P131-Computational Physics

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How to read these notes

Each section will include one or several "Exercises". In principle, these exercises would be used as examples in class, and we would work on the code toghether. However, since I'm not going to be here for the first classes, I will post the programs on the course's webpage. You should be able to compile, modify, and run them on any computer with a C compiler. I encourage you to do it and play with them, and in particular, to look at the questions asked in the exercises. The homeworks are going to be based on these programs. I will probably ask you to modify the code to study a particular problem. You are welcome to ask questions by e-mail. Don't hesitate to do it.

1 Ordinary differential equations: a review

Let's consider a simple 1st order equation:

$$\frac{dx}{dy} = f(x, y) \tag{1}$$

To solve this equation with a computer we need to <u>discretize</u> the differences: we have to convert the differential equation to a "<u>finite differences</u>" equation. The simplest solution is Euler's method.

1.1 Euler's method

Supouse that at a point x_0, the function f has a value y_0. We want to find the approximate value of y in a point x_1 close to x_0, $x_1 = x_0 + \Delta x$, with Δx

small. We assume that f, the rate of change of y, is constant in this interval Δx. Therefore we find:

$$dx \approx \Delta x = x_1 - x_0, \tag{2}$$
$$dy \approx \Delta y = y_1 - y_0, \tag{3}$$

with $y_1 = y(x_1) = x(x_0 + \Delta x)$. Then we approximate the value of y_1 as

$$y_1 = y_0 + f(x_0, y_0)(x_1 - x_0)$$

We can generalize this formula to find the value of y at $x_2 = x_1 + \Delta x$ as

$$y_2 = y_1 + f(x_1, y_1)\Delta x,$$

or in the general case:

$$y_{n+1} = y_n + f(x_n, y_n)\Delta x$$

This is a good approximation as long as Δx is "small". what is small? Depends on the problem, but it is basically defined by the "rate of change", or "smoothness" of f. $f(x)$ has to behave smoothly and without rapid variations in the interval Δx.

Notice that Euler's method is equivalent to a 1st order Taylor expansion about the point x_0. The "local error" calculating x_1 is then $O(\Delta x^2)$. If we use the method N times to calculate N consecutive points, the propagated "global" error will be $NO(\Delta x^2) \approx O(\Delta x)$. This error decreases linearly with decreasing step, so we need to halve the step size to reduce the error in half. The numerical work for each step consists of a single evaluation of f.

Exercise 1.1: Newton's law of cooling

If the temperature difference between an object and its surroundings is small, the rate of change of the temperature of the object is proportional to the temperature difference:

$$\frac{dT}{dt} = -r(T - T_s), \tag{4}$$

where T is the temperature of the body, T_s is the temperature of the environment, and r is a "cooling constant" that depends on the heat transfer mechanism, the contact area with the environment and the thermal properties of the body. The minus sign appears because if $T > T_s$, the temperature must decrease.

Write a program to calculate the temperature of a body at a time t, given the cooling constant r and the temperature of the body at time $t = 0$. Plot the results for $r = 0.1\frac{1}{min}$; $T_0 = 83°C$ using different intervals Δt and compare with exact (analytical) results.

1.2 Higher order: Taylor's series

We can go a step beyond Euler's method keeping up to second order terms in the expansion around x_0. Doing so we obtain

$$y(x + \Delta x) = y(x) + y'(x)\Delta x + \frac{1}{2}y''(x)(\Delta x)^2 + O(\Delta x^3) \tag{5}$$

from (1) we get

$$y'(x) = f(x, y), \tag{6}$$
$$y''(x) = \frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}f \tag{7}$$

Substituting in (5) we obtain

$$y_{n+1} = y_n + f\Delta x + \frac{1}{2}(\Delta x)^2[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}] + O(\Delta x^3), \tag{8}$$

where all the functions and derivatives are evaluated in (x_n, y_n).

1.3 Multistep or Predictor-Corrector methods

We can achieve higher accuracy by relating y_{n+1} not only to y_n, but also to points further in the past $y_{n-1}, y_{n-2}, ...$ To derive such formulas we can integrate exactly (1) to obtain:

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y)dx \tag{9}$$

The problem is that we don't know $f(x, y)$ over the interval (x_n, x_{n+1}). However, we can use the values of y at x_n and x_{n-1} to provide a linear extrapolation:

$$f = \frac{(x - x_{n-1})}{\Delta x}f_n - \frac{(x - x_n)}{\Delta x}f_{n-1} + O(\Delta x^2), \tag{10}$$

with $f_n = f(x_n, y_n)$. Inserting into (9) we obtain

$$y_{n+1} = y_n + \Delta x(\frac{3}{2}f_n - \frac{1}{2}f_{n-1}) + O(\Delta x^3) \tag{11}$$

Note that the value of y_0 is not sufficient information to get this algorithm started. The value of y_1 has to be obtained first by some other procedure, like the ones described previously. This means that the method is not "self-starting".

1.4 Runge-Kutta methods

1.4.1 2nd order Runge-Kutta

Euler's method rests on the idea that the slope at one point can be used to extrapolate to the next. A plausible idea to make a better estimate of the slope is to extrapolate to a point halfway across the interval, and then to use the derivative at this point to extrapolate across the whole interval. Thus,

$$k = \Delta x f(x_n, y_x), \tag{12}$$

$$y_{n+1} = y_n + \Delta x f(x + 1/2\Delta x, y_n + 1/2k) + O(\Delta x^3). \tag{13}$$

It has the same accuracy as the Taylor series (5). It requires the evaluation of f twice for each step.

1.4.2 4th order Runge-Kutta

Similar ideas can be used to derive a 3rd or 4th order Runge-Kutta method. It has been found by experience that the best balance between accuracy and computational effort is given by a fourth-order algorithm. Such a method would require evaluating f four times at each step, with a local accuracy of $O(\Delta x^5)$. It can be written as follows:

$$k_1 = \Delta x f(x_n, y_n), \tag{14}$$

$$k_2 = \Delta x f(x_n + 1/2\Delta x, y_n + 1/2k_1), \tag{15}$$

$$k_3 = \Delta x f(x_n + 1/2\Delta x, y_n + 1/2k_2), \tag{16}$$

$$k_4 = \Delta x f(x_n + \Delta x, y_n + k_3), \tag{17}$$

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) + O(\Delta x^5). \tag{18}$$

Runge-Kutta method are self-staring, meaning that they can be used to obtain the first few iterations for a non self-starting algorithm.

1.5 Equations of motion (2nd order ODEs)

We know that the motion of an object is determined by Newton's equations. In the one-dimensional case, we can define the instantaneous position $y(t)$, velocity $v(t)$ and acceleration $a(t)$ of an object using the language of differential calculus:

$$v(t) = \frac{dy}{dt}, a(t) = \frac{dv}{dt}. \tag{19}$$

The motion of the particle is defined by:

$$\frac{d^2y}{dt^2} = \frac{F(t)}{m}$$

This is a second order differential equation that can written as two first order differential equations:

$$\frac{dv}{dt} = \frac{F(t)}{m}; \tag{20}$$

$$\frac{dy}{dt} = v(t). \tag{21}$$

To solve it we can apply any of the methods described in the previous sections. If we pick Euler's, we obtain:

$$v_{n+1} = v_n + \frac{F(t)}{m}\Delta t = v_n + a_n\Delta t, \tag{22}$$

$$y_{n+1} = y_n + v_n\Delta t, \tag{23}$$

where $a_n = F(t)/m$.

Exercise 1.2: One dimensional motion

Write a program to solve the 1d equations of motion for a falling object. Input values: $y_0 = y(t = 0)$; $v_0 = v(t = 0)$. Compare results with different Δt and the exact solution. Plot $y(t)$ and $v(t)$. Use $y_0 = 10m$; $v_0 = 0$.

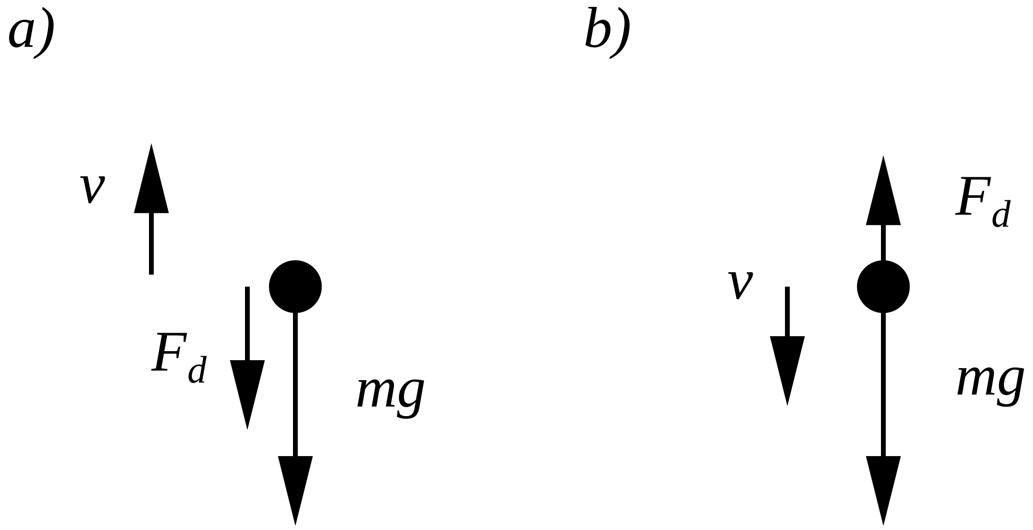

Figure 1: Forces acting on an object: a) moving upward b) falling.

