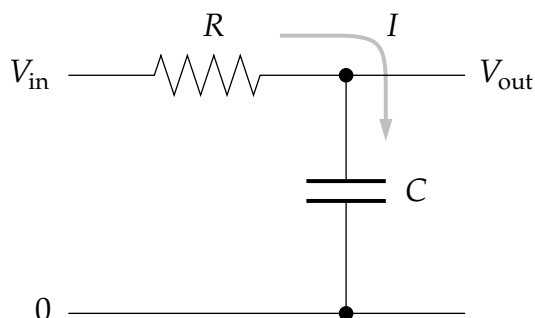


COMPUTATIONAL PHYSICS

EXERCISES FOR CHAPTER 8

Exercise 8.1: A low-pass filter

Here is a simple electronic circuit with one resistor and one capacitor:



This circuit acts as a low-pass filter: you send a signal in on the left and it comes out filtered on the right.

Using Ohm's law and the capacitor law and assuming that the output load has very high impedance, so that a negligible amount of current flows through it, we can write down the equations governing this circuit as follows. Let I be the current that flows through R and into the capacitor, and let Q be the charge on the capacitor. Then:

$$IR = V_{\text{in}} - V_{\text{out}}, \quad Q = CV_{\text{out}}, \quad I = \frac{dQ}{dt}.$$

Substituting the second equation into the third, then substituting the result into the first equation, we find that $V_{\text{in}} - V_{\text{out}} = RC (dV_{\text{out}}/dt)$, or equivalently

$$\frac{dV_{\text{out}}}{dt} = \frac{1}{RC} (V_{\text{in}} - V_{\text{out}}).$$

- a) Write a program (or modify a previous one) to solve this equation for $V_{\text{out}}(t)$ using the fourth-order Runge-Kutta method when in the input signal is a square-wave with frequency 1 and amplitude 1:

$$V_{\text{in}}(t) = \begin{cases} 1 & \text{if } \lfloor 2t \rfloor \text{ is even,} \\ -1 & \text{if } \lfloor 2t \rfloor \text{ is odd,} \end{cases} \quad (1)$$

where $\lfloor x \rfloor$ means x rounded down to the next lowest integer. Use the program to make plots of the output of the filter circuit from $t = 0$ to $t = 10$ when $RC = 0.01, 0.1$, and 1 , with initial condition $V_{\text{out}}(0) = 0$. You will have to make a decision about what value of h to use in your calculation. Small values give more accurate results, but the program will take longer to run. Try a variety of different values and choose one for your final calculations that seems sensible to you.

- b) Based on the graphs produced by your program, describe what you see and explain what the circuit is doing.

A program similar to the one you wrote is running inside most stereos and music players, to create the effect of the “bass” control. In the old days, the bass control on a stereo would have been connected to a real electronic low-pass filter in the amplifier circuitry, but these days there is just a computer processor that simulates the behavior of the filter in a manner similar to your program.

Exercise 8.2: The Lotka–Volterra equations

The Lotka–Volterra equations are a mathematical model of predator–prey interactions between biological species. Let two variables x and y be proportional to the size of the populations of two species, traditionally called “rabbits” (the prey) and “foxes” (the predators). You could think of x and y as being the population in thousands, say, so that $x = 2$ means there are 2000 rabbits. Strictly the only allowed values of x and y would then be multiples of 0.001, since you can only have whole numbers of rabbits or foxes. But 0.001 is a pretty close spacing of values, so it’s a decent approximation to treat x and y as continuous real numbers so long as neither gets very close to zero.

In the Lotka–Volterra model the rabbits reproduce at a rate proportional to their population, but are eaten by the foxes at a rate proportional to both their own population and the population of foxes:

$$\frac{dx}{dt} = \alpha x - \beta xy,$$

where α and β are constants. At the same time the foxes reproduce at a rate proportional the rate at which they eat rabbits—because they need food to grow and reproduce—but also die of old age at a rate proportional to their own population:

$$\frac{dy}{dt} = \gamma xy - \delta y,$$

where γ and δ are also constants.

- a) Write a program to solve these equations using the fourth-order Runge–Kutta method for the case $\alpha = 1$, $\beta = \gamma = 0.5$, and $\delta = 2$, starting from the initial condition $x = y = 2$. Have the program make a graph showing both x and y as a function of time on the same axes from $t = 0$ to $t = 30$. (Hint: Notice that the differential equations in this case do not depend explicitly on time t —in vector notation, the right-hand side of each equation is a function $f(\mathbf{r})$ with no t dependence. You may nonetheless find it convenient to define a Python function $f(\mathbf{r}, t)$ including the time variable, so that your program takes the same form as programs given earlier in this chapter. You don’t have to do it that way, but it can avoid some confusion. Several of the following exercises have a similar lack of explicit time-dependence.)
- b) Describe in words what is going on in the system, in terms of rabbits and foxes.

