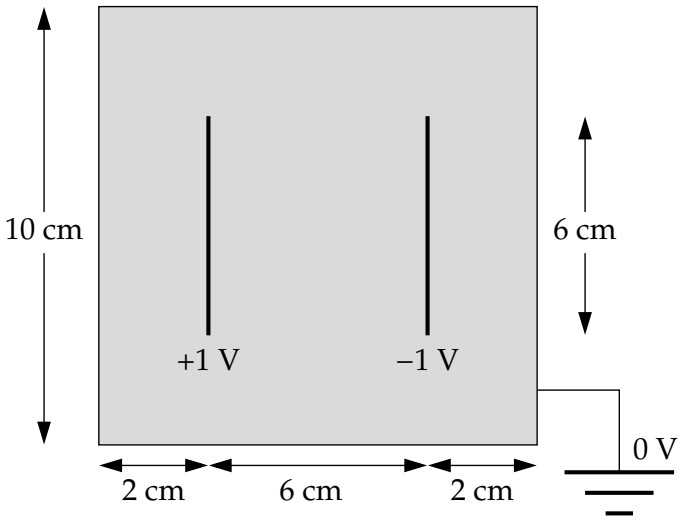
COMPUTATIONAL PHYSICS

EXERCISES FOR CHAPTER 9

Exercise 9.1: Write a program, or modify the one from Example 9.1, to solve Poisson's equation for the system described in Example 9.2. Work in units where $\epsilon_0 = 1$ and continue the iteration until your solution for the electric potential changes by less than 10^{-6} V per step at every grid point.

Exercise 9.2: Use the Gauss–Seidel method to solve Laplace's equation for the two-dimensional problem in Example 9.1—a square box 1 m on each side, at voltage $V = 1$ volt along the top wall and zero volts along the other three. Use a grid of spacing $a = 1$ cm, so that there are 100 grid points along each wall, or 101 if you count the points at both ends. Continue the iteration of the method until the value of the electric potential changes by no more than $\delta = 10^{-6}$ V at any grid point on any step, then make a density plot of the final solution, similar to that shown in Fig. 9.3. Experiment with different values of ω to find which value gives the fastest solution. As mentioned above, you should find that a value around 0.9 does well. In general larger values cause the calculation to run faster, but if you choose too large a value the speed drops off and for values above 1 the calculation becomes unstable.

Exercise 9.3: Consider the following simple model of an electronic capacitor, consisting of two flat metal plates enclosed in a square metal box:



For simplicity let us model the system in two dimensions. Using any of the methods we have studied, write a program to calculate the electrostatic potential in the box on a grid of 100×100 points, where the walls of the box are at voltage zero and the two plates (which are of negligible thickness) are at voltages ± 1 V as shown. Have your program calculate the value of the potential at each grid point to a precision of 10^{-6} volts and then make a density plot of the result.

Hint: Notice that the capacitor plates are at fixed *voltage*, not fixed charge, so this problem differs from the problem with the two charges in Exercise 9.1. In effect, the capacitor plates are part of the boundary condition in this case: they behave the same way as the walls of the box, with potentials that are fixed at a certain value and cannot change.

Exercise 9.4: Thermal diffusion in the Earth's crust

A classic example of a diffusion problem with a time-varying boundary condition is the diffusion of heat into the crust of the Earth, as surface temperature varies with the seasons. Suppose the mean daily temperature at a particular point on the surface varies as:

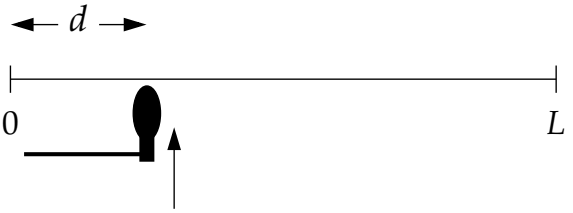
$$T_0(t) = A + B\sin\frac{2\pi t}{\tau},$$

where $\tau = 365$ days, $A = 10°\text{C}$ and $B = 12°\text{C}$. At a depth of 20 m below the surface almost all annual temperature variation is ironed out and the temperature is, to a good approximation, a constant 11°C (which is higher than the mean surface temperature of 10°C—temperature increases with depth, due to heating from the hot core of the planet). The thermal diffusivity of the Earth's crust varies somewhat from place to place, but for our purposes we will treat it as constant with value $D = 0.1\,\text{m}^2\,\text{day}^{-1}$.

