Chapter 5

Flow Maps and Dynamical Systems

Main concepts: In this chapter we introduce the concepts of continuous and discrete dynamical systems on phase space. Keywords are: classical mechanics, phase space, vector field, linear systems, flow maps, dynamical systems

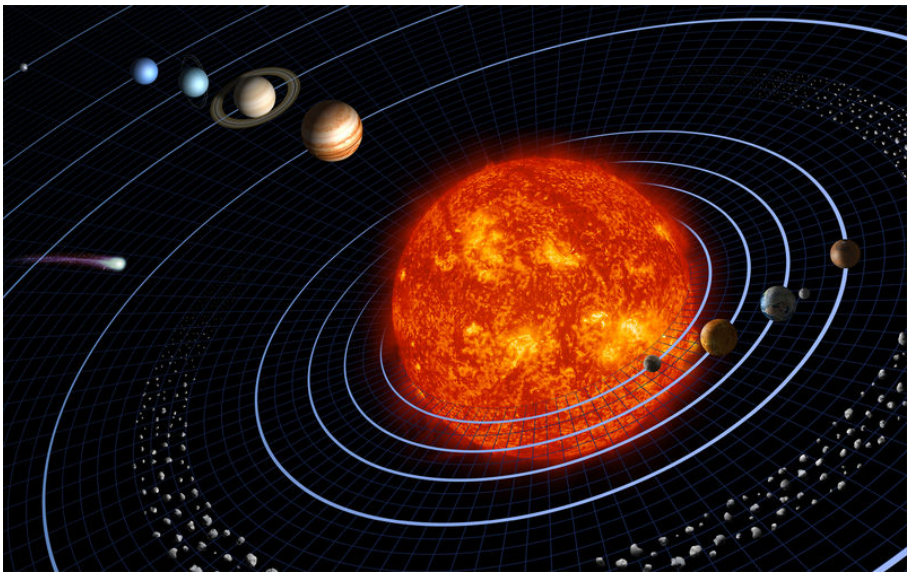

Figure 5.1: A solar system is well modelled by classical mechanics. (source: Wikimedia Commons)

In Chapter 1 we encountered a variety of ODEs in one or several variables. Only in a few cases could we write out the solution in a simple closed form. In most cases, the solutions will only be obtainable in some approximate sense, either from an asymptotic expansion or a numerical computation. Yet, as discussed in Chapter 3, many smooth systems of differential equations are known to have solutions, even globally defined ones, and so in principle we can suppose the existence of a trajectory through each point of phase space (or through "almost all" initial points). For such systems we will use the existence of such a solution to define a map called the *flow map* that takes points forward t units in time from their initial points. The concept of the flow map is very helpful in exploring the qualitative behavior of numerical methods, since it is often possible to think of numerical methods as approximations of the flow map and to evaluate methods by comparing the properties of the map associated to the numerical scheme to those of the flow map.

In this chapter we will address autonomous ODEs (recall 1.13) only:

$$y' = f(y), \qquad y, f \in \mathbb{R}^d \tag{5.1}$$

5.1 Classical mechanics

In Chapter 1 we introduced models from population dynamics. In this chapter we consider another field that is rich with dynamical systems: *classical mechanics*. Classical mechanics consists of those phenomena that can be accurately modelled using Newton's laws of motion, the second of which is:

The time rate of change of momentum of a body is equal to the net force applied to it.

If the position of the body in question is given by $x(t) \in \mathbb{R}^3$, its velocity is $\dot{x}(t) \equiv \frac{dx}{dt}$, and its momentum $p(t)$ is the product of mass m (assumed constant here) and velocity. Assuming the force F is given as a field on $\mathbb{R}^3$, the mathematical statement of the first law is

$$\frac{dp}{dt} = \frac{d}{dt}\left(m\dot{x}(t)\right) = F(x(t)).$$

The momentum can be eliminated in favor of the acceleration $\ddot{x}(t) \equiv \frac{d^2x}{dt^2}$ to give

$$m\ddot{x}(t) = F(x(t)). \tag{5.2}$$

Because of the second derivative, this is an example of a *second order differential equation*. In general we can write any *higher order differential equation* of the form

$$\frac{d^p x}{dt^p} = g(t, x, \dot{x}, \ddot{x}, \ldots, \frac{d^{p-1}x}{dt^{p-1}})$$

in the first order form (1.2) by introducing additional dependent variables. Let $X^{(1)}$ denote $x(t)$, $X^{(2)}$ denote $\dot{x}(t)$, etc. Then

$$\begin{aligned}
\dot{X}^{(1)} &= X^{(2)} \\
\dot{X}^{(2)} &= X^{(3)} \\
&\vdots \\
\dot{X}^{(p)} &= g(t, X^{(1)}, X^{(2)}, \ldots, X^{(p)}).
\end{aligned}$$

Using the momentum $p(t) = m\dot{x}(t)$, Newton's second law can be written as the first order system

$$\dot{x}(t) = \frac{1}{m}p(t) \tag{5.3a}$$

$$\dot{p}(t) = F(x(t)). \tag{5.3b}$$

To define an initial value problem for this system, we need to specify the initial position x_0 and momentum p_0 at time $t = 0$.