Exercise 8.3: The Lorenz equations

One of the most celebrated sets of differential equations in physics is the Lorenz equations:

$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = rx - y - xz, \quad \frac{dz}{dt} = xy - bz,$$

where σ , r , and b are constants. (The names σ , r , and b are odd, but traditional—they are always used in these equations for historical reasons.)

These equations were first studied by Edward Lorenz in 1963, who derived them from a simplified model of weather patterns. The reason for their fame is that they were one of the first incontrovertible examples of *deterministic chaos*, the occurrence of apparently random motion even though there is no randomness built into the equations. We encountered a different example of chaos in the logistic map of Exercise 3.6.

- a) Write a program to solve the Lorenz equations for the case $\sigma = 10$, $r = 28$, and $b = \frac{8}{3}$ in the range from $t = 0$ to $t = 50$ with initial conditions $(x, y, z) = (0, 1, 0)$. Have your program make a plot of y as a function of time. Note the unpredictable nature of the motion. (Hint: If you base your program on previous ones, be careful. This problem has parameters r and b with the same names as variables in previous programs—make sure to give your variables new names, or use different names for the parameters, to avoid introducing errors into your code.)
- b) Modify your program to produce a plot of z against x . You should see a picture of the famous “strange attractor” of the Lorenz equations, a lop-sided butterfly-shaped plot that never repeats itself.

Exercise 8.4: Building on the results from Example 8.6 above, calculate the motion of a nonlinear pendulum as follows.

- a) Write a program to solve the two first-order equations, Eqs. (8.45) and (8.46), using the fourth-order Runge–Kutta method for a pendulum with a 10 cm arm. Use your program to calculate the angle θ of displacement for several periods of the pendulum when it is released from a standstill at $\theta = 179^\circ$ from the vertical. Make a graph of θ as a function of time.
- b) Extend your program to create an animation of the motion of the pendulum. Your animation should, at a minimum, include a representation of the moving pendulum bob and the pendulum arm. (Hint: You will probably find the function rate discussed in Section 3.5 useful for making your animation run at a sensible speed. Also, you may want to make the step size for your Runge–Kutta calculation smaller than the frame-rate of your animation, i.e., do several Runge–Kutta steps per frame on screen. This is certainly allowed and may help to make your calculation more accurate.)

For a bigger challenge, take a look at Exercise 8.15 on page 398, which invites you to write a program to calculate the chaotic motion of the double pendulum.

Exercise 8.5: The driven pendulum

A pendulum like the one in Exercise 8.4 can be driven by, for example, exerting a small oscillating force horizontally on the mass. Then the equation of motion for the pendulum becomes

$$\frac{d^2\theta}{dt^2} = -\frac{g}{\ell} \sin \theta + C \cos \theta \sin \Omega t,$$

where C and Ω are constants.

- Write a program to solve this equation for θ as a function of time with $\ell = 10$ cm, $C = 2$ s⁻² and $\Omega = 5$ s⁻¹ and make a plot of θ as a function of time from $t = 0$ to $t = 100$ s. Start the pendulum at rest with $\theta = 0$ and $d\theta/dt = 0$.
- Now change the value of Ω , while keeping C the same, to find a value for which the pendulum resonates with the driving force and swings widely from side to side. Make a plot for this case also.

Exercise 8.6: Harmonic and anharmonic oscillators

The simple harmonic oscillator arises in many physical problems, in mechanics, electricity and magnetism, and condensed matter physics, among other areas. Consider the standard oscillator equation

$$\frac{d^2x}{dt^2} = -\omega^2 x.$$

- Using the methods described in the preceding section, turn this second-order equation into two coupled first-order equations. Then write a program to solve them for the case $\omega = 1$ in the range from $t = 0$ to $t = 50$. A second-order equation requires two initial conditions, one on x and one on its derivative. For this problem use $x = 1$ and $dx/dt = 0$ as initial conditions. Have your program make a graph showing the value of x as a function of time.
- Now increase the amplitude of the oscillations by making the initial value of x bigger—say $x = 2$ —and confirm that the period of the oscillations stays roughly the same.
- Modify your program to solve for the motion of the anharmonic oscillator described by the equation

$$\frac{d^2x}{dt^2} = -\omega^2 x^3.$$

Again take $\omega = 1$ and initial conditions $x = 1$ and $dx/dt = 0$ and make a plot of the motion of the oscillator. Again increase the amplitude. You should observe that the oscillator oscillates faster at higher amplitudes. (You can try lower amplitudes too if you like, which should be slower.) The variation of frequency with amplitude in an anharmonic oscillator was studied previously in Exercise 5.10.

- Modify your program so that instead of plotting x against t , it plots dx/dt against x , i.e., the “velocity” of the oscillator against its “position.” Such a plot is called a *phase space* plot.

- e) The *van der Pol oscillator*, which appears in electronic circuits and in laser physics, is described by the equation

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + \omega^2x = 0.$$

Modify your program to solve this equation from $t = 0$ to $t = 20$ and hence make a phase space plot for the van der Pol oscillator with $\omega = 1$, $\mu = 1$, and initial conditions $x = 1$ and $dx/dt = 0$. Try it also for $\mu = 2$ and $\mu = 4$ (still with $\omega = 1$). Make sure you use a small enough value of the time interval h to get a smooth, accurate phase space plot.