Write a program, or modify one of the ones given in this chapter, to calculate the temperature profile of the crust as a function of depth up to 20 m and time up to 10 years. Start with temperature everywhere equal to 10°C, except at the surface and the deepest point, choose values for the number of grid points and the time-step h, then run your program for the first nine simulated years, to allow it to settle down into whatever pattern it reaches. Then for the tenth and final year plot four temperature profiles taken at 3-month intervals on a single graph to illustrate how the temperature changes as a function of depth and time.

Exercise 9.5: FTCS solution of the wave equation

Consider a piano string of length L, initially at rest. At time $t = 0$ the string is struck by the piano hammer a distance d from the end of the string:



The string vibrates as a result of being struck, except at the ends, $x = 0$ and $x = L$, where it is held fixed.

a) Write a program that uses the FTCS method to solve the complete set of simultaneous first-order equations, Eq. (9.28), for the case $v = 100\,\text{ms}^{-1}$, with the initial condition that $\phi(x) = 0$ everywhere but the velocity $\psi(x)$ is nonzero, with profile

$$\psi(x) = C\frac{x(L-x)}{L^2}\exp\left[-\frac{(x-d)^2}{2\sigma^2}\right],$$

where $L = 1\,\text{m}$, $d = 10\,\text{cm}$, $C = 1\,\text{ms}^{-1}$, and $\sigma = 0.3\,\text{m}$. You will also need to choose a value for the time-step h. A reasonable choice is $h = 10^{-6}\,\text{s}$.

b) Make an animation of the motion of the piano string using the facilities provided by the `visual` package, which we studied in Section 3.4. There are various ways you could do this. A simple one would be to just place a small sphere at the location of each grid point on the string. A more sophisticated approach would be to use the `curve` object in the `visual` package—see the on-line documentation at `www.vpython.org` for details. A convenient feature of the curve object is that you can specify its set of x positions and y positions separately as arrays. In this exercise the x positions only need to specified once, since they never change, while the y positions will need to be specified anew each time you take a time-step. Also, since the vertical displacement of the string is much less than its horizontal length, you will probably need to multiply the vertical displacement by a fairly large factor to make it visible on the screen.

   Allow your animation to run for some time, until numerical instabilities start to appear.

Exercise 9.6: What would the equivalent of Eq. (9.7) be in three dimensions?

Exercise 9.7: The relaxation method for ordinary differential equations

There is no reason why the relaxation method must be restricted to the solution of differential equations with two or more independent variables. It can also be applied to those with one independent variable, i.e., to ordinary differential equations. In this context, as with partial differential equations, it is a technique for solving boundary value problems, which are less common with ordinary differential equations but do occur—we discussed them in Section 8.6.

Consider the problem we looked at in Example 8.8 on page 390, in which a ball of mass $m = 1\,\text{kg}$ is thrown from height $x = 0$ into the air and lands back at $x = 0$ ten seconds later. The problem is to calculate the trajectory of the ball, but we cannot do it using initial value methods like the ordinary Runge–Kutta method because we are not told the initial velocity of the ball. One approach to finding a solution is the shooting method of Section 8.6.1. Another is the relaxation method.

Ignoring friction effects, the trajectory is the solution of the ordinary differential equation

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -g,$$

where g is the acceleration due to gravity.

a) Replacing the second derivative in this equation with its finite-difference approximation, Eq. (5.109), derive a relaxation-method equation for solving this problem on a time-like "grid" of points with separation h.

b) Taking the boundary conditions to be that $x = 0$ at $t = 0$ and $t = 10$, write a program to solve for the height of the ball as a function of time using the relaxation method with 100 points and make a plot of the result from $t = 0$ to $t = 10$. Run the relaxation method until the answers change by 10^{-6} or less at every point on each step.