Exercise 1.3: Air resistance

The phenomenological form of the velocity-dependent force of the resistance of the air is given by

$$F_d = kv$$

where k is a parameter that depends on the properties of the medium and the shape of the object. Since F increases as v increases, there is a limiting terminal velocity at which $F_d = F_g = mg$ and the acceleration vanishes:

$$kv_t = mg \Rightarrow v_t = \frac{mg}{k}$$

In terms of the terminal speed, the force F_d can be rewritten as

$$F_d = mg(\frac{v}{v_t}).$$

Hence, the net force on a falling object is:

$$F = mg(1 - \frac{v}{v_t})$$

1. Sometimes, the force F_d can vary with the square of the velocity
$$F_d = k_2 v^2.$$
Derive the net force on a falling object using this expression, in units of the terminal velocity v_t

2. Compute the speed at which a pebble of mass $m = 10^{-2} kg$ reaches the ground if it's dropped from rest ate $y_0 = 50m$. Compare this speed to that of a freely falling object under the same conditions. Assume that the drag force is proportional to v^2 and the terminal speed is $v_t = 30m/s$

3. Supouse that an object is thrown vertically upward with initial velocity v_0. If we neglect air resistance, we know that the maximum height reached by the object is $v_0^2/2g$, and its velocity upon return to the earth equals v_0, the time of ascent equals the time of descent, and the total time in the air is v_0/g. Before performing a numerical simulation, give a simple qualitative analysis of the problem when it is affected by the resistance of the air. Then, perform, the numerical calculation assuming $F_d \sim v^2$ with a terminal speed $v_t = 30m/s$. Suggestions: Choose $v > 0$ when it's pointing upward, and $v < 0$ when it's pointing toward the earth.

Exercise 1.5: Gravitational force

According to Newton's law of gravitation, the action of the gravitational field of the earth on a particle is given by
$$F = \frac{GMm}{(R+y)^2} = \frac{gm}{(1+y/R)^2},$$
where y is measured from the earth's surface, R is the earth's radius, G is the gravitational constant, M is the mass of the earth, and $g = GM/R^2$. There is not simple analytical solution for this problem. Modify your code to simulate the fall of a particle from an altitude y_0 with zero initial velocity, and compute its speed when it hits the ground. Determine the value of y_0 for which this impact velocity differs by one percent from its value under a constant acceleration $g = 9.8m/s^2$. Take the radius of the earth to be $6.37 \times 10^6 m$.

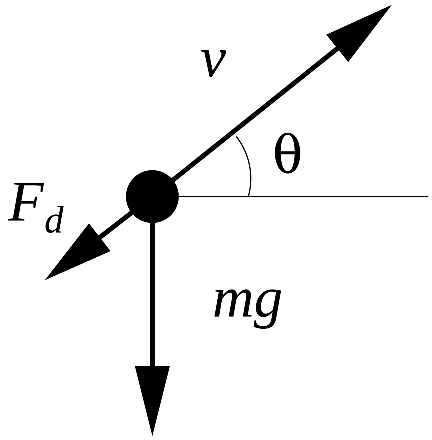

Figure 2: Object in a two dimensional trajectory under the effect of gravitational and dragging forces

Exercise 1.6: Harmonic oscillator

The two coupled first order equations

$$\frac{dy}{dt} = p; \frac{dp}{dt} = -4\pi^2 y$$

define a harmonic oscillator with period $T = 1$. Compute the position y and momentum p as a function of time using a generalization of the previous code. Plot the results for $y_0 = 1$ and p_0=0. Investigate the accuracy with which the system returns to the initial state at integral values of t.

1.6 Two dimensional trajectories

In a 2d trajectory, the direction of the drag force is opposite to the speed vector **v**. Newton's equations of motion for x and y components are written

$$m\frac{dv_x}{dt} = -F_d x; \tag{24}$$

$$m\frac{dv_y}{dt} = -mg - F_d y; \tag{25}$$

Using $F_d = kv^2$, $v_x = v\cos\theta$ and $v_y = v\sin\theta$, we find

$$\frac{dv_x}{dt} = -\frac{k}{m} v v_v, \tag{26}$$

$$\frac{dv_x}{dt} = -g - \frac{k}{m} v v_v, \tag{27}$$

where $v^2 = v_x^2 + v_y^2$. Hence, we cannot calculate the vertical motion of the object without reference to the horizontal component.

Exercise 1.7: Trajectory of a shot

Modify your code so that the 2d trajectory of an object can be computed, and graphs of y as a function of x can be made.

1. As a check on your program, first neglect the effect of air resistance so that you an compare to known results. Supouse that the object is thrown and t_0 with an angle θ_0 with an initial velocity $v_0 = 15\text{m/s}$. Vary θ_0 and show that the maximum range occurs at $\theta_0 = 45°$ Compare your result with the exact value v_0^2/g

2. Consider the effects of air resistance. Compute the maximum range, and the corresponding angle using $k/m = 0.1$, $v_0 = 30\text{m/s}$.

1.7 Stability

A major consideration in integrating differential equations is the numerical stability of the algorithm used. Since we have replaced the differential equation by a difference equation, we know that our results will not be exact. Discrepancies will arise when using different step sizes, for instance. This is the "truncation error" and depends on the method employed. Other errors that do not originate in the method correspond to the roundoffs performed by the computer, since it does not work with real numbers, but with a finite number of digits determined by the hardware. These roundoff errors will accumulate and can become significant in some cases.

In practice we determine the accuracy of our solutions by reducing the value of the step until the solutions unchanged at the desired level of accuracy.

In addition to accuracy, another important factor is the stability of the algorithm. For instance, it may occur that the numerical results are very good for short times, but diverge from the "true" solution for longer times. Such an algorithm is said to be "unstable" for the particular problem.

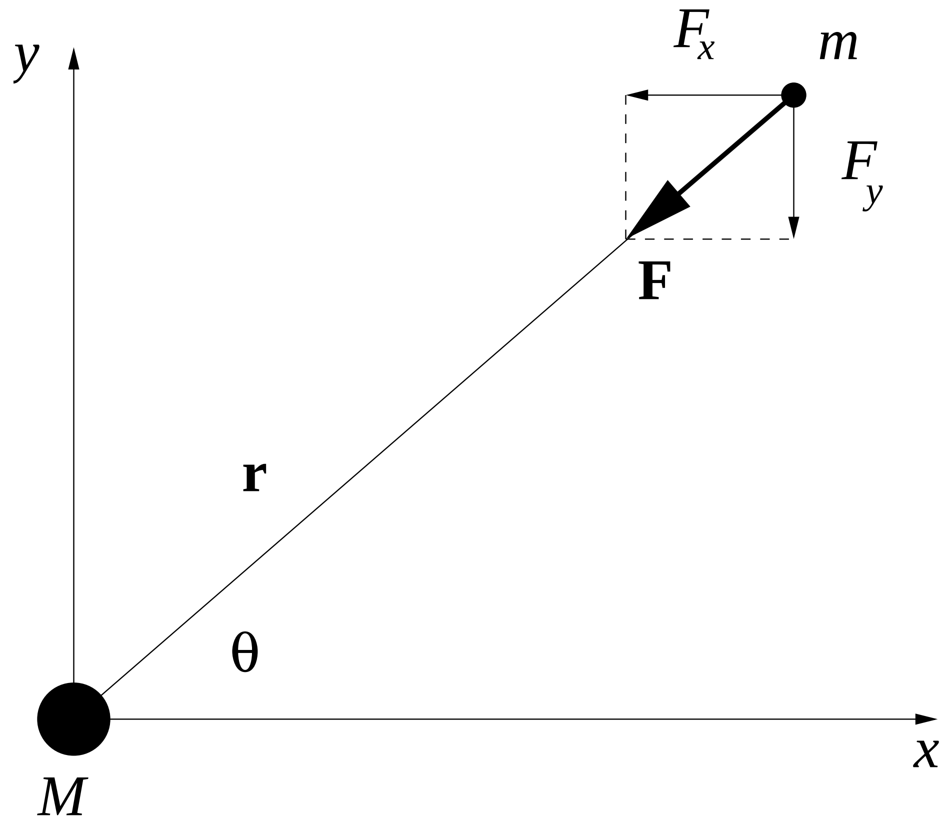

Figure 3: An object of mass m under the effects of a central force F

2 Motion in a central potential

2.1 Kepler's problem

The motion of the sun and the earth is an example of a "two-body problem". This is a relatively simple problem that can be solved analytically (it interesting to notice here, however, that adding a new object to the problem, the moon for instance, make it completely intractable. This is the famous "three body problem"). We can assume that, to a good approximation, the sun is stationary and is a convenient origin of our coordinate system. This is equivalent to changing to a "center of mass" coordinate system, where most of the mass is concentrated in the sun. The problem can be reduced to an equivalent one body problem involving an object of reduced mass μ given by

$$\mu = \frac{mM}{m+M}$$

Since the mass of the earth is $m = 5.99 \times 10^{24}$ kg and the mass of the sun is $M = 1.99 \times 10^{30}$ kg we find that for most practical purposes, the reduced mass of the earth-sun system is that of the earth. Hence, in the following we are going to consider the problem of a single particle of mass m moving about a fixed center of force, which we take as the origin of the coordinate system. The gravitational force on the particle m is given by