Exercise 8.7: Trajectory with air resistance

Many elementary mechanics problems deal with the physics of objects moving or flying through the air, but they almost always ignore friction and air resistance to make the equations solvable. If we're using a computer, however, we don't need solvable equations.

Consider, for instance, a spherical cannonball shot from a cannon standing on level ground. The air resistance on a moving sphere is a force in the opposite direction to the motion with magnitude

$$F = \frac{1}{2}\pi R^2 \rho C v^2,$$

where R is the sphere's radius, ρ is the density of air, v is the velocity, and C is the so-called *coefficient of drag* (a property of the shape of the moving object, in this case a sphere).

- a) Starting from Newton's second law, $F = ma$, show that the equations of motion for the position (x, y) of the cannonball are

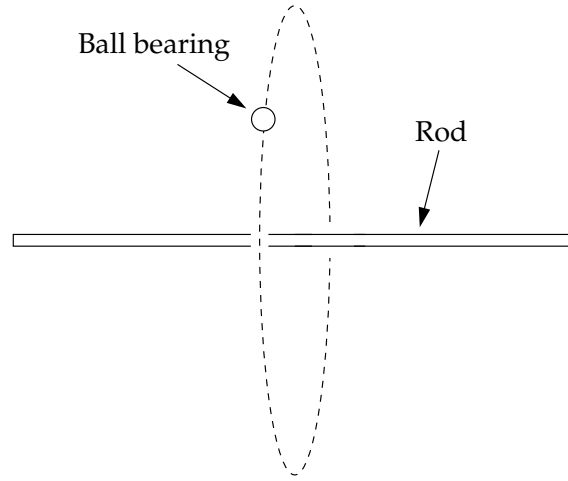
$$\ddot{x} = -\frac{\pi R^2 \rho C}{2m} \dot{x} \sqrt{\dot{x}^2 + \dot{y}^2}, \quad \ddot{y} = -g - \frac{\pi R^2 \rho C}{2m} \dot{y} \sqrt{\dot{x}^2 + \dot{y}^2},$$

where m is the mass of the cannonball, g is the acceleration due to gravity, and \dot{x} and \ddot{x} are the first and second derivatives of x with respect to time.

- b) Change these two second-order equations into four first-order equations using the methods you have learned, then write a program that solves the equations for a cannonball of mass 1 kg and radius 8 cm, shot at 30° to the horizontal with initial velocity 100 ms^{-1} . The density of air is $\rho = 1.22 \text{ kg m}^{-3}$ and the coefficient of drag for a sphere is $C = 0.47$. Make a plot of the trajectory of the cannonball (i.e., a graph of y as a function of x).
- c) When one ignores air resistance, the distance traveled by a projectile does not depend on the mass of the projectile. In real life, however, mass certainly does make a difference. Use your program to estimate the total distance traveled (over horizontal ground) by the cannonball above, and then experiment with the program to determine whether the cannonball travels further if it is heavier or lighter. You could, for instance, plot a series of trajectories for cannonballs of different masses, or you could make a graph of distance traveled as a function of mass. Describe briefly what you discover.

Exercise 8.8: Space garbage

A heavy steel rod and a spherical ball-bearing, discarded by a passing spaceship, are floating in zero gravity and the ball bearing is orbiting around the rod under the effect of its gravitational pull:



For simplicity we'll assume that the rod is of negligible cross-section and heavy enough that it doesn't move significantly, and that the ball bearing is orbiting around the rod's mid-point in a plane perpendicular to the rod.

- a) Treating the rod as a line of mass M and length L and the ball bearing as a point mass m , show that the attractive force F felt by the ball bearing in the direction toward the center of the rod is given by

$$F = \frac{GMm}{L} \sqrt{x^2 + y^2} \int_{-L/2}^{L/2} \frac{dz}{(x^2 + y^2 + z^2)^{3/2}},$$

where G is Newton's gravitational constant and x and y are the coordinates of the ball bearing in the plane perpendicular to the rod. The integral can be done in closed form and gives

$$F = \frac{GMm}{\sqrt{(x^2 + y^2)(x^2 + y^2 + L^2/4)}}.$$

Hence show that the equations of motion for the position x, y of the ball bearing in the xy -plane are

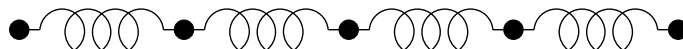
$$\frac{d^2x}{dt^2} = -GM \frac{x}{r^2 \sqrt{r^2 + L^2/4}}, \quad \frac{d^2y}{dt^2} = -GM \frac{y}{r^2 \sqrt{r^2 + L^2/4}},$$

where $r = \sqrt{x^2 + y^2}$.