Note that, unlike the shooting method, the relaxation method does not give us the initial value of the velocity needed to achieve the required solution. It gives us only the solution itself, although one could get an approximation to the initial velocity by calculating a numerical derivative of the solution at time $t = 0$. On balance, however, the relaxation method for ordinary differential equations is most useful when one wants to know the details of the solution itself, but not the initial conditions needed to achieve it.

Exercise 9.8: The Schrödinger equation and the Crank–Nicolson method

Perhaps the most important partial differential equation, at least for physicists, is the Schrödinger equation. This exercise uses the Crank–Nicolson method to solve the full time-dependent Schrödinger equation and hence develop a picture of how a wavefunction evolves over time. The following exercise, Exercise 9.9, solves the same problem again, but using the spectral method.

We will look at the Schrödinger equation in one dimension. The techniques for calculating solutions in two or three dimensions are basically the same as for one dimension, but the calculations take much longer on the computer, so in the interests of speed we'll stick with one dimension. In one dimension the Schrödinger equation for a particle of mass M with no potential energy reads

$$-\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} = \mathrm{i}\hbar\frac{\partial\psi}{\partial t}.$$

For simplicity, let's put our particle in a box with impenetrable walls, so that we only have to solve the equation in a finite-sized space. The box forces the wavefunction ψ to be zero at the walls, which we'll put at $x = 0$ and $x = L$.

Replacing the second derivative in the Schrödinger equation with a finite difference and applying Euler's method, we get the FTCS equation

$$\psi(x,t+h) = \psi(x,t) + h\frac{\mathrm{i}\hbar}{2ma^2}\bigl[\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)\bigr],$$

where a is the spacing of the spatial grid points and h is the size of the time-step. (Be careful not to confuse the time-step h with Planck's constant $\hbar$.) Performing a similar step in reverse, we get the implicit equation

$$\psi(x,t+h) - h\frac{\mathrm{i}\hbar}{2ma^2}\bigl[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h)\bigr] = \psi(x,t).$$

And taking the average of these two, we get the Crank–Nicolson equation for the Schrödinger equation:

$$\begin{aligned}\psi(x,t+h) - h\frac{\mathrm{i}\hbar}{4ma^2}&\bigl[\psi(x+a,t+h) + \psi(x-a,t+h) - 2\psi(x,t+h)\bigr]\\ &= \psi(x,t) + h\frac{\mathrm{i}\hbar}{4ma^2}\bigl[\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)\bigr].\end{aligned}$$

This gives us a set of simultaneous equations, one for each grid point.

The boundary conditions on our problem tell us that $\psi = 0$ at $x = 0$ and $x = L$ for all t. In between these points we have grid points at a, $2a$, $3a$, and so forth. Let us arrange the values of ψ at these interior points into a vector

$$\boldsymbol{\psi}(t) = \begin{pmatrix} \psi(a,t) \\ \psi(2a,t) \\ \psi(3a,t) \\ \vdots \end{pmatrix}.$$

Then the Crank–Nicolson equations can be written in the form

$$\mathbf{A}\boldsymbol{\psi}(t+h) = \mathbf{B}\boldsymbol{\psi}(t),$$

where the matrices $\mathbf{A}$ and $\mathbf{B}$ are both symmetric and tridiagonal:

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & & & \\ a_2 & a_1 & a_2 & & \\ & a_2 & a_1 & a_2 & \\ & & a_2 & a_1 & \\ & & & & \ddots \end{pmatrix}, \qquad \mathbf{B} = \begin{pmatrix} b_1 & b_2 & & & \\ b_2 & b_1 & b_2 & & \\ & b_2 & b_1 & b_2 & \\ & & b_2 & b_1 & \\ & & & & \ddots \end{pmatrix},$$

with

$$a_1 = 1 + h\frac{\mathrm{i}\hbar}{2ma^2}, \qquad a_2 = -h\frac{\mathrm{i}\hbar}{4ma^2}, \qquad b_1 = 1 - h\frac{\mathrm{i}\hbar}{2ma^2}, \qquad b_2 = h\frac{\mathrm{i}\hbar}{4ma^2}.$$

(Note the different signs and the factors of 2 and 4 in the denominators.)

