\partial H}{\partial q_2} - \ldots - \frac{\partial}{\partial p_k}\frac{\partial H}{\partial q_k}$$

which vanishes due to equality of mixed partial derivatives.

The remarkable feature of divergence-free vector fields is that the flow maps associated to these vector fields are volume preserving.

16.2.1 Volume-preserving flows and Liouville's theorem

Recall the change of variables theorem tells us that, if we are given a map $\Phi : \mathbf{R}^d \to \mathbf{R}^d$, and a suitable domain $V \subset \mathbf{R}^d$, then

$$\mathrm{vol}\ V = \int_V d\mathbf{x}, \qquad \mathrm{vol}\ \Phi(V) = \int_V \left|\det \frac{\partial \Phi}{\partial \mathbf{x}}\right| d\mathbf{x} = \int_V |\det M|\ d\mathbf{x}$$

where $M = \Phi'$ is the Jacobian of Φ. It follows that the map Φ preserves volume provided $|\det M| = 1$. We would like to examine the Jacobian determinant of the flow map of a system. The flow map itself satisfies

$$\frac{d}{dt}\Phi_t(y) = f(\Phi_t(y))$$

On each side of this equation, we have a vector valued function of y and t; compute the Jacobian matrix of each side, and swap the order of differentiation with respect to t and y:

$$\frac{d}{dt}\Phi_t'(y) = f'(\Phi_t(y))\Phi_t'(y)$$

Or $dM/dt = f'(\Phi_t(y))M$. Assuming M is invertible, multiply on the right on both sides by M^{-1}. Compute the trace of each side:

$$\mathrm{tr}(\dot{M}M^{-1}) = \mathrm{tr}[f'(\Phi_t(y))]$$

It is a short exercise to show that $\mathrm{tr} f' = \mathrm{div} f$. *Jacobi's formula* for the derivative of a determinant gives

$$\mathrm{tr}(\dot{M}M^{-1}) = \frac{\frac{d}{dt}\det M}{\det M}$$

Since $M(0) = \Phi_0'(y) = I$, it follows that

$$\det \Phi_t'(y) \equiv 1$$

Thus we have proved the following theorem:

Theorem 16.2.1 (Liouville's Theorem) *Let a vector field f be divergence free. Then Φ_t is a volume preserving map (for all t).*

In particular, all Hamiltonian flow maps preserve volume in phase space. This is a sort of (qualitative) invariant property, but not a first integral.

16.2.2 Volume-preserving numerical methods

We now ask if there are numerical methods that preserve volume in phase space, i.e. mimicking the corresponding property for the flow map.

The obvious requirement for such a numerical method Ψ_h is that

$$\text{div} f = 0 \Rightarrow \det(\Psi_h') = 1.$$

Let us start with Euler's method, $y_{n+1} = y_n + hf(y_n)$. The Jacobian matrix of the flow map is

$$\Psi_h' = I + hf'(y_n)$$

which only has unit determinant in extraordinary situations. For example, the determinant is one for Euler's method applied to the following example:

$$\begin{aligned} \frac{dx}{dt} &= 0 \\ \frac{du}{dt} &= f(x) \end{aligned}$$

However, it is *not* one when Euler's method is applied to the harmonic oscillator:

$$\begin{aligned} \frac{dx}{dt} &= u \\ \frac{du}{dt} &= -x \end{aligned}$$

On the other hand, there are certain methods that do conserve volume, sometimes under special conditions.

16.3 Symplectic Structure

It can be shown that Hamiltonian flows possess an even deeper property than volume preservation: the flow map is a symplectic map. Given any two vectors ξ and η in $\mathbb{R}^{2d}$, define the quantity

$$\omega_i(\xi, \eta) = \xi_i \eta_{d+i} - \xi_{d+i}\eta_i.$$

This quantity can be given a geometric interpretation. The vectors ξ and η span a 2-dimensional parallelogram in $\mathbb{R}^{2d}$. The quantity ω_i is the *oriented area of the orthogonal projection of this parallelogram on the (q_i, p_i) plane*. Here, the word *oriented* means that the sign of ω_i may be either positive or negative, based on the 'right-hand rule' convention for vector multiplication.