- b) Convert these two second-order equations into four first-order ones using the techniques of Section 8.3. Then, working in units where $G = 1$, write a program to solve them for $M = 10, L = 2$, and initial conditions $(x, y) = (1, 0)$ with velocity of $+1$ in the y direction. Calculate the orbit from $t = 0$ to $t = 10$ and make a plot of it, meaning a plot of y against x . You should find that the ball bearing does not orbit in a circle or ellipse as a planet does, but has a precessing orbit, which arises because the attractive force is not a simple $1/r^2$ force as it is for a planet orbiting the Sun.

Exercise 8.9: Vibration in a one-dimensional system

In Example 6.2 on page 235 we studied the motion of a system of N identical masses (in zero gravity) joined by identical linear springs like this:



As we showed, the horizontal displacements ξ_i of masses $i = 1 \dots N$ satisfy equations of motion

$$\begin{aligned} m \frac{d^2 \xi_1}{dt^2} &= k(\xi_2 - \xi_1) + F_1, \\ m \frac{d^2 \xi_i}{dt^2} &= k(\xi_{i+1} - \xi_i) + k(\xi_{i-1} - \xi_i) + F_i, \\ m \frac{d^2 \xi_N}{dt^2} &= k(\xi_{N-1} - \xi_N) + F_N. \end{aligned}$$

where m is the mass, k is the spring constant, and F_i is the external force on mass i . In Example 6.2 we showed how these equations could be solved by guessing a form for the solution and using a matrix method. Here we'll solve them more directly.

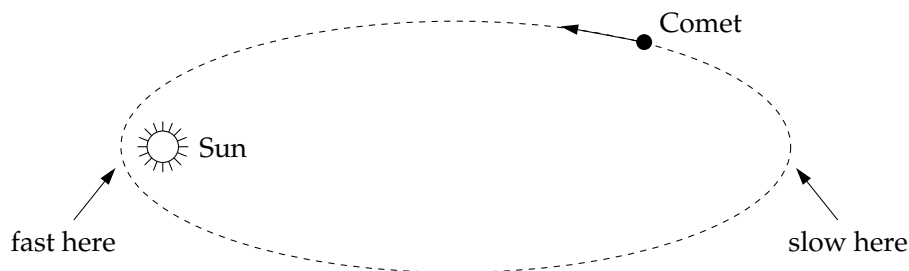
- a) Write a program to solve for the motion of the masses using the fourth-order Runge–Kutta method for the case we studied previously where $m = 1$ and $k = 6$, and the driving forces are all zero except for $F_1 = \cos \omega t$ with $\omega = 2$. Plot your solutions for the displacements ξ_i of all the masses as a function of time from $t = 0$ to $t = 20$ on the same plot. Write your program to work with general N , but test it out for small values— $N = 5$ is a reasonable choice.

You will need first of all to convert the N second-order equations of motion into $2N$ first-order equations. Then combine all of the dependent variables in those equations into a single large vector \mathbf{r} to which you can apply the Runge–Kutta method in the standard fashion.

- b) Modify your program to create an animation of the movement of the masses, represented as spheres on the computer screen. You will probably find the rate function discussed in Section 3.5 useful for making your animation run at a sensible speed.

Exercise 8.10: Cometary orbits

Many comets travel in highly elongated orbits around the Sun. For much of their lives they are far out in the solar system, moving very slowly, but on rare occasions their orbit brings them close to the Sun for a fly-by and for a brief period of time they move very fast indeed:



This is a classic example of a system for which an adaptive step size method is useful, because for the large periods of time when the comet is moving slowly we can use long time-steps, so that the program runs quickly, but short time-steps are crucial in the brief but fast-moving period close to the Sun.

The differential equation obeyed by a comet is straightforward to derive. The force between the Sun, with mass M at the origin, and a comet of mass m with position vector \mathbf{r} is GMm/r^2 in direction $-\mathbf{r}/r$ (i.e., the direction towards the Sun), and hence Newton's second law tells us that

$$m \frac{d^2 \mathbf{r}}{dt^2} = - \left(\frac{GMm}{r^2} \right) \frac{\mathbf{r}}{r}.$$

Canceling the m and taking the x component we have

$$\frac{d^2 x}{dt^2} = -GM \frac{x}{r^3},$$

and similarly for the other two coordinates. We can, however, throw out one of the coordinates because the comet stays in a single plane as it orbits. If we orient our axes so that this plane is perpendicular to the z -axis, we can forget about the z coordinate and we are left with just two second-order equations to solve:

$$\frac{d^2 x}{dt^2} = -GM \frac{x}{r^3}, \quad \frac{d^2 y}{dt^2} = -GM \frac{y}{r^3},$$

where $r = \sqrt{x^2 + y^2}$.

- a) Turn these two second-order equations into four first-order equations, using the methods you have learned.
- b) Write a program to solve your equations using the fourth-order Runge–Kutta method with a *fixed* step size. You will need to look up the mass of the Sun and Newton's gravitational constant G . As an initial condition, take a comet at coordinates $x = 4$ billion kilometers and $y = 0$ (which is somewhere out around the orbit of Neptune) with initial velocity $v_x = 0$ and $v_y = 500 \text{ m s}^{-1}$. Make a graph showing the trajectory of the comet (i.e., a plot of y against x).