$$\mathbf{F} = -\frac{GMm}{r^3}\mathbf{r},$$

where the vector $\mathbf{r}$ is directed from M to m, and G is the gravitation constant

$$G = 6.67 \times 10^{-11} \frac{m^3}{kg.s^2}$$

The negative sign implies that the gravitational force is attractive, and decreases with the separation r. The gravitational force is a “central force”: its magnitude depends on the separation between the particles and its direction is along the line that connects them. The assumption is that the motion is confined to the xy plane. The angular momentum $\mathbf{L}$ lies on the third direction z and is a constant of motion, *i.e.* it is conserved:

$$L_z = (\mathbf{r} \times m\mathbf{v})_z = m(xv_y - yv_x) = \text{const.}$$

An additional constant of motion ins the total energy E given by

$$E = \frac{1}{2}mv^2 - \frac{GmM}{r}$$

If we fix the coordinate system in the sun, the equation of motion is

$$m\frac{d^2\mathbf{r}}{dt^2} = -\frac{mMG}{r^3}\mathbf{r}$$

For computational purposes it is convenient to write it down in cartesian components:

$$F_x = -\frac{GMm}{r^2}\cos\theta = -\frac{GMm}{r^3}x, \tag{28}$$

$$F_y = -\frac{GMm}{r^2}\sin\theta = -\frac{GMm}{r^3}y. \tag{29}$$

Hence, the equations of motions in cartesian coordinates are:

$$\frac{d^2x}{dt} = -\frac{GM}{r^3}x, \tag{30}$$

$$\frac{d^2y}{dt} = -\frac{GM}{r^3}y, \tag{31}$$

where $r^2 = x^2 + y^2$. These are coupled differential equations, since each differential equation contains both x and y.

Circular motion

Since many planetary orbits are nearly circular, it is useful to obtain the condition for a circular orbit. In this case, the magnitude of the acceleration $\mathbf{a}$ is related to the radius by

$$a = \frac{v^2}{r}$$

where v is the speed of the object. The acceleration is always directed toward the center. Hence

$$\frac{mv^2}{r} = \frac{mMG}{r^2}$$

or

$$v = (\frac{MG}{r})^{1/2}. \tag{32}$$

This is a general condition for the circular orbit. We can also find the dependence of the period T on the radius of a circular orbit. Using the relation

$$T = \frac{2\pi r}{v},$$

we obtain

$$T^2 = \frac{4\pi^2 r^3}{GM}$$

Elliptical orbits

An ellipse has two foci F_1 and F_2, and has the property that for any point the distance $F_1P + F_2P$ is a constant. It also has a horizontal semi-axis a and a vertical b. It is common in astronomy to characterize an orbit by its "eccentricity" e, given by the ratio of the distance between the foci, and the length of the major axis $2a$. Since $F_1P + F_2P = 2a$, it is easy to show that (consider a point P at $x = 0$,$y = b$)

$$e = \sqrt{1 - \frac{b^2}{a^2}},$$

with $0 < e < 1$. A special case is $a = b$ for which the ellipse reduces to a circle and $e = 0$. The earth orbit has eccentricity $e = 0.0167$.

Astronomical units

It is useful to choose a system of units where the product GM is of the order of unity. To describe the earth's motion, the convention is to choose the earth's semi-major axis as the unit of length, called "astronomical unit" (AU) and is

$$1AU = 1.496 \times 10^{11} m.$$

The unit of time is taken to be "one year", or 3.15×10^7s. In these units, $T = 1$yr, $a = 1AU$, and we can write

$$GM = \frac{4\pi^2 a^3}{T^2} = 4\pi^2 AU^3/yr^2.$$

Exercise 2.1: Simulation of the orbit

1. Write a program to simulate motion in a central force field. Verify the case of circular orbit using (in astronomical units) ($x_0 = 1$, $y_0 = 0$ and $v_x(t = 0) = 0$. Use the condition (32 to calculate $v_y(t = 0)$ for a circular orbit. Choose a value of Δt such that to a good approximation the total energy E is conserved. Is your value of Δt small enough to reproduce the orbit over several periods?

2. Run the program for different sets of initial conditions x_0 and $v_y(t = 0)$ consistent with the condition for a circular orbit. Set $y_0 = 0$ and $v_x(t = 0) = 0$. For each orbit, measure the radius and the period to verify Kepler's third law ($T^2/a^3 = $ const.). Think of a simple condition which allows you to find the numerical value of the period.

3. Show that Euler's method does not shield stable orbits for the same choice of Δt used in the previous items. Is it sufficient to simply choose a smaller Δt or Euler's method is no stable for this dynamical system?

Use the average velocity $1/2(v_n + v_{n+1})$ to obtain x_{n+1}. Are the results any better?

4. Set $y_0 = 0$ and $v_x(t = 0) = 0$. By trial and error find several choices of x_0 and $v_y(t = 0)$ which yield coonvinient elliptical orbits. Determine total energy, angular momentum, semi-major and semi-nimor axes, eccentricity, and period for each orbit.

5. You probably noticed that Euler's algorithm with a fixed Δt breaks down if you get to close to the sun. How are you able to visually confirm this? What is the cause of the failure of the method? Think of a simple modification of your program that can improve your results.

2.2 A mini solar system

The presence of other planets implies that the total force on a planet is no longer a central force. Furthermore, since the orbits are not exactly on the same plane, the analysis must be extended to 3D. However, for simplicity, we are going to consider a two-dimensional solar system, with two planets in orbit around the sun.

The equations of motion of the two planets of mass m_1 and m_2 can be written in vector form as

$$m_1 \frac{d^2\mathbf{r}_1}{dt^2} = -\frac{m_1 MG}{r_1^3}\mathbf{r}_1 + \frac{m_1 m_2 G}{r_{21}^3}\mathbf{r}_{21}, \tag{33}$$

$$m_2 \frac{d^2\mathbf{r}_2}{dt^2} = -\frac{m_2 MG}{r_2^3}\mathbf{r}_2 + \frac{m_1 m_2 G}{r_{21}^3}\mathbf{r}_{21}, \tag{34}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are directed form the sun to the planets, and $\mathbf{r}_{21} = \mathbf{r}_2 - \mathbf{r}_1$ is the vector from planet 1 to planet 2. This is a problem with no analytical solution, but its numerical solution can be obtained extending our previous analysis for the two-body problem.

Exercise 2.2: A three body problem

Let us consider astronomical units, and values for the masses $m_1/M = 0.001$ and $m_2/M = 0.01$. Consider initial positions $r_1 = 1$ and $r_2 = 4/3$ and velocities $\mathbf{v}_{1,2} = (0, \sqrt{GM/r_{1,2}})$.

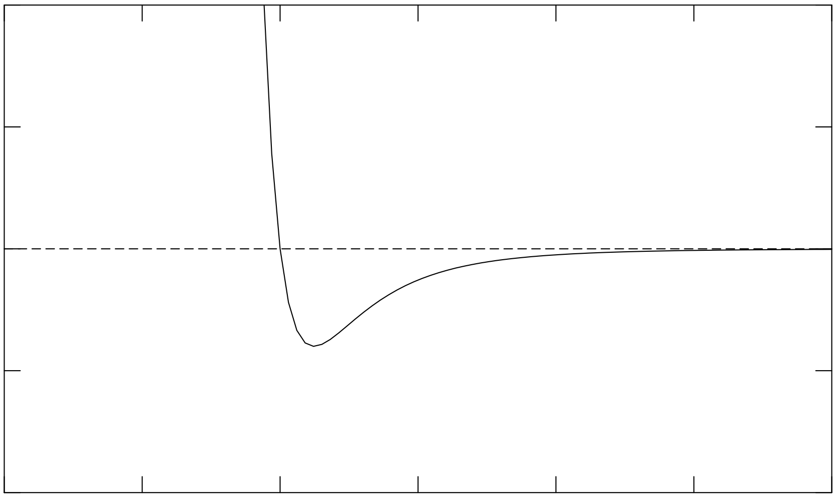

Figure 4: The Lennard-Jones potential

1. Write a program to calculate the trajectories of the two planets, and plot them.

2. What would the shape and the periods of the orbits be if the don't interact? What is the qualitative effect of the interaction. Why is one planet affected more by the interaction that the other? Are the angular momentum and energy of planet 1 conserved? Is the total momentum an energy of the two planets conserved?

2.3 Scattering by a central potential

In this section, we will investigate the classical scattering of a particle of mass m by a central potential. In a scattering event, the particle, with initial kinetic energy E and impact parameter b approaches the potential from a large distance (see Fig. 5). It is deflected during its passage near the force center and eventually emerges with the same energy, but moving at an angle Θ with respect to the original direction. This problem is very similar in many aspects to the orbital motion, but in this case the potential is repulsive, and it is not necessarily a function of the inverse square of the

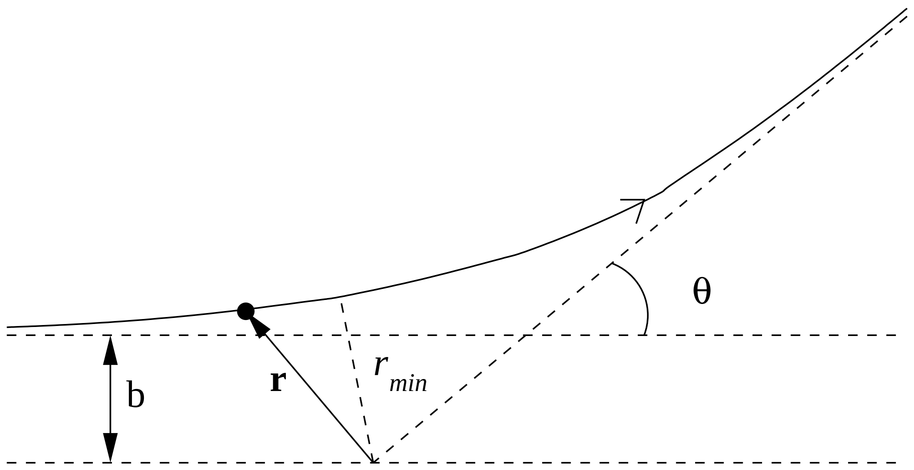

Figure 5: Quantities involved in the scattering of a particle by a central potential.

distance. The energy and momentum are conserved, and the trajectory lies in the plane.