Next, define the bilinear form

$$\omega(\xi, \eta) = \sum_{i=1}^{d} \omega_i(\xi, \eta).$$

which is the sum of the projected oriented areas of ξ and η. This form can also be written, making use of the matrix J from (16.3), as

$$\omega(\xi, \eta) = \xi^T J \eta$$

A *symplectic matrix* A is one that preserves the bilinear form ω in the sense that

$$\omega(A\xi, A\omega) = \omega(\xi, \omega).$$

In other words,

$$\xi^T A^T J A \eta = \xi^T J \eta.$$

Since this must hold for arbitrary vectors ξ and η in $\mathbb{R}^2 d$, it follows that the condition for a matrix to be symplectic is

$$A^T J A = J.$$

Similarly, a map $g(y) : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is said to be a *symplectic transformation* if its Jacobian $g'(y)$ satisfies

$$g'(y)^T J g'(y) = J.$$

The fundamental property of Hamiltonian systems is that the flow map is a symplectic transformation:

$$(\Phi_t')^T J \Phi_t' = J$$

Such a map is said to be *symplectic.* To see that this holds, recall that, with $M = \Phi_t'$,

$$\dot{M} = f'(\Phi_t(y))M$$

In the case of a Hamiltonian system, we have

$$f(y) = J\nabla H(y)$$

hence

$$f'(y) = J H_{yy},$$

with H_{yy} the (symmetric) Hessian matrix of second derivatives $\frac{\partial^2 H}{\partial y_i \partial y_j}$, and

$$\dot{M} = J H_{yy} M$$

Differentiate the matrix

$$R = M^T J M$$

with respect to time:

$$\dot{R} = \dot{M}^T J M + M^T J \dot{M}$$

so

$$\dot{R} = M^T H_{yy} J^T J M + M^T J J H_{yy} M$$

Noting that $J^2 = -I$ and $J^T J = I$, we have

$$\dot{R} = M^T H_{yy} M - M^T H_{yy} M = 0.$$

Since $M(0) = \Phi_0'(y) = I$, we must have

$$R(0) = M(0)^T J M(0) = J$$

Since the matrix R is constant for all time, we must have the desired identity

$$M^T J M = J.$$

16.4 Symplectic Integrators

It is possible to verify by direct computation that certain numerical methods are symplectic whenever the differential equation being solved is Hamiltonian; in general this means checking that

$$(\Psi_h')^T J \Psi_h' = J.$$

Within the class of Runge-Kutta methods, it can be shown that the subclass of symplectic methods is equivalent to the subsclass of methods that conserve arbitrary quadratic invariants. That is, the methods which satisfy (14.2). In particular, the implicit midpoint rule is symplectic.

An especially fruitful means of constructing symplectic integrators is considered next.

16.4.1 Symplectic splitting methods

The idea of splitting has many practical uses. In some instances it allows us to construct methods with some desirable property. In this section we illustrate this for Hamiltonian systems, where splitting may be used to construct symplectic integrators.

Consider a Hamiltonian system

$$\frac{dy}{dt} = J\nabla H(y), \qquad H(y) = H_1(y) + H_2(y)$$

and suppose the flows

$$\frac{dy}{dt} = J\nabla H_1(y), \qquad \frac{dy}{dt} = J\nabla H_2(y)$$

can be exactly integrated. Define the corresponding flow maps $\phi_{t,1}(y)$ and $\phi_{t,2}(y)$. Since the exact solution of a Hamiltonian system defines a symplectic map, we have

$$\phi_{t,1}'(y)^T J \phi_{t,1}'(y) = J, \qquad \phi_{t,2}'(y)^T J \phi_{t,2}'(y) = J.$$

Next consider the numerical method defined by composing these two exact flow maps:

$$\psi_h := \phi_{t,2} \circ \phi_{t,1}$$

This map is also symplectic, since

$$\begin{aligned} \psi_h'(y)^T J \psi_h'(y)^T &= (\phi_{t,2}'(y^*)\phi_{t,1}'(y))^T J \phi_{t,2}'(y^*)\phi_{t,1}'(y) \\ &= \phi_{t,1}'(y)^T \phi_{t,2}'(y^*)^T J \phi_{t,2}'(y^*)\phi_{t,1}'(y) \\ &= \phi_{t,1}'(y)^T J \phi_{t,1}'(y) = J. \end{aligned}$$

That is, the composition of symplectic maps is again a symplectic map.

Example. A *separable* Hamiltonian system is one for which $H(q,p) = T(p) + U(q)$. For this case, the splitting method based on splitting the Hamiltonian into kinetic and potential energy terms is given by

$$q_{n+1} = q_n + hT'(p_n), \qquad p_{n+1} = p_n + hU'(q_{n+1}).$$

This scheme is referred to as *symplectic Euler*.

The second order, symmetric variant is called the *Störmer-Verlet method*

$$q_{n+1/2} = q_n + \frac{h}{2}T'(p_n), \quad p_{n+1} = p_n + hU'(q_{n+1/2}), \quad q_{n+1} = q_{n+1/2} + \frac{h}{2}T'(p_{n+1}).$$

16.5 Exercises

1. Show that the Harmonic oscillator and the Kepler problem are all expressible as Hamiltonian systems. [Hint: in each case, start by reformulating the differential equations in terms of positions and momenta, by using the relation $p = mv$ where m is mass and v is velocity.]

2. Write the differential equations for the N-body problem.