Choose a fixed step size h that allows you to accurately calculate at least two full orbits of the comet. Since orbits are periodic, a good indicator of an accurate calculation is that successive orbits of the comet lie on top of one another on your plot. If they do not then you need a smaller value of h . Give a short description of your findings. What value of h did you use? What did you observe in your simulation? How long did the calculation take?

- c) Make a copy of your program and modify the copy to do the calculation using an adaptive step size. Set a target accuracy of $\delta = 1$ kilometer per year in the position of the comet and again plot the trajectory. What do you see? How do the speed, accuracy, and step size of the calculation compare with those in part (b)?
- d) Modify your program to place dots on your graph showing the position of the comet at each Runge–Kutta step around a single orbit. You should see the steps getting closer

together when the comet is close to the Sun and further apart when it is far out in the solar system.

Calculations like this can be extended to cases where we have more than one orbiting body—see Exercise 8.16 for an example. We can include planets, moons, asteroids, and others. Analytic calculations are impossible for such complex systems, but with careful numerical solution of differential equations we can calculate the motions of objects throughout the entire solar system.

Exercise 8.11: Write a program to solve the differential equation

$$\frac{d^2x}{dt^2} - \left(\frac{dx}{dt}\right)^2 + x + 5 = 0$$

using the leapfrog method. Solve from $t = 0$ to $t = 50$ in steps of $h = 0.001$ with initial condition $x = 1$ and $dx/dt = 0$. Make a plot of your solution showing x as a function of t .

Exercise 8.12: Orbit of the Earth

Use the Verlet method to calculate the orbit of the Earth around the Sun. The equations of motion for the position $\mathbf{r} = (x, y)$ of the planet in its orbital plane are the same as those for any orbiting body and are derived in Exercise 8.10 on page 361. In vector form, they are

$$\frac{d^2\mathbf{r}}{dt^2} = -GM\frac{\mathbf{r}}{r^3},$$

where $G = 6.6738 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$ is Newton's gravitational constant and $M = 1.9891 \times 10^{30} \text{ kg}$ is the mass of the Sun.

The orbit of the Earth is not perfectly circular, the planet being sometimes closer to and sometimes further from the Sun. When it is at its closest point, or *perihelion*, it is moving precisely tangentially (i.e., perpendicular to the line between itself and the Sun) and it has distance $1.4710 \times 10^{11} \text{ m}$ from the Sun and linear velocity $3.0287 \times 10^4 \text{ m s}^{-1}$.

- Write a program to calculate the orbit of the Earth using the Verlet method, Eqs. (8.77) and (8.78), with a time-step of $h = 1$ hour. Make a plot of the orbit, showing several complete revolutions about the Sun. The orbit should be very slightly, but visibly, non-circular.
- The gravitational potential energy of the Earth is $-GMm/r$, where $m = 5.9722 \times 10^{24} \text{ kg}$ is the mass of the planet, and its kinetic energy is $\frac{1}{2}mv^2$ as usual. Modify your program to calculate both of these quantities at each step, along with their sum (which is the total energy), and make a plot showing all three as a function of time on the same axes. You should find that the potential and kinetic energies vary visibly during the course of an orbit, but the total energy remains constant.
- Now plot the total energy alone without the others and you should be able to see a slight variation over the course of an orbit. Because you're using the Verlet method, however, which conserves energy in the long term, the energy should always return to its starting value at the end of each complete orbit.

Exercise 8.13: Planetary orbits

This exercise asks you to calculate the orbits of two of the planets using the Bulirsch–Stoer method. The method gives results significantly more accurate than the Verlet method used to calculate the Earth’s orbit in Exercise 8.12.

The equations of motion for the position x, y of a planet in its orbital plane are the same as those for any orbiting body and are derived in Exercise 8.10 on page 361:

$$\frac{d^2x}{dt^2} = -GM\frac{x}{r^3}, \quad \frac{d^2y}{dt^2} = -GM\frac{y}{r^3},$$

where $G = 6.6738 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$ is Newton’s gravitational constant, $M = 1.9891 \times 10^{30} \text{ kg}$ is the mass of the Sun, and $r = \sqrt{x^2 + y^2}$.

Let us first solve these equations for the orbit of the Earth, duplicating the results of Exercise 8.12, though with greater accuracy. The Earth’s orbit is not perfectly circular, but rather slightly elliptical. When it is at its closest approach to the Sun, its perihelion, it is moving precisely tangentially (i.e., perpendicular to the line between itself and the Sun) and it has distance $1.4710 \times 10^{11} \text{ m}$ from the Sun and linear velocity $3.0287 \times 10^4 \text{ ms}^{-1}$.