Our basic interest is on the deflection function $\Theta(b)$, giving the final scattering angle Θ as a function of the impact parameter. This function also depends upon the incident energy. The differential cross section for scattering at an angle Θ, $d\sigma/d\Omega$ is an experimental observable that is related to the deflection function by

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\Theta}|\frac{db}{d\Theta}|. \tag{35}$$

Thus, if $d\Theta/db$ can be computed, the cross section is known.

Expressions for the deflection function can be found analytically only for a few potentials, so that numerical methods usually must be employed. There are some simplification that can me made using the fact that the angular momentum is conserved, which connects the angular and the radial motion, making the problem one-dimensional. However, in this section we are going to use the tools learned in the previous sections, and solve the four first-order differential equations for the two coordinates and their velocities in the xy plane.

In the following we are going to consider a Lennard-Jones potential:

$$V(r) = 4V_0[(\frac{a}{r})^{12} - (\frac{a}{r})^6], \tag{36}$$

The potential is attractive for long distances, and strongly repulsive approaching the core (see Fig. 4), with a minimum occurring at $r_{min} = 2^{(1/6)}a$ with a depth V_0.

Exercise 2.3

1. Before beginning any numerical computation, it is important to have some idea of what the results should look like. Sketch what you think the deflection function should look like at relatively low energies, $E \leq V_0$, where the the peripheral collisions at large $b \leq r_{max}$ will take place in a predominantly attractive potential and the more central collisions will "bounce" against the repulsive core. What happens at much higher energies $E \gg V_0$, where the attractive pocket in V can be neglected? Note that the values of b where the deflection function has a maximum or a minimum, Eq. (35) shows that the cross section should be infinite,as occurs in the rainbow formed when light scatters from water drops.

2. Write a program that calculates, for a given kinetic energy E, the deflection function solving the equations of motion a a number of equally spaced b values between 0 and r_{max}.

3. Use your program to calculate the deflection function for scattering from a Lennard-Jones potential at selected values of E ranging from $0.1V_0$ to $100V_0$. Reconcile your answers in step 1) with the results obtained. Calculate the differential cross sections a function of $Theta$ at these energies.

4. If your program is working correctly you should observe for energies $E \leq V_0$ a singularity in the deflection function where Θ appear to approach $-\infty$ at some critical value of b, b_{crit}, that depends on E. This singularity, which disappears when E becomes larger that about V_0 is characteristic of "orbiting", and the scattering angle becomes logarithmically infinite. What happens is that the particle spends a very long time spiralling around the center. Calculate some trajectories

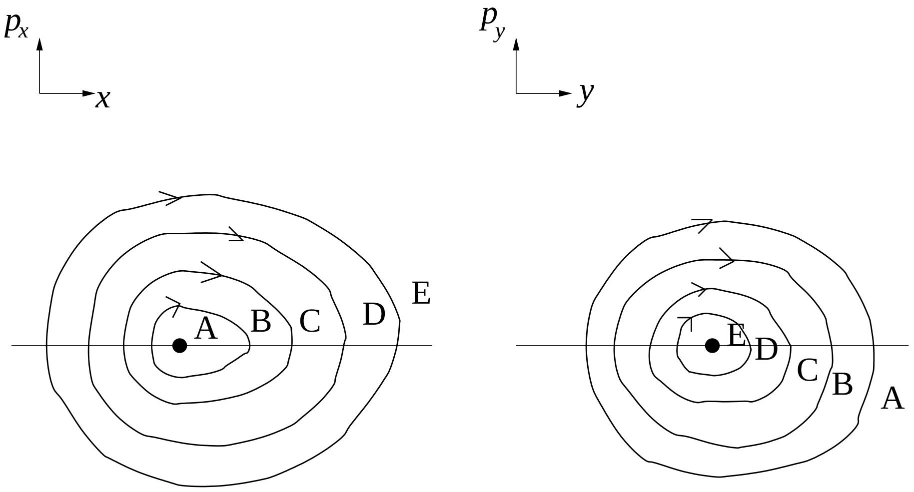

Figure 6: Trajectories of a particle in a two-dimensional separable potential as they appear in the (x, p_x) and (y, p_y) planes. Several trajectories corresponding to the same energy but different initial conditions are shown. Trajectories A and E area the limiting ones having vanishing E_x and E_y, respectively

around this point and convince yourself that this is precisely what's happening. Determine the maximum energy for which the Lennard-Jones potential exhibits orbiting by solving the correct set of equations involving V and its derivatives.

2.4 Trajectories in phase space and integrability

Let's "complicate" things a little bit. We know that all the problems described above can be expressed elegantly using the Hamiltonian formalism. Let us consider a particle of mass m moving in a potential V in two dimensions ans assume that V is such that the particle remains confined if the energy is low enough. The momenta conjugate to the two coordinates (x, y) area (p_x, p_y). The Hamiltonian (the energy!) takes the form

$$H = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y). \tag{37}$$

Given any particular initial values of the coordinates and momenta, the particle's trajectory is specifies by their time evolution, that is governed by four first-order differential equations (Hamilton's equations):

$$\frac{dx}{dt} = \frac{\partial H}{\partial p_x} = p_x, \frac{dy}{dt} = \frac{\partial H}{\partial p_y} = p_y; \tag{38}$$

$$\frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}, \frac{dp_y}{dt} = -\frac{\partial H}{\partial y} = -\frac{\partial V}{\partial y}. \tag{39}$$

For any V, these equations conserve the energy E so that the constraint

$$H(x, y, p_x, p_y, t) = E$$

restricts the trajectory to a three-dimensional manifold embedded in the four dimensional phase space.

The Hamiltonian is said to be "integrable" when there is a second function of the coordinates and momenta that is also a constant of motion; the motion is thus constrained to a two-dimensional manifold in phase space. Two familiar kinds of integrable systems are *separable* and *central* potentials.

In the separable case

$$V(x, y) = V_x(x) + V_y(y)$$

where $V_{x,y}$ are independent functions of only one variable, so that the Hamiltonian separates in two parts and each coordinate can be solved independently,

$$H = H_x + H_y; H_{x,y} = \frac{1}{2}p_{x,y}^2 + V_{x,y}.$$

The motions of x and y are therefore decoupled form each other and each of the Hamiltonians is separately a constant of motion.

In the case of a central potential,

$$V(x, y) = V(r); r = \sqrt{x^2 + y^2},$$

so that the angular momentum $L_z = xp_y - yp_x$ is the second constant of motion and the Hamiltonian can be written as

$$H = \frac{1}{2}p_r^2 + V(r) + \frac{p_\theta^2}{2r^2}.$$

where p_r is the momentum conjugate to r. The additional constraint on the trajectory makes the system tractable reducing the problem to les variables.

All the familiar analytically soluble problems in classical mechanics are those that are integrable. An analysis of phase space suggests a way to detect integrability. Consider for instance the case of a separable potential, Because the motions of each of the two coordinates are independent, plots of the trajectory in (x, p_x) and (y, p_y) planes should look as in Fig.6. Here, we assumed that each potential has a minimum value of 0 at particular values of x and y respectively. The particle moves on a closed contour in each of these two-dimensional projections of the four-dimensional phase space, each of them looking as a on-dimensional motion. The areas of these contours is associated to the total energy (E_x and E_y). Since the total energy must be conserved, as one varies the initial conditions, one contour shrinks, and the other grows. In each plane there is a limiting contour that is approached when all the energy is in one coordinate. The fact that these contours are closed signals the integrability of the system.

How can we obtain this information from the trajectory alone? Supouse that at every time we observe one of the coordinates, say x, pass through zero, we plot the location of the particle in the (y, p_y) plane. If the periods of the x and y motions are incommensurate (*i.e.* their ratio is an irrational number), then, as the trajectory proceeds, these observations will trace out the full (y, p_y) contour; if the periods are commensurate (*i.e.* a rational ratio), then a series of discrete points around the contour will result.

3 Oscillatory Motion

3.1 The harmonic oscillator

We know that simple oscillatory motion is described by a general quadratic potential of the form

$$V = \frac{1}{2}kx^2,$$

where k is a "force constant". In a spring, this is a measure of the stiffness of the spring. In a pendulum, it is given by

$$k = \frac{mg}{L}$$

where m is the mass of the particle and L its length. From this potential we can extract the force

$$F = -\frac{dV}{dx} = -kx$$

and the equation of motion can be written as

$$\frac{d^2x}{dt^2} = -\omega_0^2 x, \tag{40}$$

where the quantity ω_0 is defined by

$$\omega_0 = \frac{k}{m}$$

The dynamical motion described by these equations is called "simple harmonic motion" and can be solved analytically:

$$x(t) = A\cos\omega_0 t + \delta, \tag{41}$$

where a is the amplitude of th oscillations and δ is a phase that depends on the initial conditions.