Let us consider the specific example of a mass on a spring. The force exerted by a spring is proportional to its displacement (this is essentially the definition of a "spring" in mechanics).

$$F(x(t)) = -k^2 x(t), \quad x, F \in \mathbb{R}$$

Applying Newton's second law gives

$$m\ddot{x} = -k^2 x$$

Assume $m = 1$. The first order system that arises is also known as the *harmonic oscillator*

$$\dot{x} = p, \qquad \dot{p} = -k^2 x. \tag{5.4}$$

The solution

$$x(t) = x_0 \cos kt + \frac{p_0}{k} \sin kt.$$

is periodic with frequency k.

More complex mechanical models have nonlinear forces $F(x(t))$ and may involve the coupling of a number of bodies. For example, in molecular dynamics, one may study the motion of a large number of interacting atomic particles. Atomic motion has several different types of forces. There are long range attracting forces and short range repelling forces. The Lennard-Jones model incorporates both of these. If we consider two particles iteracting on a line via a Lennard-Jones potential, and take one particle fixed in space, the force on the other particle at a distance $x(t) \in \mathbb{R}$ away is $F(x) = 12(x^{-13} - x^{-7})$. This yields the *Lennard-Jones oscillator*

$$\dot{x} = p, \qquad \dot{p} = 12(x^{-13} - x^{-7}). \tag{5.5}$$

The motion $x(t) \in \mathbb{R}^2$ of a satellite of mass m subject to the gravitational pull of a cellestial body positioned at the origin is governed by the *Kepler problem*

$$\dot{x} = \frac{1}{m} p, \qquad \dot{p} = -g \frac{x}{(x^T x)^{3/2}}. \tag{5.6}$$

This system has dimension $d = 4$.

5.2 Phase Space

In multidimensional autonomous systems (5.1) we sometimes refer to the underlying space $\mathbb{R}^d$ as the **phase space**. The *phase portrait* for a differential equation is the collective graph of trajectories of the differential equation in the phase plane. Obviously we cannot draw all the trajectories, so in typical parlance, the phase portrait is just a simplified graph showing several trajectories. The phase portrait for the Lennard-Jones oscillator (5.5) in $\mathbb{R}^2$ is shown in the left panel of Figure 5.2. For this system, all of the trajectories are closed curves, indicating that the solutions of the Lennard-Jones oscillator are periodic in time.

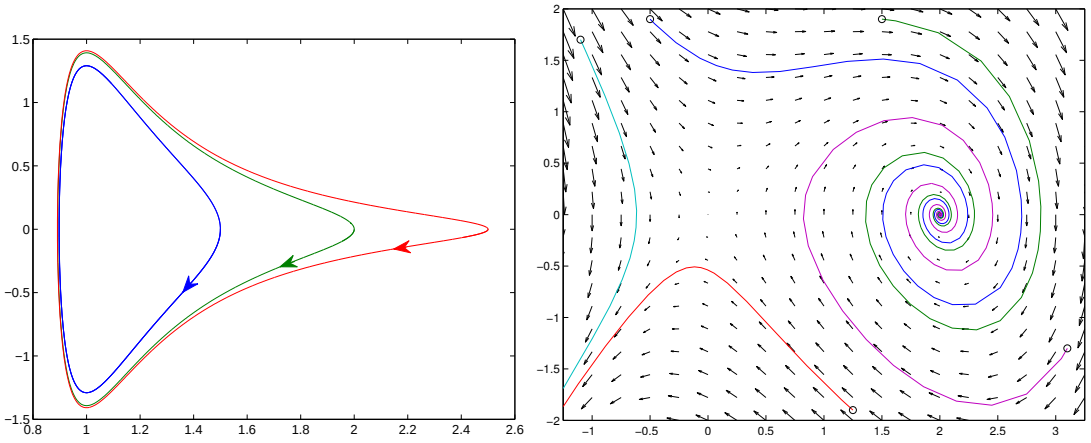

Figure 5.2: On the left, the phase portrait of the Lennard-Jones oscillator (5.5). On the right, vector field for the differential equation $\ddot{x} = 2x - x^2 - \dot{x}/2$ with some trajectories.