- a) Write a program, or modify the one from Example 8.7, to calculate the orbit of the Earth using the Bulirsch–Stoer method to a positional accuracy of 1 km per year. Divide the orbit into intervals of length $H = 1$ week and then calculate the solution for each interval using the combined modified midpoint/Richardson extrapolation method described in this section. Make a plot of the orbit, showing at least one complete revolution about the Sun.
- b) Modify your program to calculate the orbit of the dwarf planet Pluto. The distance between the Sun and Pluto at perihelion is $4.4368 \times 10^{12} \text{ m}$ and the linear velocity is $6.1218 \times 10^3 \text{ ms}^{-1}$. Choose a suitable value for H to make your calculation run in reasonable time, while once again giving a solution accurate to 1 km per year.

You should find that the orbit of Pluto is significantly elliptical—much more so than the orbit of the Earth. Pluto is a Kuiper belt object, similar to a comet, and (unlike true planets) it’s typical for such objects to have quite elliptical orbits.

Exercise 8.14: Quantum oscillators

Consider the one-dimensional, time-independent Schrödinger equation in a harmonic (i.e., quadratic) potential $V(x) = V_0 x^2/a^2$, where V_0 and a are constants.

- a) Write down the Schrödinger equation for this problem and convert it from a second-order equation to two first-order ones, as in Example 8.9. Write a program, or modify the one from Example 8.9, to find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50 \text{ eV}$, and $a = 10^{-11} \text{ m}$. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic

oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution—there is no need to use an adaptive method for this problem.

The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

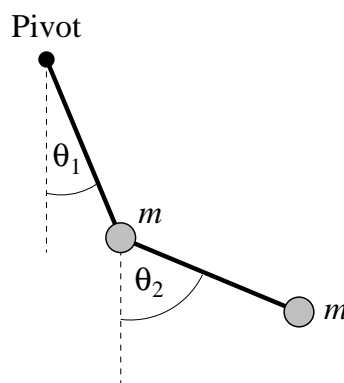
- b) Now modify your program to calculate the same three energies for the anharmonic oscillator with $V(x) = V_0 x^4 / a^4$, with the same parameter values.
- c) Modify your program further to calculate the properly normalized wavefunctions of the anharmonic oscillator for the three states and make a plot of them, all on the same axes, as a function of x over a modest range near the origin—say $x = -5a$ to $x = 5a$.

To normalize the wavefunctions you will have to evaluate the integral $\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ and then rescale ψ appropriately to ensure that the area under the square of each of the wavefunctions is 1. Either the trapezoidal rule or Simpson's rule will give you a reasonable value for the integral. Note, however, that you may find a few very large values at the end of the array holding the wavefunction. Where do these large values come from? Are they real, or spurious?

One simple way to deal with the large values is to make use of the fact that the system is symmetric about its midpoint and calculate the integral of the wavefunction over only the left-hand half of the system, then double the result. This neatly misses out the large values.

Exercise 8.15: The double pendulum

If you did Exercise 8.4 you will have created a program to calculate the movement of a nonlinear pendulum. Although it is nonlinear, the nonlinear pendulum's movement is nonetheless perfectly regular and periodic—there are no surprises. A *double pendulum*, on the other hand, is completely the opposite—chaotic and unpredictable. A double pendulum consists of a normal pendulum with another pendulum hanging from its end. For simplicity let us ignore friction, and assume that both pendulums have bobs of the same mass m and massless arms of the same length ℓ . Thus the setup looks like this:



The position of the arms at any moment in time is uniquely specified by the two angles θ_1 and θ_2 . The equations of motion for the angles are most easily derived using the Lagrangian formalism, as follows.

The heights of the two bobs, measured from the level of the pivot are

$$h_1 = -\ell \cos \theta_1, \quad h_2 = -\ell(\cos \theta_1 + \cos \theta_2),$$

so the potential energy of the system is

$$V = mgh_1 + mgh_2 = -mg\ell(2 \cos \theta_1 + \cos \theta_2),$$

where g is the acceleration due to gravity. The (linear) velocities of the two bobs are given by

$$v_1 = \ell \dot{\theta}_1, \quad v_2^2 = \ell^2 [\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)],$$

where $\dot{\theta}$ means the derivative of θ with respect to time t . (If you don't see where the second velocity equation comes from, it's a good exercise to derive it for yourself from the geometry of the pendulum.) Now the total kinetic energy is

$$T = \frac{1}{2}mv_1^2 + \frac{1}{2}mv_2^2 = m\ell^2 [\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)],$$

and the Lagrangian of the system is

$$\mathcal{L} = T - V = m\ell^2 [\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)] + mg\ell(2 \cos \theta_1 + \cos \theta_2).$$

Then the equations of motion are given by the Euler–Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_1} \right) = \frac{\partial \mathcal{L}}{\partial \theta_1}, \quad \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_2} \right) = \frac{\partial \mathcal{L}}{\partial \theta_2},$$

which in this case give

$$\begin{aligned} 2\ddot{\theta}_1 + \ddot{\theta}_2 \cos(\theta_1 - \theta_2) + \dot{\theta}_2^2 \sin(\theta_1 - \theta_2) + 2\frac{g}{\ell} \sin \theta_1 &= 0, \\ \ddot{\theta}_2 + \ddot{\theta}_1 \cos(\theta_1 - \theta_2) - \dot{\theta}_1^2 \sin(\theta_1 - \theta_2) + \frac{g}{\ell} \sin \theta_2 &= 0, \end{aligned}$$

where the mass m has canceled out.