The equation $\mathbf{A}\boldsymbol{\psi}(t+h) = \mathbf{B}\boldsymbol{\psi}(t)$ has precisely the form $\mathbf{A}\mathbf{x} = \mathbf{v}$ of the simultaneous equation problems we studied in Chapter 6 and can be solved using the same methods. Specifically, since the matrix $\mathbf{A}$ is tridiagonal in this case, we can use the fast tridiagonal version of Gaussian elimination that we looked at in Section 6.1.6.

Consider an electron (mass $M = 9.109 \times 10^{-31}\,\mathrm{kg}$) in a box of length $L = 10^{-8}\,\mathrm{m}$. Suppose that at time $t = 0$ the wavefunction of the electron has the form

$$\psi(x,0) = \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]\mathrm{e}^{\mathrm{i}\kappa x},$$

where

$$x_0 = \frac{L}{2}, \qquad \sigma = 1 \times 10^{-10}\,\mathrm{m}, \qquad \kappa = 5 \times 10^{10}\,\mathrm{m}^{-1},$$

and $\psi = 0$ on the walls at $x = 0$ and $x = L$. (This expression for $\psi(x,0)$ is not normalized—there should really be an overall multiplying coefficient to make sure that the probability density for the electron integrates to unity. It's safe to drop the constant, however, because the Schrödinger equation is linear, so the constant cancels out on both sides of the equation and plays no part in the solution.)

a) Write a program to perform a single step of the Crank–Nicolson method for this electron, calculating the vector $\boldsymbol{\psi}(t)$ of values of the wavefunction, given the initial wavefunction above and using $N = 1000$ spatial slices with $a = L/N$. Your program will have to

perform the following steps. First, given the vector $\boldsymbol{\psi}(0)$ at $t = 0$, you will have to multiply by the matrix $\mathbf{B}$ to get a vector $\mathbf{v} = \mathbf{B}\boldsymbol{\psi}$. Because of the tridiagonal form of $\mathbf{B}$, this is fairly simple. The ith component of $\mathbf{v}$ is given by

$$v_i = b_1\psi_i + b_2(\psi_{i+1} + \psi_{i-1}).$$

You will also have to choose a value for the time-step h. A reasonable choice is $h = 10^{-18}$ s.

Second you will have to solve the linear system $\mathbf{A}\mathbf{x} = \mathbf{v}$ for $\mathbf{x}$, which gives you the new value of $\boldsymbol{\psi}$. You could do this using a standard linear equation solver like the function `solve` in `numpy.linalg`, but since the matrix $\mathbf{A}$ is tridiagonal a better approach would be to use the fast solver for banded matrices given in Appendix E, which can be imported from the file `banded.py` (which you can find in the on-line resources). Note that although the wavefunction of a particle in principle has a complex value, in this case the wavefunction is always real—all the coefficients in the equations above are real numbers so if, as here, the wavefunction starts off real, then it remains real. Thus you do not need to use a complex array to represent the vector $\boldsymbol{\psi}$. A real one will do the job.

Third, once you have the code in place to perform a single step of the calculation, extend your program to perform repeated steps and hence solve for ψ at a sequence of times a separation h apart. Note that the matrix $\mathbf{A}$ is independent of time, so it doesn't change from one step to another. You can set up the matrix just once and then keep on reusing it for every step.

b) Extend your program to make an animation of the solution by displaying the real part of the wavefunction at each time-step. You can use the function `rate` from the package `visual` to ensure a smooth frame-rate for your animation—see Section 3.5 on page 117.

There are various ways you could do the animation. A simple one would be to just place a small sphere at each grid point with vertical position representing the value of the real part of the wavefunction. A more sophisticated approach would be to use the `curve` object from the `visual` package—see the on-line documentation at `www.vpython.org` for details. Depending on what coordinates you use for measuring x, you may need to scale the values of the wavefunction by an additional constant to make them a reasonable size on the screen. (If you measure your x position in meters then a scale factor of about 10^{-9} works well for the wavefunction.)

c) Run your animation for a while and describe what you see. Write a few sentences explaining in physics terms what is going on in the system.