Two trajectories in phase space may not intersect, as this would imply that the solution is nonunique at the point of intersection. Furthermore, the solution traverses a curve in phase space in one direction only. It cannot "turn around" as this too would contradict uniqueness.

The function $f(y) : \mathbb{R}^d \to \mathbb{R}^d$ defines a **vector field** on the phase space. That is, to each point $y \in \mathbb{R}^d$ is associated a vector $f(y) \in \mathbb{R}^d$. An example for a representative ODE is shown in the right panel of Figure 5.2. Every solution of (5.1) is everywhere tangent to the vector field f, as depicted in the figure. A solution is said to be a *trajectory* or *orbit* or *integral curve* of the vector field.

5.3 The Group of Flow Maps

Consider the solution (4.7) of the linear ODE (4.3). One way of using this function is to compute the time evolution of an initial value problem associated with (4.3). In other words, given y_0, the function

$$y(t) = \exp(tA)y_0 + t\theta(tA)b, \qquad 0 \le t \le T,$$

maps out a continuous curve in the phase space $\mathbb{R}^d$.

However, we could use the solution in a different way. Specifically, consider a fixed time $t = \tau$ and the function

$$\Phi_\tau(y) = \exp(\tau A)y + \tau\theta(\tau A)b :$$

The function $\Phi_\tau : \mathbb{R}^d \to \mathbb{R}^d$ maps initial conditions of (4.3) to final conditions after an interval $[0, \tau]$.

To generalize this idea, let us take an autonomous ODE system (5.1). Given a fixed time τ, we can consider any point of phase space, y_0, as a starting point of a trajectory $(y(t; y_0))$ which is continued up to time τ, assuming the solution exists on the entire interval. We think of the action of solving the differential equation as defining a map from starting points of trajectories to their endpoints. Associated to a differential equation (5.1) we define the **flow map**

$$\Phi_\tau(y_0) = y(\tau)$$

where $y(t)$ is the solution of the initial value problem

$$y'(t) = f(y), \quad y(0) = y_0, \quad t \in [0, \tau].$$

When the system is nonlinear there is usually not a simple formula for the flow map. Nonetheless the concept is valuable.

Consider solving the ODE (5.1) with initial condition $y(0) = y_0$ for a time t_1. Denote solution at t_1 by y_1. Next, solve initial value problem (5.1) with initial condition $y(0) = y_1$ on the interval $[0, t_2]$. Denote the solution at time t_2 by y_2. Because of the invariance of the autonomous system to a translation of time, it is clear that y_2 is also the same solution you would obtain if you would solve (5.1) with initial condition $y(0) = y_0$ over the interval $[0, t_1 + t_2]$. In terms of the flow map,

$$\Phi_{t_2} \circ \Phi_{t_1} = \Phi_{t_1+t_2} = \Phi_{t_1} \circ \Phi_{t_2}, \qquad t_1, t_2 > 0.$$

Thus the composition of the two maps is another map of the same family. If we can solve the differential equations for all positive or negative time, then we can write

$$\Phi_t \circ \Phi_{-t} = \Phi_{t+-t} = \Phi_0,$$

but Φ_0 is evaluated by solving the differential equations over a zero length interval, so is just the identity map. Hence we see that $\Phi_{-t} = \Phi_t^{-1}$. The set of all such maps $\{\Phi_t \,|\, t \in \mathbf{R}\}$ is what is termed a *one-parameter group* with the (commutative) group operation being composition of maps.

The flow map can also be applied to an open set $B \subset \mathbb{R}^d$, and then we view the flow map as a function taking sets on phase space to other sets on phase space, t time units later. In other words, each element of B is taken as the initial condition of (5.1), and is mapped to the solution at the end of the interval of time t.

$$\Phi_\tau(B) = \{z \in \mathbb{R}^d : z = \Phi_\tau(y); y \in B\}$$

Implicit in this usage is the assumption that the trajectories through every point of B exist for at least t units of time.

For example, in Figure 5.3 a rectangular set of initial conditions in $\mathbb{R}^2$ is mapped under the flow map Φ_τ of the Lennard-Jones oscillator (5.5) for $\tau = 0, 0.35, 0.9$. In general, and especially in higher dimensions, such a set will become stretched and folded in on itself in a very complicated way.