These are second-order equations, but we can convert them into first-order ones by the usual method, defining two new variables, ω_1 and ω_2 , thus:

$$\dot{\theta}_1 = \omega_1, \quad \dot{\theta}_2 = \omega_2.$$

In terms of these variables our equations of motion become

$$\begin{aligned} 2\dot{\omega}_1 + \dot{\omega}_2 \cos(\theta_1 - \theta_2) + \omega_2^2 \sin(\theta_1 - \theta_2) + 2\frac{g}{\ell} \sin \theta_1 &= 0, \\ \dot{\omega}_2 + \dot{\omega}_1 \cos(\theta_1 - \theta_2) - \omega_1^2 \sin(\theta_1 - \theta_2) + \frac{g}{\ell} \sin \theta_2 &= 0. \end{aligned}$$

Finally we have to rearrange these into the standard form of Eq. (8.29) with a single derivative on the left-hand side of each one, which gives

$$\dot{\omega}_1 = -\frac{\omega_1^2 \sin(2\theta_1 - 2\theta_2) + 2\omega_2^2 \sin(\theta_1 - \theta_2) + (g/\ell) [\sin(\theta_1 - 2\theta_2) + 3 \sin \theta_1]}{3 - \cos(2\theta_1 - 2\theta_2)},$$

$$\dot{\omega}_2 = \frac{4\omega_1^2 \sin(\theta_1 - \theta_2) + \omega_2^2 \sin(2\theta_1 - 2\theta_2) + 2(g/\ell) [\sin(2\theta_1 - \theta_2) - \sin \theta_2]}{3 - \cos(2\theta_1 - 2\theta_2)}.$$

(This last step is quite tricky and involves some trigonometric identities. If you're not certain of how the calculation goes you may find it useful to go through the derivation for yourself.)

These two equations, along with the equations $\dot{\theta}_1 = \omega_1$ and $\dot{\theta}_2 = \omega_2$, give us four first-order equations which between them define the motion of the double pendulum.

- Derive an expression for the total energy $E = T + V$ of the system in terms of the variables $\theta_1, \theta_2, \omega_1$, and ω_2 , plus the constants g, ℓ , and m .
- Write a program using the fourth-order Runge–Kutta method to solve the equations of motion for the case where $\ell = 40$ cm, with the initial conditions $\theta_1 = \theta_2 = 90^\circ$ and $\omega_1 = \omega_2 = 0$. Use your program to calculate the total energy of the system assuming that the mass of the bobs is 1 kg each, and make a graph of energy as a function of time from $t = 0$ to $t = 100$ seconds.

Because of energy conservation, the total energy should be constant over time (actually it should be zero for this particular set of initial conditions), but you will find that it is not perfectly constant because of the approximate nature of the solution of the differential equation. Choose a suitable value of the step size h to ensure that the variation in energy is less than 10^{-5} Joules over the course of the calculation.

- Make a copy of your program and modify the copy to create a second program that does not produce a graph, but instead makes an animation of the motion of the double pendulum over time. At a minimum, the animation should show the two arms and the two bobs.

Hint: As in Exercise 8.4 you will probably find the function rate useful in order to make your program run at a steady speed. You will probably also find that the value of h needed to get the required accuracy in your solution gives a frame-rate much faster than any that can reasonably be displayed in your animation, so you won't be able to display every time-step of the calculation in the animation. Instead you will have to arrange the program so that it updates the animation only once every several Runge–Kutta steps.

Exercise 8.16: The three-body problem

If you mastered Exercise 8.10 on cometary orbits, here's a more challenging problem in celestial mechanics—and a classic in the field—the *three-body problem*.

Three stars, in otherwise empty space, are initially at rest, with the following masses and positions, in arbitrary units:

	Mass	x	y
Star 1	150	3	1
Star 2	200	-1	-2
Star 3	250	-1	1

(All the z coordinates are zero, so the three stars lie in the xy plane.)

- a) Show that the equation of motion governing the position \mathbf{r}_1 of the first star is

$$\frac{d^2\mathbf{r}_1}{dt^2} = Gm_2 \frac{\mathbf{r}_2 - \mathbf{r}_1}{|\mathbf{r}_2 - \mathbf{r}_1|^3} + Gm_3 \frac{\mathbf{r}_3 - \mathbf{r}_1}{|\mathbf{r}_3 - \mathbf{r}_1|^3}$$

and derive two similar equations for the positions \mathbf{r}_2 and \mathbf{r}_3 of the other two stars. Then convert the three second-order equations into six equivalent first-order equations, using the techniques you have learned.

- b) Working in units where $G = 1$, write a program to solve your equations and hence calculate the motion of the stars from $t = 0$ to $t = 2$. Make a plot showing the trails of all three stars (i.e., a graph of y against x for each star).
- c) Modify your program to make an animation of the motion on the screen from $t = 0$ to $t = 10$. You may wish to make the three stars different sizes or colors (or both) so that you can tell which is which.