We can now define a period T such as

$$x(t+T) = x(t).$$

Since $\omega_0 T$ corresponds to one cycle, we obtain

$$T = \frac{2\pi}{\omega_0} = \frac{2\pi}{\sqrt{k/m}}.$$

The frequancy ν is the number of cycles per unit of time and is given by $\nu = 1/T$. Note that the period of the motion depends on the ration k/m and is completely independent of the initial conditions.

Exercise 3.1: Energy conservation

1. In Exercise 1.6 we wrote program to simulate simple harmonic motion. Now use the program to calculate the relative change in the total energy during one cycle $\Delta_n = (E_n - E_0)/E_0$. Is the function Δ uniformly small during the cycle? Choose $x_0 = 1$, $v_0 = 0$, and $\omega_0^2 = 9$ Compare using Euler's method and 2nd. order Runge-Kutta.

2. Plot position and velocity as a function of the time t.

3. Compute the amplitude A for the initial conditions $x_0 = 4$, $v_0 = 0$, and $x_0 = 0$, $v_0 = 4$; choose $\omega_0^2 = 4$ in both cases. What quantity determines the value of A?.

4. Compute the average value of the kinetic energy and the potential energy during a complete cycle. Is there a relation between the two averages?

5. Plot the path of the oscillator in phase space (x, v). Set $\omega_0^2 = 9$ and use different initial conditions $(x_0, v_0) = (1, 0); (0, 1); (4, 0)$. Do you find different paths for each of them? What physical quantity distinguishes or characterizes each path? What is the shape of the phase paths? Is the motion of a representative point (x, v) always in the clockwise or counterclockwise direction?

Exercise 3.2: Large oscillations

The pendulum responds to the equation of motion (40) only in the limit of small angles. In the case of large oscillations, the equation has to ve modified becoming

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta.$$

The enrgy of the pendulum is then given by

$$E = \frac{1}{2}mL^2(\frac{d\theta}{dt})^2 + mgL(1 - \cos\theta)$$

1. Modify your program to simulate large amplitude oscillations in a pendulum. Set $g/L = 9$ and choose Δt so that the numerical solution is stable, *i.e.* it does no diverge with time from the "true" solution. Check the stability by clculating the total energy and ensuring thatt it does not drift from its initial value.

2. Set $d\theta/dt|_{t=0} = 0$ and make plots of $\theta(t)$ and $d\theta/dt(t)$ for the initial conditions $\theta(t = 0) = 0.1$, 0.2, 0.4, 0.8, 1.0. Describle the qualitative behavior of θ and $d\theta/dt$. What is the period T and the maximum amplitude θ_max in each case? Plot T versus θ_max and discuss the qualitative dependence of the period on the amplitude. How do the results compare in the linear and non-linear cases, *e.g.* which period is larger? Explain the relative values of T in physical terms.

Exercise 3.3: Damped oscillations

If a drag force is included in the problem, the equation of motion becomes:

$$\frac{d^2x}{dt^2} = -\omega_0^2 x - \gamma\frac{dx}{dt},$$

where the "damping coefficient" gamma is a measure of the friction. Note that the drag force opposes the motion.

1. Incorporate the effects of damping in yout program and plot the time dependece of position and velocity. Make runs for $\omega_0^2 = 9$, $x_0 = 1$, $v_0 = 0$, and $\gamma = 0.5$.

2. Compare the period and angular frquency to the undamped case. is the period longer or shorter? Make additional runs for $\gamma = 1, 2, 3$. Does the frequency increase or decrease with greater damping?

3. Define the amplitude as the maximum value of x in one cycle. Compute the "relaxation time" τ, the time it takes for the amplitude to change from its maximum to $1/e \approx 0.37$ of its maximum value. To do this, plot the maximum amplitud of each cycle, and fit it with an exponential of the form $A_0 \exp -t/\tau$. Compute τ for each of the values of γ use in th previous item and discuss the qualitative dependence of τ with γ.

4. Plot the total energy as a function of time for the values of γ considered previously. If the decrease of the energy is not monotonic, explainthe cause of the time-dependence.

5. Compute the average value of the kinetic energy, potential energy, and total energy over a complete cycle. Plot these averages as a function of the number of cycles. Due to the presence of damping, these averages decrease with time. Is the decrease uniform?

6. Compute the time-dependence of $x(t)$ and $v(t)$ for $\gamma = 4, 5, 6, 7, 8$. Is the motion oscillatory for all γ? Consider a condition for equilibrium $x < 0.0001$; how quickly does $x(t)$ decay to equilibrium? For fixed ω_0, the oscillator is said to be "critically damped" at the smallest values of γ for which the decay to equilibrium is monotonic. For what value of γ does critical damping occur for $\omega_0^2 = 9$ and $\omega_0^2 = 4$? For each value of ω_0 compute the value of γ for which the system approaches equilibrium more quickly.

7. Construct the phase space diagram for cases $\omega_0^2 = 9$ and $\gamma = 0.5$, 2, 4, 6, 8. Area the qualitative features of the paths independent of γ? If not, discuss the qualitative differences.

Exercise 3.4: Linear response to external forces

How can we determine the period of a pendulum that is not already in motion? The obvious way is to disturb the system, for instance, apply a small displacement and observe the resulting motion. We will find that the "response" of a system is actually an intrinsic property of the system and can tell us about its nature in the absence of perturbations.

Consider a damped linear oscillator with an external force $F(t)$

$$\frac{d^2x}{dt^2} = -\omega_0^2 x - \gamma \frac{dx}{dt} + \frac{1}{m} F(t).$$

Is is customary to interpret the reponse of the system in terms of the displacement x. The time dependence in $F(t)$ is arbitrary. A particular case is when the force is harmonic:

$$\frac{1}{m} F(t) = A_0 \cos \omega t, \tag{42}$$

where ω is the angular frequency of the driving force.

When a weak driving force has frequency ω equal to the natural frequency ω_0, it is possible to have a periodic steady motion with frequency ω_0. In this case it is possible to pick the magnitude of the external force such that after the initial transient dies off, the average energy put into the system during one period exactly balances the energy dissipated by friction. This leads to a "limiting cycle" in which the motion is stable even in the presence of damping.

However, when the magnitude of the force f is large, the driving overpowers the natural motion of the system and the steady state motion is at the frequency of the driving force. This is a case of "mode locking". The force can lock the system in an excited "overtone", a vibrational mode with higher frequency. In this case the driving and the natural frquencies are rationally related:

$$\frac{\omega}{\omega_0} = \frac{n}{m},$$

where n and m are integers.

1. Modify your program so that an external force of the form (42) is included. Set $\omega_0^2 = 9$, $\gamma = 0.5$, $A_0 = 1$ and $\omega = 2$ (we'll use these values fro the rest of the exercise). These values correspond to a lightly damped oscillator. Plot $x(t)$ versus t for the initial conditions $(x_0 = 1, v_0 = 0)$. How does the qualitative behavior differ from the unperturbed case? What is the period and angular frequency of $x(t)$ after several oscillations? Obtain a similar plot with $(x_0 = 0, v_0 = 1)$. What is the period and angular frequancy after several oscillations? Does $x(t)$ approach a limiting behavior that is independent of the initial conditions? Identify a "transient" part of $x(t)$ which depends on the initial conditions and decays in time, and a "steady state" part which dominates at longer times and which is independent of the initial conditions.

2. Compute $x(t)$ for $\omega = 1$ and $\omega = 4$. What is the period and angular frequancy of the steady state in each case?

3. Compute $x(t)$ for $\omega_0 = 4$. What is the angular frequancy of the steady state motion? Onthe basis of these results, explain which parameters determine the frequency of the steady state behavior/

4. Verify that the steady state behavior is given by

$$x(t) = A(\omega) \cos \omega t + \delta,$$

where δ is the phase difference between the applied force and the steady state motion. Compute δ for $\omega_0^2 = 9, \gamma = 0.5$,$\omega = 0$, 1.0, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4. repeat the computation for $\gamma = 1.5$ and plot δ versus ω for the two values of γ. Discuss the qualitative dependence of $\delta(\omega)$ in the two cases.

Exercise 3.5: Resonance

The long term behavior of the driven harmonic oscillator depends on the frequency of the driving force. One measure of this behavior is the maximum of the steady state displacement $A(\omega)$.

1. Adopt the initial condition $(x_0 = 0, v_0 = 0)$. Compute $A(\omega)$ for $\omega = 0$, 1.0, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4 with $\omega_0 = 3$ and $\gamma = 0.5$. Plot $A(\omega)$ versus ω and describe its qualitative behavior. If $A(\omega)$ has a maximum, determine the "resonance angular frequency" ω_{max}, which is the frequency at the maximum of A. Is the value of ω_{max} close to the natural angular frequency ω_0?

2. Compute A_{max}, the value of the amplitude at ω_{max}, and the ratio $\Delta\omega/\omega_{max}$, where $\Delta\omega$ is the "width" of the resonance. Define $\Delta\omega$ as the frequency interval between points on the amplitude curve which are $1/\sqrt{2}A_{max}$. Set $\omega_0 = 3$ and consider $\gamma = 0.1$, 0.5, 1.0, 2.0. Describe the qualitative dependence of A_{max} and $\Delta\omega/\omega_{max}$ on γ. The quantity $\Delta\omega/\omega_{max}$ is proportional to $1/Q$, where Q is the "quality factor" of the oscillator.

