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Introduction

This book is about numerical methods for use in simulating dynamical phenomena governed by conservative processes. In this chapter, we review a few basic principles regarding conservative models. In general, we are concerned here with initial value problems for systems of ordinary differential equations (ODEs) of the form

$$\frac{d}{dt}z = \boldsymbol{f}(z), \qquad\qquad z(t_0) = z^0,$$

where $z : \mathbb{R} \to \mathbb{R}^k$. The basic questions encountered early on in a first course on ODEs concern existence and uniqueness of solutions, a topic addressed, for example, by Picard's theorem. Discussion then turns to various techniques for analytically solving the differential equations when $\boldsymbol{f}$ has a prescribed form. In particular, the scalar case $k = 1$ is an instance of a *separable differential equation* and such models are in principle solvable in quadratures (i.e. by evaluating certain integrals and solving certain algebraic equations). Linear systems are exactly solvable after determination of the eigenvalues and eigenvectors (or generalized eigenvectors, in the degenerate case). Beyond these and a few other special cases, most models are not exactly integrable. In this book we are mostly interested in complex models that do not admit exact solutions.

The emphasis of this book is on the particular models which are formulated naturally as *conservative systems* of ODEs, most importantly *Hamiltonian systems*. As a general rule, mechanical systems resulting from physical principles are Hamiltonian until (usually for prudent modeling purposes) subjected to simplifying reductions or truncations. For example, in typical fluid dynamics applications, the incorporation of diffusive effects due to friction with a boundary plays an essential role in the modeling. However, in many situations, the conservative paradigm can be retained and remains the most appropriate foundation for the construction of models, since it is in no small measure due to properties such as conservation of energy and angular momentum that matter behaves as it does.

The existence of Kepler's laws which approximately describe the motion of the planets in the solar system are reflections of the conservative nature of

gravitational dynamics. The celebrated Kolmogorov–Arnold–Moser theory which discusses the local stability of nonlinear dynamical systems in the vicinity of certain critical points applies only to conservative systems. Even dissipative systems typically retain certain conservation laws (for example conservation of mass in fluid dynamics), and many of the ideas developed in this book are still applicable to such problems.

1.1 *N*-body problems

Conservative dynamical systems most often originate through application of Newton's second law which describes the motion of a body in an applied force field. In a classical *N*-body system (Fig. 1.1), several point masses are involved and the forces acting on any one body arise from the presence of neighboring bodies or some external field.

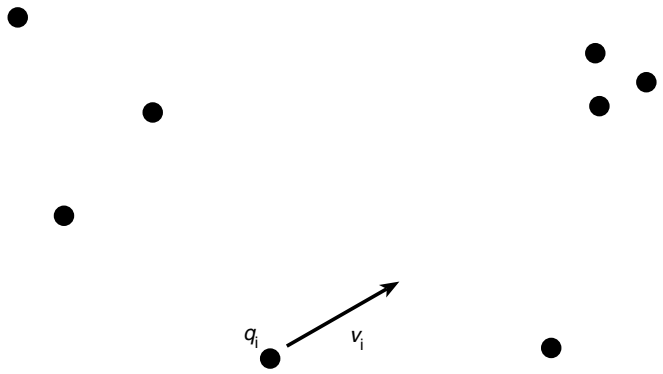

Figure 1.1 An *N*-body system.

Let the ith body be assigned a mass m_i, an instantaneous position $\boldsymbol{q}_i$ (with respect to some appropriate reference frame), and a velocity $\boldsymbol{v}_i$, $i = 1, \ldots, N$. Let $\boldsymbol{F}_i$ represent the force acting on body i (due, for example, to interactions with the other particles). We assume that the force can be obtained as the negative gradient of a potential energy function V with respect to the ith particle position $\boldsymbol{q}_i$, i.e.

$$\boldsymbol{F}_i = -\nabla_{\boldsymbol{q}_i} V(\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_N).$$

The N-point particles then move according to Newton's equations of motion

$$\frac{d}{dt}\boldsymbol{q}_i = \boldsymbol{v}_i, \tag{1.1}$$

$$m_i \frac{d}{dt}\boldsymbol{v}_i = \boldsymbol{F}_i, \qquad i = 1, 2, \ldots, N. \tag{1.2}$$