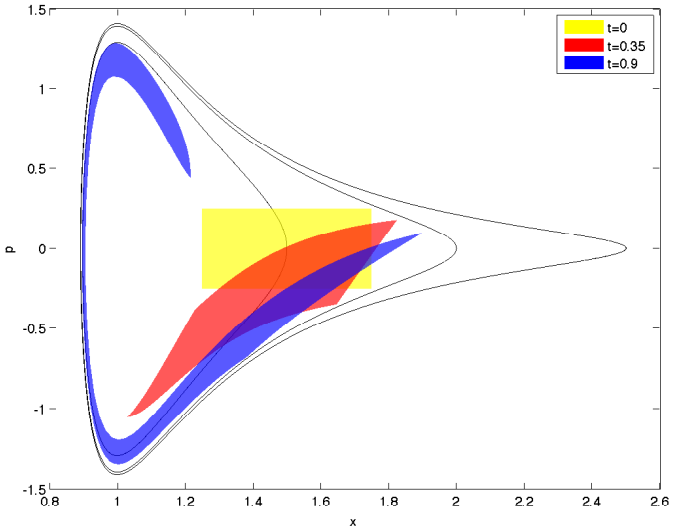

Figure 5.3: Evolution of a rectangular set B under the flow map of the Lennard-Jones oscillator (5.5) at times $t = 0$ (yellow), $t = 0.35$ (red) and $t = 0.9$ (blue).

5.4 Dynamical systems

It is important to note that the flow map $\Phi_\tau(y)$ only makes sense if the solution through y exists up to time t. In Chapter 3 we showed that a sufficient condition for existence of a solution on a set $D \subseteq \mathbb{R}^d$ is that the vector field f be Lipschitz on D. However, this condition alone does not specify to what time t the solution will continue to exist. We will be interested in two special cases in which the solution is known to exist for all time $t > 0$. First, we say a vector field f is **globally Lipschitz** if it is Lipschitz with constant $L < \infty$ on all of $\mathbb{R}^d$. In this case, a solution through any point y exists and is unique for all time. This is often not a very realistic assumption. Instead, consider a set D with the property: A set $D \subset \mathbb{R}^d$ is said to be **positively invariant** under the flow map Φ_t if

$$\Phi_t(D) \subseteq D \qquad \forall t \geq 0.$$

(The stipulation "for all $t > 0$" is not really restrictive. It is sufficient if $\Phi_t : D \to D$ on any interval $[0, \tau)$, $\tau > 0$, since this implies invariance for all $t > 0$.) If f is Lipschitz on a set D that is positively invariant under the flow map, then there the unique solution for any initial condition $y_0 \in D$ exists for all time. Given a set $D \subseteq \mathbb{R}^d$, a map $\Phi_t : D \to D$ defines a **dynamical system** on D. Clearly the flow map of a differential equation defines a dynamical system whenever the vector field f is globally Lipschitz, or Lipschitz on a positively invariant set.

For some differential equations, the solution may also exist for negative time $t < 0$ and hence for all time $t \in \mathbb{R}$. If D is invariant under the negative time flow of a differential equation, we say D is *negatively invariant*. A set that is both positively and negatively invariant is said to be *invariant*.

The **ω-limit set** of y is the set of points x such that there exists a sequence of times $t_n \to \infty$, such that $\Phi_{t_n}(y) \to x$. This set is denoted $\omega(y)$. Similarly the **α-limit set** of y is the set of such

points for $t_n \to -\infty$. Examples of such sets are equilibrium points, limit cycles, periodic orbits and attractors. We also use $\omega(B)$ and $\alpha(B)$ to denote the union of the ω and α limit sets of all initial conditions in an open set B.

For example, in the right panel of Figure 1.2, solutions of the predation model (1.5) are shown. For the values $r = 0.1$ and $r = 0.6$, the set $D = \{n_0 > 0\}$ has $\omega(D)$ a single point. For $r = 0.25$, $\omega(D)$ contains two points. For the Lotka-Volterra model (1.6), all solutions are periodic, the ω and α limit sets coincide, and are precisely the solution curves.

5.5 Discretization and Approximate Flow Maps

When we discretize an ODE, we normally replace it by a difference equation which describes in an approximate sense how the solution evolves from timestep to timestep. For example, recall Euler's method (2.1) from Chapter 2

$$y_{n+1} = y_n + hf(y_n).$$

Here y_n represents a numerical approximation of $y(t_n)$.

We could regularly sample the exact solution on a succession of time intervals of length h, according to the rule

$$y(t_{n+1}) = \Phi_h(y(t_n))$$

If $y(t; y_0)$ represents the solution of the differential equation (5.1) with initial condition $y(0) = y_0$ after t units of time, we can write

$$y(h; y_0) = \Phi_h(y_0).$$

Moreover,

$$y(2h; y_0) = \Phi_h \circ \Phi_h(y_0),$$

and so on. This means that we can view the iteration of Φ_h as producing snapshots of the solution at equally spaced points in time. Similarly, Euler's method can be seen as iteration of a map

$$\Psi_h(y) = y + hf(y)$$

which approximates the flow map Φ_h. We refer to Ψ_h as the **numerical flow map** for Euler's method.