3. Decribe the qualitative behavior of the steady state amplitude $A(\omega)$ near $\omega = 0$ and $\omega \gg \omega_0$. Why is $A(\omega = 0) > A(\omega)$ for small ω? Why does $A(\omega) \to 0$ for $\omega \gg \omega_0$?

3.2 Chaotic structure in phase space

In the examples of the previous sections we investigated several cases of harmonic oscillators under different circumstances. In the exercises we have seen the behavior of the trajectories in phase space. Look at the plots you created, and you will identify the following characteristic structures:

- **Limit cycles:** ellipse-like figures with frequencies grater than ω_0. There may be sporadic changes among the limiting cycles.

- **Strange attractors:** well-defined, yet complicated semi-periodic behaviors that appear to be uncorrelated to the motion at an earlier time. These are highly sensitive to the initial conditions. Even after millions od observations, the motion remains *attracted* to these paths.

- **Predictable attractors:** well-defined, yet fairly simple periodic behaviors that are not particularly sensitive to the initial conditions. These are orbits, such as fixed points and limit cycles, into which the system prefers to settle. If your location in phase space is close to a predictable attractor, ensuing times will bring you to it.

- **Chaotic paths:** regions of phase space that appear as filled-in bands rather than lines. The continuity between the bands implies some very complicated behaviors, yet the general motion still has some underlying structure.

4 Molecular Dynamics

Thus far we have studied the dynamics behavior of systems with only a few particles. However, many systems in nature such as gases, liquids and solids contain many mutually interacting particles. A typical problem involves $10^{23} - 10^{25}$ molecules which, to a good approximation, obey the laws of classical physics. Although the intermolecular forces produce a complicated trajectory for each particle, the observable properties of the whole are averages that do not depend on the individual behavior. The motion is completely determined by the classical equations of motion, and all the physics is contained in the intramolecular potential, *i.e.* the interactions.

The problem consists in understanding the properties of the whole, starting from the known interactions.. The most direct approach is to simulate the problem with a computer. The problem of simulating a system with $10^{23} - 10^{25}$ particles requires the power of a supercomputer, and using parallelization techniques. However we can learn the principles using a fraction of that number, say 10^4 particles, that is tractable in a PC. Not only we can learn about about many of the instead of statistical mechanics, but also the basic simulation techniques. The technique that we will learn in this section does not differ in essence from that used in supercomputers, and it is called "molecular dynamics".

4.1 The intermolecular potential

Our first goal is to identify the model we want to simulate. The first simplification is to consider the molecules spherical, chemically inert, and that they move according to the laws of classical mechanics. We also assume that the force between molecules depends only on the distance between them. The form of this potential for electrically neutral atoms can be constructed from a detailed first principles quantum mechanical calculation. Such calculation can be complicated, so we will consider a phenomenological form. The most important features are: **strong repulsion at short distances, weak attraction at large separations**. The repulsion originates from the electrostatic interaction between equally charged particles, and the long range attraction from the mutual polarization of the electronic clouds, known as "van de Waals" force.

Below we list some model potentials:

Hard Spheres	$V(r) = \infty$ if $r < r_o$ $V(r) = 0$ if $r \geq r_o$	First approximation in many applications
Lennard-Jones	$V(r) = 4\epsilon \left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6} \right]$	Noble gas atoms; nearly spherical molecules
Harmonic	$V(r) = A(r - r_o)^2$	Intramolecular bonds

4.2 Tricks of the trade

4.2.1 Units

Meters and kilograms are not meant to measure molecules. Using these units would imply the clumsy manipulation of small numbers. We want to choose units of mass, energy, and length such that the values of the quantities are always of the order 1. For instance, in the case of the Lennard-Jones potential is wise to use σ as a unit of length, ϵ as a unit of energy, and $m_0 = 1AMU$ as the unit of mass. Re-scaling by these quantities, the potentia would be

$$V^*(r) = 4\left[u^{-12} - u^{-6}\right],$$

where $V^* = V/\epsilon$ and $u = r/\sigma$. The advantages are that the Lennard-Jones parameters never show in the formulas, and that we are spared of many computationally expensive calculations. With this choice of units, we find that time is measured in units of $t_0 = \sqrt{m_0\sigma^2/\epsilon}$. For the electrical charge, the natural unit is the charge of the electron e, and for temperature, ϵ/k. After finishing the simulation, we transform the results back to the original units to be compared with the experimental data.

4.2.2 Boundary conditions

Since the size of our system is typically 10-100 molecular diameters, this is certainly not a good representation for a macroscopic sample because most of the particles will be situated near a "wall" or "boundary". To minimize the effects of the boundaries and to simulate more closely the properties of the macroscopic system, it is convenient to choose "periodic boundary conditions". These means that our basic box containing N particles is surrounded by images (or replicas) of itself. This is equivalent to wrap the coordinates around the boundaries: when one particles hits a wall, instead of bouncing

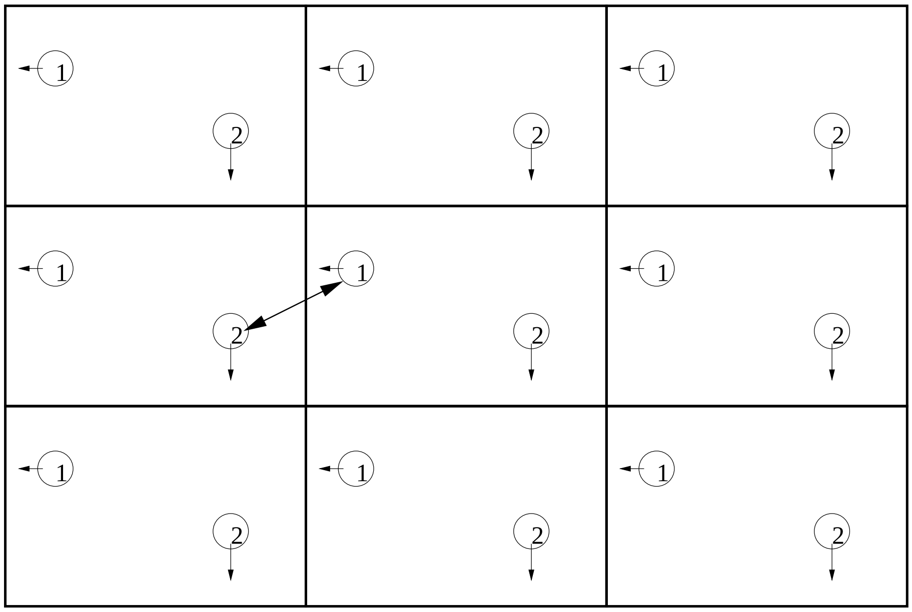

Figure 7: Example of periodic boundary conditions in 2D. Note that particle 1 is about to leave the left face of the central cell and to enter the center cell trhough the right face. The minimum image distance convention inplies that the separation between particles 1 and 2 is given by the bold line

pack, it reappears on the other side of the box. This means that the system has the topology of a torus. If the linear size of the box is L, the maximum separation between particles is $L/2$.

The rule can be summarized as follows: instead of the coordinate x_i of some particle, we have to adopt

$$(x_i + 2L)\text{mod}L. \tag{43}$$

In this way the number of particles in a given box is always conserved. A particle crossing the right boundary is automatically replaced by a particle entering the left, and vice versa.. (Adding $2L$ before the modulo operation is to catch any runaway particles with $x_i < -L$)

To compute the potential energy or the force between two particles i and j one augments the periodic boundary conditions we have to adopt the so-called "nearest image convention". Imagine that the two particles on opposite sides of the box. The convention dictates that we have to adopt the minimum distance across the walls, or between images in the neighboring replicas. If $\Delta x_{ij} = x_j - x_i$ is larger than $L/2$, then the particle j will be disregarded as an interaction partner of i, with its left image, having coordinate $x_j - L$ in its place. In practice this means simply that when calculating $V(r_{ij})$ we have to use the quantity $\Delta x_{ij} - L$ instead of Δx_{ij}. An analogous rule holds for $\Delta x_{ij} \leq -L/2$ and for the other coordinates.

The rule can be expressed by

$$\Delta x = \Delta x - L\text{int}\left(\frac{\Delta x}{L}\right). \tag{44}$$

Expressions (44) and (43) can be replaced by ifs expressions. In a parallel code this is counter productive, but in a serial code may be preferable. The optimal choice should be base on benchmarks.