N-body problems can be naturally formulated to describe motion in any Euclidean space $\mathbb{R}^\nu$, $\nu > 0$, i.e. with $\boldsymbol{q}_i$, $\boldsymbol{v}_i$, and $\boldsymbol{F}_i$ all in $\mathbb{R}^\nu$. Such a system is said to have νN *degrees of freedom*. We will say that the *phase space* of an N-body problem is the $2\nu N$-dimensional set consisting of all possible positions $\boldsymbol{q} = (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_N)^T$ and velocities $\boldsymbol{v} = (\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_N)^T$ of the particles. Under mild smoothness assumptions on the potential energy function V, there exists, at least locally through any point $(\boldsymbol{q}^0, \boldsymbol{v}^0)$ of phase space, a unique *trajectory* of the mechanical system: a solution of the equations (1.1)–(1.2) subject to the initial conditions $\boldsymbol{q}(0) = \boldsymbol{q}^0$, $\boldsymbol{v}(0) = \boldsymbol{v}^0$. At a *critical point* $\boldsymbol{q} = \bar{\boldsymbol{q}}$, all of the forces acting on the particles in the system vanish; hence the trajectory through $(\bar{\boldsymbol{q}}, \boldsymbol{0})$ reduces to a single point.

The total energy associated to the mechanical system (1.1)–(1.2) is the sum of kinetic and potential terms

$$E(\boldsymbol{q}, \boldsymbol{v}) = \frac{1}{2} \sum_{i=1}^{N} m_i \|\boldsymbol{v}_i\|^2 + V(\boldsymbol{q}).$$

It is easy to see that the energy is constant along a trajectory, since

$$\begin{aligned} \frac{d}{dt} E &= \sum_{i=1}^{N} m_i \boldsymbol{v}_i \cdot \dot{\boldsymbol{v}}_i + \sum_{i=1}^{N} \nabla_{\boldsymbol{q}_i} V(\boldsymbol{q}) \cdot \dot{\boldsymbol{q}}_i \\ &= \sum_{i=1}^{N} m_i \boldsymbol{v}_i \cdot \left(\frac{1}{m_i} \boldsymbol{F}_i \right) - \sum_{i=1}^{N} \boldsymbol{F}_i \cdot \boldsymbol{v}_i = 0. \end{aligned}$$

(Refer to the preface for details on the notation used in this derivation and later in the book.) A system with an energy function constant along solutions is referred to as a *conservative* system.

1.2 Problems and applications

Let us briefly survey a few of the most important recurring N-body applications. Examples of these problems, along with a number of other types of models, are developed in more detail in various places in the book.

The historical origin of the N-body problem lies in *gravitational modeling*, and these problems remain of substantial current interest. Simulations are being conducted on a wide variety of astronomical systems, including planetary systems (for understanding both their formation and their long-term stability), systems of interacting stars or binaries, galaxies, and globular clusters. Closely related problems arise in semi-classical studies of atomic systems. As an example, the

three-body gravitational problem involving bodies of unequal mass has the potential energy

$$V(\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3) = -\frac{Gm_1m_2}{\|\boldsymbol{q}_1 - \boldsymbol{q}_2\|} - \frac{Gm_2m_3}{\|\boldsymbol{q}_2 - \boldsymbol{q}_3\|} - \frac{Gm_1m_3}{\|\boldsymbol{q}_1 - \boldsymbol{q}_3\|},$$

where G is the universal gravitational constant. Such a three-body problem has no general, analytical solution, so simulation is needed to enhance understanding, sometimes in conjunction with partial theoretical analysis, for example to determine the stability of certain configurations of the bodies. Chaotic solutions of the three-body problem may include arbitrarily close approaches of the bodies, in which case the singularity in the potential may cause significant difficulty for numerical simulation and some sort of regularizing transformations of time and/or coordinates are needed. We will return to consider some of these issues in one of the book's later chapters.

Classical mechanics is also the basis of many *molecular models* in chemistry, physics, and biology, including those commonly used for studying liquids and gases, materials, proteins, nucleic acids, and other polymers. In these applications, V is composed of a sum of several heterogeneous nonlinear contributions based on the distances between pairs of particles, varying both in functional form and in relative intensity. These terms may be "local" ("short-range") meaning that they effectively involve only contributions from nearby particles, or they may be "long-range." A commonly treated system with only local interactions is the simplified model of a gas or liquid, consisting of N identical atoms of a certain prescribed mass, interacting in a *Lennard–Jones* pair potential

$$\varphi_{\text{L.J.}}(r) = \epsilon \left[\left(\frac{\bar{r}}{r}\right)^{12} - 2\left(\frac{\bar{r}}{r}\right)^{6} \right]. \tag{1.3}$$