To do this calculation properly you will need to use an adaptive step size method, for the same reasons as in Exercise 8.10—the stars move very rapidly when they are close together and very slowly when they are far apart. An adaptive method is the only way to get the accuracy you need in the fast-moving parts of the motion without wasting hours uselessly calculating the slow parts with a tiny step size. Construct your program so that it introduces an error of no more than 10^{-3} in the position of any star per unit time.

Creating an animation with an adaptive step size can be challenging, since the steps do not all correspond to the same amount of real time. The simplest thing to do is just to ignore the varying step sizes and make an animation as if they were all equal, updating the positions of the stars on the screen at every step or every several steps. This will give you a reasonable visualization of the motion, but it will look a little odd because the stars will slow down, rather than speed up, as they come close together, because the adaptive calculation will automatically take more steps in this region.

A better solution is to vary the frame-rate of your animation so that the frames run proportionally faster when h is smaller, meaning that the frame-rate needs to be equal to C/h for some constant C . You can achieve this by using the rate function from the visual package to set a different frame-rate on each step, equal to C/h . If you do this, it's a good idea to not let the value of h grow too large, or the animation will make some large jumps that look uneven on the screen. Insert extra program lines to ensure that h never exceeds a value h_{\max} that you choose. Values for the constants of around $C = 0.1$ and $h_{\max} = 10^{-3}$ seem to give reasonable results.

Exercise 8.17: Cometary orbits and the Bulirsch–Stoer method

Repeat the calculation of the cometary orbit in Exercise 8.10 (page 361) using the adaptive Bulirsch–Stoer method of Section 8.5.6 to calculate a solution accurate to $\delta = 1$ kilometer per

year in the position of the comet. Calculate the solution from $t = 0$ to $t = 2 \times 10^9$ s, initially using just a single time interval of size $H = 2 \times 10^9$ s and allowing a maximum of $n = 8$ modified midpoint steps before dividing the interval in half and trying again. Then these intervals may be subdivided again, as described in Section 8.5.6, as many times as necessary until the method converges in eight steps or less in each interval.

Make a plot of the orbit (i.e., a plot of y against x) and have your program add dots to the trajectory to show where the ends of the time intervals lie. You should see the time intervals getting shorter in the part of the trajectory close to the Sun, where the comet is moving rapidly.

Hint: The simplest way to do this calculation is to make use of recursion, the ability of a Python function to call itself. (If you're not familiar with the idea of recursion you might like to look at Exercise 2.13 on page 83 before doing this exercise.) Write a user-defined function called, say, `step(r, t, H)` that takes as arguments the position vector $\mathbf{r} = (x, y)$ at a starting time t and an interval length H , and returns the new value of \mathbf{r} at time $t + H$. This function should perform the modified midpoint/Richardson extrapolation calculation described in Section 8.5.5 until either the calculation converges to the required accuracy or you reach the maximum number $n = 8$ of modified midpoint steps. If it fails to converge in eight steps, have your function call itself, twice, to calculate separately the solution for the first then the second half of the interval from t to $t + H$, something like this:

```
r1 = step(r, t, H/2)
r2 = step(r1, t+H/2, H/2)
```

(Then *these* functions can call themselves, and so forth, subdividing the interval as many times as necessary to reach the required accuracy.)

Exercise 8.18: Oscillating chemical reactions

The *Belousov–Zhabotinsky reaction* is a chemical oscillator, a cocktail of chemicals which, when heated, undergoes a series of reactions that cause the chemical concentrations in the mixture to oscillate between two extremes. You can add an indicator dye to the reaction which changes color depending on the concentrations and watch the mixture switch back and forth between two different colors for as long as you go on heating the mixture.

Physicist Ilya Prigogine formulated a mathematical model of this type of chemical oscillator, which he called the “Brusselator” after his home town of Brussels. The equations for the Brusselator are

$$\frac{dx}{dt} = 1 - (b + 1)x + ax^2y, \quad \frac{dy}{dt} = bx - ax^2y.$$

Here x and y represent concentrations of chemicals and a and b are positive constants.

Write a program to solve these equations for the case $a = 1$, $b = 3$ with initial conditions $x = y = 0$, to an accuracy of at least $\delta = 10^{-10}$ per unit time in both x and y , using the adaptive Bulirsch–Stoer method described in Section 8.5.6. Calculate a solution from $t = 0$ to $t = 20$, initially using a single time interval of size $H = 20$. Allow a maximum of $n = 8$ modified midpoint steps in an interval before you divide in half and try again.

Make a plot of your solutions for x and y as a function of time, both on the same graph, and have your program add dots to the curves to show where the boundaries of the time intervals

lie. You should find that the points are significantly closer together in parts of the solution where the variables are changing rapidly.

Hint: The simplest way to perform the calculation is to make use of recursion, as described in Exercise 8.17.