4.2.3 Starting configuration

Since the size of our system is typically 10-100 molecular diameters, this is certainly not a good representation for a macroscopic sample because most of the particles will be situated near a "wall" or "boundary". To minimize the effects of the boundaries and to simulate more closely the Since the size of our system is typically 10-100 molecular diameters, this is certainly not a good representation for a macroscopic sample because most of the

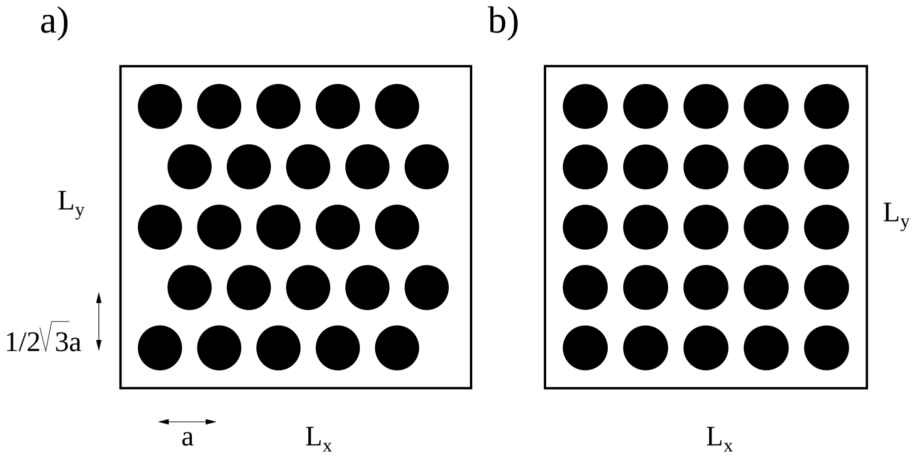

Figure 8: Initial configuration with particles in vertices of a a) triangular; b) rectangular lattice

particles will be situated near a "wall" or "boundary". To minimize the effects of the boundaries and to simulate more closely the Picking the right starting configuration is not trivial. The first choice would be to place the molecules randomly distributed, but this would give rice to large starting energies and forces, since many pairs would be placed at unphysical short distances. It is therefore customary to place the particles in the vertices of a some crystal lattice (face centered cubic –or triangular–, for instance). The x and y components of the velocities can be picked randomly in an interval $[-v_{\max}, v_{\max}]$. Before starting the proper simulation and the measurement of the physical quantities, it is necessary to perform a "thermalization" run to let the system relax to a situation of dynamical and thermal equilibrium.

4.2.4 Adjusting density and temperature

Since the number of particles is usually fixes and conserved, the way to achieve the desired density os to adjust the volume. This is done scaling all coordinates by a suitable factor.

In Molecular Dynamics, the temperature is a measurable quantity. Kinetic theory tells us that

$$T = m\langle|\mathbf{v}|^2\rangle/3k,$$

where k is the Boltzmann's constant, and $\langle|\mathbf{v}|^2\rangle$ is the averaged square of the velocity. In a simulation, we have to average this quantity over a number of MD steps to get a measurement of T. If we want to simulate a particular temperature, we rescale each component of the velocity vector of every particle by $\sqrt{T_{desired}/T_{actual}}$. Obviously T is a fluctuating quantity and can therefore be adjusted only approximately.

4.3 MD simulation of Hard Spheres

To set the initial conditions let us consider the N spheres to be distributed in a lattice, and with random initial velocities. An addtional requirement is that the total energy should be consistent with some desired temperature according to $E = 3NkT/2$. Furthermore, is advantageous to make the total momentum (which will be conserved in the simulation) equal to zero.

Next, we compute for each pair of particles (i, j) in the system the time t_{ij} that would take the pair to meet:

$$t_{ij} = \frac{-b - \sqrt{b^2 - v^2(r^2 - d^2)}}{v^2}$$

where d is the sphere diameter, r is the distance between the centers of i and j , and

$$\begin{aligned} b &= (\mathbf{r}_j - \mathbf{r}_i).(\mathbf{v}_j - \mathbf{v}_i) \\ v &= |(\mathbf{v}_j - \mathbf{v}_i)| \end{aligned}$$

For each particle i the smallest positive collision time $t(i) = \min(\{t_{ij}\})$ and the corresponding collision partner $j(i)$ are memorized. If the particle has no collision partner at positive times, we set $j(i) = -1$ and $t(i) = 10^{16}$ or the largest representable number.

Evidently this calculation is quite costly, since there are $N(N-1)/2$ pairs to be scanned. However this double loop over all indices has to be performed only once, at the start of the simulation.

Next we identify the smallest among the N "next collision times", calling it $t(i_0)$ This will give us the time that will pass until the next collision occurring in the entire system. Let the partners in this collision be i_0 and j_0.

Now all the particle positions are incremented according to the free motion law

$$\mathbf{r}_i = \mathbf{r}_i + \mathbf{v}_i t(i_0)$$

and all the $t(i)$ are decreased by $t(i_0)$.

The elastic collision between the spheres $i = i_0$ and $j = j_0$ leads to new velocities of these two particles

$$\mathbf{v}'_i = \mathbf{v}_i + \Delta\mathbf{v}, \quad \mathbf{v}'_j = \mathbf{v}_j - \Delta\mathbf{v}$$

where

$$\Delta\mathbf{v} = b\frac{\mathbf{r}_{ij}}{d^2}$$

All pairwise collision times t_{ij} that involve either i_0 or j_0 must now be recalculated using the new velocities. For this purpose no more than $2N-3$ pairs have to be scanned.

The elementary step of a hard sphere MD calculations now completed. The next step is started by once more searching all the t_i for the smallest element.

Exercise 4.1: MD for Hard Spheres

Write the MD code for a two dimensional system of hard disks. Set the simple initial configuration with the disk in the vertices of a square lattice. Use a small density and take snapshots. Notice that sometimes, due to the periodic boundary conditions, some particles suddenly appear overlapping another. Limit the time allowed for free flight such that for each particle and each coordinate α the free motion displacement fulfills $\Delta x_\alpha \equiv v_\alpha \Delta t \leq L/2 - d$. To avoid this difficulty one may as well use reflecting boundary conditions, doing a "billiard dynamics" simulation.

4.4 MD simulation: Continuous potentials

The interaction between hard particles was considered as an instantaneous collision process, with forces of infinite strength actin instantaneously during infinitely short times. A dynamical equation is of no use in such model, and it was therefore appropriate to calculate the collision laws to obtain the new velocities. In between collisions, the particles fly freely without acceleration. In contrast, for a continuous varying potential, the particles are either in a force field, or interact with some other particle at long distances and at any time. Therefore

$$\ddot{\mathbf{r}} = \frac{1}{m}\mathbf{F}_i = \frac{1}{m}\sum_{j\neq i}\mathbf{f}_{ij}(t)$$

with

$$\mathbf{f}_{ij} = -\nabla_i V(r_{ij})$$

where V is the interaction potential (*e.g.* Lennard-Jones).

When evaluating the total force acting on a particle we apply periodic boundary conditions and the nearest image convention. In this way we may determine the sum of all the forces acting on a particle. A popular method to integrate the equations of motion is the Verlet algorithm:

$$\mathbf{r}_i(t_{n+1}) = 2\mathbf{r}_i(t_n) - \mathbf{r}_i(t_{n-1}) + \mathbf{F}_i(t_n)(\Delta t)^2$$

(Notice that this is not a self starting algorithm)

Exercise 4.2: Approach to equilibrium I

Write the code for simulating a two dimensional system of particles interacting via a Lennard-Jones potential. Consider $N = 12$ particles in a box of linear dimensions $L_x = L_y = 8$. For this choice of N and L the density $\rho = 12/64 = 0.19$. Suppose that the particles are initially constrained to be in the left part of the box and placed on a rectangular grid. At $t = 0$ the constraint is removed and the particles move freely throughout the entire box. Use $v_{\max} = 1.0$, the maximum initial speed, and $\Delta t = 0.02$.

1. Observe a sufficient number of snapshots for the particles to move significantly from their original positions (It will take of the order of 100-200 time steps). Does the system become more or less random?

2. From the visual snapshots of the trajectories, estimate the time for the system to reach equilibrium. What is your qualitative criterion for equilibrium?

3. Compute $n(t)$ the number of particles on the left hand side of the box. Plot its value as a function of time. What is the qualitative behavior of $n(t)$? What is the mean number of particles on the left side?

Exercise 4.3: Approach to equilibrium II

Consider $N = 12$ particles in a box of linear dimensions $L_x = L_y = 8$. Consider the initially the particles are placed in a rectangular grid and the velocities are random with $v_{\max} = 1.0$.

1. Do a number of MD steps (50,100) and average the quantity $|\mathbf{v}^*|^2$ to estimate the actual temperature. To adjust the temperature to a desired value, scale all velocity components for all particles in a suitable way. Repeat this procedure up to 10 times. After 500-1000 steps the fluid will be well equilibrated and the temperature will be steady (although fluctuating slightly). Use $\Delta t = 0.02$.

2. Plot the temperature averaged over intervals of 5 time steps as a function of time for each of the previous temperatures. What is the qualitative dependence of the temperature fluctuations?

3. Calculate the kinetic and potential energies as a function of time. Are the kinetic and potential energies conserved separately?

Exercise 4.4: Distribution of speeds

Our goal is to calculate the equilibrium probability $P(v)\Delta v$ of finding a particle with speed between v and $v + \Delta v$. Obtain an estimate of the maximum speed of the particles from the initial configuration. Choose windows with width Δv. Each particle will belong to the k-th window, with $k = v/\Delta v$. A reasonable choice of Δv is $0.1\sqrt{T}$, where T is the temperature.

1. Record the histogram of velocities $P(v)$ and plot is versus v. What is the qualitative form of $P(v)$? What is the most probable value for v? What is the approximate "width" of $P(v)$? This probability distribution is known as the Maxwell-Boltzman distribution.

2. Determine the distribution for each component of the velocity. Make sure to distinguish between positive and negative values. What are the most probable values for the x and y components? What are the average values?