The total potential energy is

$$V = \sum_{1 \le i < j \le N} \varphi_{\text{L.J.}}(\|\boldsymbol{q}_i - \boldsymbol{q}_j\|). \tag{1.4}$$

Note that such models are always simplifications of vastly more complex quantum-mechanical models. The parameters ϵ and $\bar{r}$ of the Lennard–Jones potential provide a fit to experiment, but would depend on the temperature and pressure at which the simulation is performed. Strictly speaking, the pair interactions between atoms would include all pairs, no matter how distant, but since the energy decays like r^{-6}, the forces are generally found to be so small outside of some critical radius that the potential can simply be cut off beyond this distance. In practice, this is usually done by introducing a smooth transition of the potential energy function to a constant value.

Regardless of what other potentials may be present, the presence of the Lennard–Jones potential ensures that the particle forces are ultimately strongly repulsive at short range. These repulsive forces are a very important aspect of molecular systems. The potential will be singular where particle positions overlap, but otherwise, the potential is smooth and the solution is *globally defined*: solutions started away from singularities can be extended without bound in t. Thus molecular systems do not undergo the extreme collisions encountered in strictly Coulombic problems such as gravitation.

Still other classes of conservative systems arise through discretization of *partial differential equations*. A semi-linear wave equation of the form

$$u_{tt} = u_{xx} - f(u), \qquad u = u(x,t),$$

is conservative under certain prescriptions of boundary and initial data. If we assume, for example, that solutions are defined on the interval $[0, L]$ and are periodic with period L, then the energy functional is

$$E[u] = \int_0^L \left[\frac{1}{2}u_t^2 + \frac{1}{2}u_x^2 + F(u)\right] dx,$$

where $F(u) = \int_0^u f(s)ds$. The equations of motion could be written in the "Newton-like" form

$$v_t = -\delta_u V[u], \qquad u_t = v,$$

where $V[u] = \int_0^L \left[\frac{1}{2}u_x^2 + F(u)\right] dx$ represents the potential energy, and δ_u, termed the *variational derivative*, is the analogue of the gradient appearing in the Newtonian equations of motion,

$$(\delta_u G[u], \delta u) = \lim_{\varepsilon \to 0} \frac{G[u + \varepsilon \delta u] - G[u]}{\varepsilon}, \tag{1.5}$$

where G is a functional, like the potential energy V, that assigns a real number to functions $u(x)$ and the equality holds for all sufficiently regular periodic functions $\delta u(x)$, i.e. $\delta u(x) = \delta u(x+L)$. This definition is formally equivalent to the defining relation for the gradient mentioned in the preface with $\langle ., . \rangle$ replaced by the L_2 inner product,

$$(u, v) = \int_0^L u(x)v(x)dx.$$

Note that $\delta_u G[u]$ is itself a function of x.

The simplest centered finite difference spatial discretization takes the form, for $i = 1, 2, \ldots, N$,

$$\frac{d}{dt}u_i = v_i,$$
$$\frac{d}{dt}v_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} - f(u_i),$$

where $u_i \approx u(i\Delta x, t)$, $\Delta x = L/N$, and the periodic boundary condition leads to the definitions $u_0 \equiv u_N$, $u_{N+1} \equiv u_1$. This is in the form of a standard N-body system in one dimension with positions $\boldsymbol{u} = (u_1, u_2, \ldots, u_N)^T$, velocities $\boldsymbol{v} = (v_1, v_2, \ldots, v_N)^T$, and potential

$$V(\boldsymbol{u}) = \sum_{i=1}^{N} \left(\frac{u_{i+1} - u_i}{\Delta x} \right)^2 + \sum_{i=1}^{N} F(u_i).$$

1.3 Constrained dynamics

In the setting of modern applications, we will need to consider generalizations of the traditional N-body problem in which the basic modeling unit is not the point particle moving in Euclidean space but an object moving in some *constrained* space.