Do the mappings Ψ_h form a one-parameter group? The answer is no. Quite simply,

$$\Psi_{h_1} \circ \Psi_{h_2} \neq \Psi_{h_1+h_2}.$$

Indeed, even

$$\Psi_h \circ \Psi_h \neq \Psi_{2h}.$$

This is a fundamental difference between the exact flow map and its numerical approximation.

There are a wide variety of numerical methods available for solving the ODE (1.2) or (5.1). In some cases these are based on using the values of solutions computed at two or more successive points in time (so-called *multistep methods*). While such schemes offer benefits for certain types of computations, only in the case that the numerical method computes the approximation based only on the approximate solution at the previous time point can we directly compare the method's properties to those of the flow map. For this reason, we restrict in this course to *generalized one-step methods* which can always be associated to the recurrence relation

$$y_{n+1} = \Psi_h(y_n). \tag{5.7}$$

The discrete approximation would satisfy

$$y_1 = \Psi_h(y_0), \qquad y_2 = \Psi_h(y_1) = \Psi_h \circ \Psi_h(y_0),$$

and so on. It is useful to have a notation for applying a map n times, recursively. We will use a superscript to indicate this:

$$\Psi_h^2 = \Psi_h \circ \Psi_h, \qquad \Psi_h^3 = \Psi_h \circ \Psi_h \circ \Psi_h,$$

etc.

For explicit methods such as Euler's method, the numerical flow map is obvious. For implicit methods such as the Trapezoidal rule (2.2) introduced in Chapter 2, it is unclear in advance whether such a map is well-defined. It follows from the implicit function theorem that for h small enough and appropriate f, there exists a solution to the trapezoidal rule, but it may not be unique. Typically, there is a branch of solutions that converge to y_n as $h \to 0$. If we take this branch, then the flow map (5.7) is well-defined.

As in the case of the continuous flow map, we use the notation $\Psi_h(B)$ to denote the set obtained by applying Ψ_h to every element of an open set B. Given a set $D \subseteq \mathbb{R}^d$, if a discrete map Ψ_h satisfies $\Psi_h(D) \subseteq D$, then it defines a **discrete dynamical system** on D.

In this course we will study the dynamics of numerical flows Ψ_h. This will give us an appreciation of the qualitative behavior of different methods. Generally we will attempt to compare the properties of Ψ_h with those of the exact flow Φ_t. However, since the numerical map does not satisfy the group property, the size of h plays a special role in numerics. In particular there are practical restrictions on the maximum allowable step size h. And in general we will have to compare the iterated map Ψ_h^n with the exact flow Φ_{nh}. In the theory of continuous dynamical systems, one is often concerned with the limit behavior of solutions as $t \to \pm\infty$, and roughly speaking, we would like to recover this behavior in the iterated numerical map. Besides the dynamics of the numerical flow map, however, there is an additional issue—unique to numerics—of *approximation*. Whereas when studying dynamics we are often interested in the *dynamic limit*

$$T \to \infty, \quad h \text{ fixed}, \tag{5.8}$$

when studying approximation we look instead at the *approximation limit*

$$h \to 0, \quad T \text{ fixed}. \tag{5.9}$$

Before turning to the dynamical systems limit, we will first be concerned with the approximation limit in the next few chapters.

5.6 References

The definitive work on dynamical systems aspects of numerical integrators is

> A. M. Stuart and A. R. Humphries, *Dynamical Systems and Numerical Analysis*, Cambridge, 1996.

5.7 Exercises

1. Can a globally Lipschitz vector field have a solution that grows unbounded? Give an example or counterexample to support your answer.
2. Show that for any H the ellipse $E(H) = \{(x, p) : k^2x^2 + p^2 = H\}$ is invariant under the flow map of the harmonic oscillator (5.4). Is such an ellipse also invariant under the flow map of Euler's method (2.1) applied to this problem? Trapezoidal rule (2.2)?
3. Show that any ellipsoidal disc $D(H) = \{(x, p) : k^2x^2 + p^2 \leq H\}$ is invariant under the flow map of the damped spring (**??**). Is such a disc also invariant under the flow map of Euler's method applied to this problem? For what range of stepsizes?
4. Consider the logistic equation (1.4) and the open interval $X = (0, 1)$. What is $\omega(X)$? What is $\alpha(X)$?