Exercise 9.9: The Schrödinger equation and the spectral method

This exercise uses the spectral method to solve the time-dependent Schödinger equation

$$-\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t}$$

for the same system as in Exercise 9.8, a single particle in one dimension in a box of length L with impenetrable walls. The wavefunction in such a box necessarily goes to zero on the walls and hence one possible (unnormalized) solution of the equation is

$$\psi_k(x,t) = \sin\left(\frac{\pi k x}{L}\right) \mathrm{e}^{\mathrm{i}Et/\hbar},$$

where the energy E can be found by substituting into the Schrödinger equation, giving

$$E = \frac{\pi^2\hbar^2 k^2}{2ML^2}.$$

As with the vibrating string of Section 9.3.4, we can write a full solution as a linear combination of such individual solutions, which on the grid points $x_n = nL/N$ takes the value

$$\psi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1} b_k \sin\left(\frac{\pi k n}{N}\right) \exp\left(\mathrm{i}\frac{\pi^2\hbar k^2}{2ML^2}t\right),$$

where the b_k are some set of (possibly complex) coefficients that specify the exact shape of the wavefunction and the leading factor of $1/N$ is optional but convenient.

Since the Schrödinger equation (unlike the wave equation) is first order in time, we need only a single initial condition on the value of $\psi(x,t)$ to specify the coefficients b_k, although, since the coefficients are in general complex, we will need to calculate both real and imaginary parts of each coefficient.

As in Exercise 9.8 we consider an electron (mass $M = 9.109 \times 10^{-31}$ kg) in a box of length $L = 10^{-8}$ m. At time $t = 0$ the wavefunction of the electron has the form

$$\psi(x,0) = \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]\mathrm{e}^{\mathrm{i}\kappa x},$$

where

$$x_0 = \frac{L}{2}, \qquad \sigma = 1 \times 10^{-10}\,\mathrm{m}, \qquad \kappa = 5 \times 10^{10}\,\mathrm{m}^{-1},$$

and $\psi = 0$ on the walls at $x = 0$ and $x = L$.

a) Write a program to calculate the values of the coefficients b_k, which for convenience can be broken down into their real and imaginary parts as $b_k = \alpha_k + \mathrm{i}\eta_k$. Divide the box into $N = 1000$ slices and create two arrays containing the real and imaginary parts of $\psi(x_n,0)$ at each grid point. Perform discrete sine transforms on each array separately and hence calculate the values of the α_k and η_k for all $k = 1 \ldots N-1$.

   To perform the discrete sine transforms, you can use the fast transform function `dst` from the package `dcst`, which you can find in the on-line resources in the file named `dcst.py`. A copy of the code for the package can also be found in Appendix E. The function takes an array of N real numbers and returns the discrete sine transform as another array of N numbers.

   (Note that the first element of the input array should in principle always be zero for a sine transform, but if it is not the `dst` function will simply pretend that it is. Similarly the first

element of the returned array is always zero, since the $k = 0$ coefficient of a sine transform is always zero. So in effect, the sine transform really only takes $N - 1$ real numbers and transforms them into another $N - 1$ real numbers. In some implementations of the discrete sine transform, therefore, though not the one in the package `dsct` used here, the first element of each array is simply omitted, since it's always zero anyway, and the arrays are only $N - 1$ elements long.)

b) Putting $b_k = a_k + i\eta_k$ in the solution above and taking the real part we get

$$\text{Re}\,\psi(x_n, t) = \frac{1}{N}\sum_{k=1}^{N-1}\left[a_k \cos\left(\frac{\pi^2\hbar k^2}{2ML^2}t\right) - \eta_k \sin\left(\frac{\pi^2\hbar k^2}{2ML^2}t\right)\right]\sin\left(\frac{\pi k n}{N}\right)$$

for the real part of the wavefunction. This is an inverse sine transform with coefficients equal to the quantities in the square brackets. Extend your program to calculate the real part of the wavefunction $\psi(x, t)$ at an arbitrary time t using this formula and the inverse discrete sine transform function `idst`, also from the package `dcst`. Test your program by making a graph of the wavefunction at time $t = 10^{-16}$ s.

c) Extend your program further to make an animation of the wavefunction over time, similar to that described in part (b) of Exercise 9.8 above. A suitable time interval for each frame of the animation is about 10^{-18} s.

d) Run your animation for a while and describe what you see. Write a few sentences explaining in physics terms what is going on in the system.