For instance, in molecular dynamics, the bond stretch between two atoms is typically modeled by a spring with rest length $L > 0$, say

$$V_{12}(\boldsymbol{q}_1, \boldsymbol{q}_2) = \frac{\alpha}{2} \left(\|\boldsymbol{q}_1 - \boldsymbol{q}_2\| - L \right)^2,$$

where $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ are the positions of the atoms and α is a positive parameter. When α is large, the vibrational frequency is also large, while the variation in the length of the stretch from L will typically be small. It is then common practice to replace one or more of these bonds by rigid length constraints, i.e. to introduce a constraint of the form

$$\|\boldsymbol{q}_1 - \boldsymbol{q}_2\|^2 = L^2.$$

If enough constraints among a set of particles are imposed simultaneously, the group becomes completely rigid. Such *rigid bodies* have very interesting dynamical properties in and of themselves. For example, in molecular dynamics, it is standard practice to replace small polyatomic molecules (for example, H_2O) by rigid bodies. As another illustration, while it may be appropriate to treat the bodies in the solar system as point masses for many purposes, in more delicate situations, the nonspherical rigid body structure of the planets may need to be taken into consideration.

Let us begin by extending Newton's equations for particle motion to the constrained case. Imagine a particle of mass m moving on a constraint surface defined as the zero set of some smooth function g. At any time, the particle is acted on by two types of forces: *applied forces* defined in the usual way by a potential energy function V, and *constraint* forces which act in such a way as to make the particle lie on the constraint surface. Although we do not in general know anything about the directionality of the applied force, we may take as our starting point the *principle of D'Alembert*: *the constraint force acts along the normal direction to the constraint surface*, i.e. along the direction of the gradient to the function g at the point of contact (Fig. 1.2).

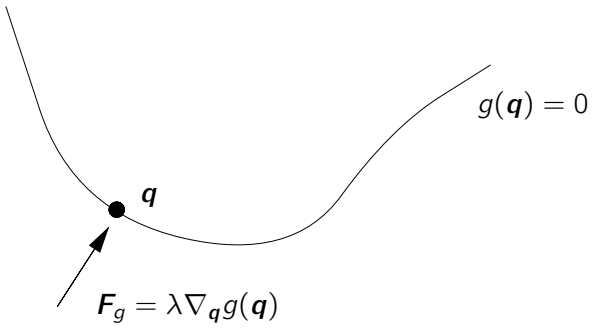

Figure 1.2 D'Alembert's Principle: the constraint force acts in the normal direction to the constraint surface at the point of contact.

Thus, if we denote the constraint forces by $\boldsymbol{F}_g$, we have

$$\boldsymbol{F}_g \quad || \quad \nabla_{\boldsymbol{q}} g(\boldsymbol{q}),$$

or

$$\boldsymbol{F}_g = \lambda \nabla_{\boldsymbol{q}} g(\boldsymbol{q}),$$

where λ is a scalar.

Using Newton's second law, the equations of motion then take the form

$$m\dot{\boldsymbol{v}} = -\nabla_{\boldsymbol{q}} V(\boldsymbol{q}) + \lambda \nabla_{\boldsymbol{q}} g(\boldsymbol{q}), \tag{1.6}$$

$$\dot{\boldsymbol{q}} = \boldsymbol{v}, \tag{1.7}$$

$$g(\boldsymbol{q}) = 0. \tag{1.8}$$

The parameter λ is an unknown which is uniquely determined by the condition that $\boldsymbol{q}(t)$ satisfy (1.8) at all points on the trajectory and that the trajectory be smooth. Specifically, if we differentiate the equation $g(\boldsymbol{q}(t)) = 0$ twice with respect to time, we find first

$$\frac{d}{dt} g(\boldsymbol{q}) = \nabla_{\boldsymbol{q}} g(\boldsymbol{q}) \cdot \dot{\boldsymbol{q}} = \nabla_{\boldsymbol{q}} g(\boldsymbol{q}) \cdot \boldsymbol{v} = 0, \tag{1.9}$$

and, then

$$\frac{d^2}{dt^2}g(\boldsymbol{q}) = \langle \boldsymbol{v}, g_{\boldsymbol{qq}}(\boldsymbol{q})\boldsymbol{v}\rangle + m^{-1}\nabla_{\boldsymbol{q}}g(\boldsymbol{q})\cdot[-\nabla_{\boldsymbol{q}}V(\boldsymbol{q}) + \lambda\nabla_{\boldsymbol{q}}g(\boldsymbol{q})] = 0, \qquad (1.10)$$

where $g_{\boldsymbol{qq}}(\boldsymbol{q})$ represents the Hessian matrix of g. Provided that $\nabla_{\boldsymbol{q}}g(\boldsymbol{q}) \neq 0$, the equation (1.10) has a unique solution $\lambda = \Lambda(\boldsymbol{q}, \boldsymbol{v})$

$$\Lambda(\boldsymbol{q}, \boldsymbol{v}) = \frac{m}{\|\nabla_{\boldsymbol{q}}g(\boldsymbol{q})\|^2}\left(\frac{1}{m}\langle\nabla_{\boldsymbol{q}}g(\boldsymbol{q}), \nabla_{\boldsymbol{q}}V(\boldsymbol{q})\rangle - \langle \boldsymbol{v}, g_{\boldsymbol{qq}}(\boldsymbol{q})\boldsymbol{v}\rangle\right).$$

Equations (1.6)–(1.8) are a special case of the constrained Euler–Lagrange equations. As a simple illustration, we mention the example of a bead (of mass m) moving in gravity in two dimensions (coordinates (x, z)) along a wire described by the curve $\Gamma : z = f(x)$. The constraint is $g(x, z) := z - f(x)$, and the equations of motion take the form

$$m\ddot{x} = -\lambda f'(x), \qquad (1.11)$$
$$m\ddot{z} = -mg + \lambda, \qquad (1.12)$$
$$z = f(x). \qquad (1.13)$$

Here g represents the earth's gravitational constant.

As a second illustration, consider the spherical pendulum consisting of a bob of mass m suspended from a fixed point on a rigid massless rod of length $L > 0$. We formulate the problem in cartesian coordinates (x, y, z) with energy

$$E = \frac{1}{2m}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + mgz,$$

and equations of motion

$$\begin{aligned} m\ddot{x} &= 2\lambda x,\\ m\ddot{y} &= 2\lambda y,\\ m\ddot{z} &= -mg + 2\lambda z,\\ 0 &= x^2 + y^2 + z^2 - L^2. \end{aligned}$$

1.4 Exercises

1. *Scalar nonlinear models.* Consider a single-degree-of-freedom problem of the form

$$\begin{aligned} \dot{q} &= v,\\ m\dot{v} &= -\varphi'(q). \end{aligned}$$

a. Write the energy function $E(q, v)$ for the above system and verify that it is conserved along trajectories of the system.

b. Set the energy function to a constant value, say E_0, and show that the resulting equation can be solved for v as a function of q, subject to a choice of the sign of v. Using this, together with the differential equations, show that the equations of motion reduce to a first-order differential equation for q of the form

$$\dot{q} = \pm\sqrt{\left(\frac{2}{m}\right)(E_0 - \varphi(q))}.$$

(Observe that this equation is separable, and hence the solution can in principle be recovered by integration.)

Discuss first the case $v \neq 0$ and continue with an investigation of the solution behavior in the vicinity of $v = 0$.

2. *Morse oscillator.* (See problem 1 above.) The Morse oscillator is a one-degree-of-freedom conservative system consisting of a single particle of unit mass moving in the potential $\varphi(q) = D(1 - e^{-\beta q})^2$. In the following set $D = 1$ and $\beta = 1$.

a. Sketch the graph of φ as a function of q.

b. Sketch several of the level curves ($E(q, v) = E_0$, E_0 fixed) of the energy function. In particular, observe that the system has bounded trajectories for $E < E_*$. What is E_*? What can be said about an orbit with energy $E = E_*$?

c. Sketch the graphs of several solution curves as functions of t. [Hint: the velocity field can be sketched by using the result of problem 1b.]

3. *Pendulum.* The planar version of the pendulum is described by the equations

$$\begin{aligned} m\ddot{x} &= 2\lambda x, \\ m\ddot{y} &= -mg + 2\lambda y, \\ 0 &= x^2 + y^2 - L^2. \end{aligned}$$

Introduce coordinates $x = L\sin\theta$, $y = -L\cos\theta$ and show that the equations of motion can be reduced to a single second-order differential equation for θ which is in the form of a nonlinear oscillator.

4. *Bead-on-wire.* Consider the "bead-on-wire" problem (1.11)–(1.13). Show that the equations of motion can be reduced to a second-order unconstrained differential equation for x of the form

$$\ddot{x} = -f'(x)\frac{g + f''(x)\dot{x}^2}{1 + f'(x)^2}.$$

5. *Variational derivative.* Using the definition (1.5) of the variational derivative and integration by parts, verify that

$$\delta_u V[u] = -u_{xx} + F'(u),$$

for

$$V[u] = \int_0^L \left[\frac{1}{2}u_x^2 + F(u)\right] dx.$$