4.5 Evaluation of observables

In the previous exercises we have used the number of particles in the left side of the box, and the measure of the temperature T to characterize the equilibrium of the system. Other parameter that can be used are the mean pressure P and as well as the total energy E.

Other thermal quantity is the heat capacity $C_V = (\partial E/\partial T)_V$. C_V is a measure of the amount of heat needed to produce a change in the temperature. Since this is and extensive quantity (depends on the size of the system) it is convenient to use the specific heat $c_V = C_V/N$ instead. The easiest way to obtain it is to determine the mean potential energies at neighboring temperatures T and $T + \Delta T$.

In order to determine the mean pressure, suppouse for a moment that the container has rigid walls. We know that the collisions of particles with the walls will cause a mean net force to be exerted on each element of the wall. The mean force per unit of area is the pressure P of the gas. The force can be found by relating the force in the horizontal direction to the rate of change of the linear component of the linear momentum of the particles hitting the wall.

We can use a similar argument to calculate the pressure in the absence of walls. Since the pressure is uniform at equilibrium, we can relate the pressure to the transfer of momentum across an element of area anywhere in the system. Consider an element of area dA and let $\mathbf{K}_+$ be the mean momentum crossing the surface per unit of time from left to right, and let $\mathbf{K}_-$ be the mean momentum crossing the surface per unit of time from right to left. The the mean force $\mathbf{F}$ is

$$\mathbf{F} = \mathbf{K}_+ - \mathbf{K}_-$$

and the mean pressure is given by

$$P = \frac{dF_\alpha}{dA}$$

where F_α is the component of the force normal to the element of area. (For two dimensions, the pressure is defined per unit of length)

An alternative way of calculating the pressure is from the virial theorem:

$$PV = NkT + \frac{1}{d}\langle \sum_i^N \mathbf{r}_i \cdot \mathbf{F}_i \rangle$$

Exercise 4.5: Equation of state of a non-ideal gas

In this problem we compute the pressure and hence the "equation of state" (the relation between pressure, temperature and volume) of a gas

1. Consider $L_x = L_y = 6, N = 16$. Choose the initial configuration to be an equilibrium configuration. Compute the mean pressure using the net momentum transfer method and the virial theorem. Allow at least 100 time steps for equilibration and 200 to compute averages. Is the pressure constant or fluctuates? How does the pressure compare with the ideal gas result? Which method of computing the pressure is more accurate?

2. An approximate equation of state for dense gases and liquids is the "van der Waals" equation:

$$P = kT\frac{\rho}{1 - b\rho} - a\rho^2.$$

The phenomenological parameters a and b are related to the repulsive and attractive parts of the interaction respectively and are approximately independent of the temperature.. Use the same configuration to find the dependence of P on T. Plot P versus T and use the van der Waals equation to obtain an estimate for the parameters a and b.

Exercise 4.6: Ground state energy

Although the use of periodic boundary conditions minimizes surface effects, it is also important to choose the symmetry of the central "unit cell" to be consistent with the symmetry of the solid phase of the system. This choice of cell is essential if we wish to do simulations of the high density, low-temperature behavior. We know that the equilibrium structure of a crystalline solid at $T = 0$ is the configuration of lowest energy.

1. Consider a triangular lattice of with L_x and height $L_y = \frac{\sqrt{3}}{2}L_x$. Each column of the triangular lattice is separated by a distance $a = L_x/n_c$, where n_c is the number of particles per row and $N = n_c^2$. For a square lattice to have the same density, we have to choose the linear dimension to be $L = \sqrt{L_x L_y}$. Choose $n_c = 6$ and determine the energy for each lattice using the Lennard-Jones potential. Use $L_x = 5$ and 7. What is the density of the system for each case? Are your results for E/N independent of the since of the lattice? Which lattice has lower energy? Why?

2. Consider $n_c = 6$ and $L_x = 10, 20$, and $2^{1/6} n_c$. Which lattice structure has lowest energy in each case? In all these cases the net force on a particle is zero. Why? The latter density correspond to the case where the force between nearest neighbors is zero. Convince yourself that at this density the lattice is unstable, since the force on any particle which deviates from its equilibrium position in the lattice is negative. Consequently, the system will collapse to a higher density, where the triangular lattice is always favored.

3. Repeat the previous calculations for $V(r) = 1/r^6$ and $1/r^4$. Is the triangular lattice still favored?

Exercise 4.7: The solid state and melting

1. Choose the parameters $N = 16$, $\Delta t = 0.01$, $L_x = 4$, and $L_y = 2\sqrt{3}$. Place the particles on a triangular lattice which fills the container and give each particle initial zero velocity. Measure the temperature and pressure as a function of time and plot several "snapshots" of the system. What is the total energy of the system? Does it remain a solid?

2. Give the particles a random initial velocity with $v_{\max} = 0.1$. What is the total energy? Equilibrate the system for approximately 50 time steps and average the pressure and temperature over 100 time steps.

3. Pick an equilibrium configuration from the previous item and rescale all velocities by a factor 2. What is the new total energy? Take snapshots of the system every 25 time steps and describe the behavior of the motion of the particles. What is the equilibrium temperature and pressure of the system? After equilibrium is reached, rescale the velocities again in the same way. repeat this rescaling and measure $P(T)$ and $E(T)$ for size different temperatures.

4. Plot $E(T) - E(0)$ and the pressure $P(T)$ as a function of T. What is the dependence of difference ΔE with T?

5. Decrease the density by multiplying L_x, L_y , and the particle coordinates by a factor 1.1. What are your results for temperature and pressure? What is the nature of the snapshots? Continue rescaling the density and the positions until the system "melts". What is your qualitative criterion for melting?

4.6 Simple transport properties

Suppose that we follow the trajectory of a particle and we determine its displacement $\mathbf{r}_i(t_2) - \mathbf{r}_i(t_1)$. We know that if the particle suffers zero net force, this displacement will increase linearly. However, a particle in a fluid undergoes collisions and on the average its net displacement will be zero. A more interesting quantity is the mean square displacement $R(t)^2$ defined by

$$R(t)^2 = \langle |\mathbf{r}_i(t_2) - \mathbf{r}_i(t_1)|^2 \rangle, \tag{45}$$

where $t = t_2 - t_1$ and we have averaged over all particles. Since the system is at equilibrium, this quantity depends only on the time difference. According to Einstein relation

$$R(t)^2 = 2dDt \qquad (t \to \infty)$$

where D is the "self-diffusion constant".

Another single -particle property is the "velocity autocorrelation function" $Z(t)$. Suppose that a particle has velocity $\mathbf{v}_i(t_1)$ at time t_1. If it suffers zero net force, its velocity will remain constant, and hence, its velocity at a later time will remain "correlated" with its initial velocity. However, the interactions with the other particles in the fluid will alter its velocity, and we expect that after some time its velocity will no longer be strongly correlated. Hence, we define $Z(t)$ as

$$Z(t) = \langle \mathbf{v}_i(t_2) \cdot \mathbf{v}_i(t_1) \rangle$$

where $t = t_2 - t_1$. If we define the self-diffusion constant D by relation (45), it can be shown that D is related to $Z(t)$ by

$$D = \frac{1}{d} \int_{-\infty}^{+\infty} Z(t) dt.$$

This relation is an example of a general relation between transport coefficients such as viscosity and thermal conductivity and autocorrelation functions.

4.7 How much complicated can it get?

- External fields
- Three dimensions

- Complicated geometries
- Different types of particles
- Internal degrees of freedom (rotations)
- Quantum mechanics

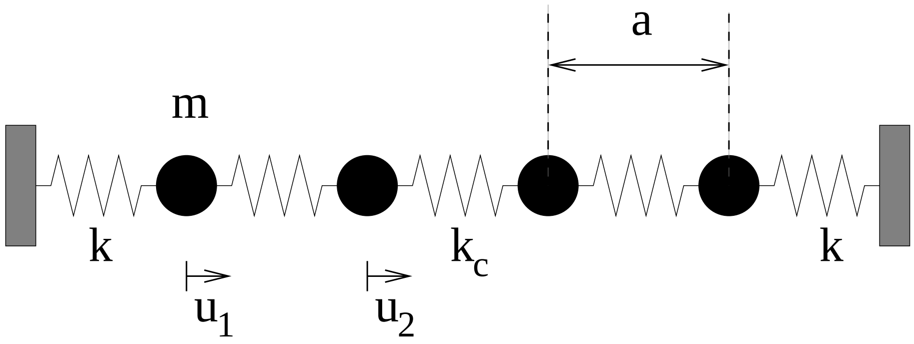

Figure 9: Coupled oscillators in one dimension

5 Waves!

Imagine a pulse propagating in a string. As the wave travels each segment of the string moves up and down perpendicular to the direction of propagation. At the macroscopic level, we observe a transverse wave that moves along the string, and the individual motion of the segments is not relevant.. In contrast, at the microscopic level, we see discrete particles undergoing oscillatory motion perpendicular to the motion of the wave.

In a string, or a solid, or a fluid, the collective motion of the particles determine the velocity of sound in the medium, as well as the thermal transport properties.

5.1 Coupled oscillators

Let us first consider a one-dimensional chain of N particles of mass m with equal equilibrium separation a. The particles are coupled to massless springs with force constant k_c, except for the first and last springs at the two ends of the chain which have spring constant k. the individual displacement of the particle i from its equilibrium position along the x axis is called u_i. The ends of the fist and last spring are assumed fixed:

$$u_0 = u_{N+1} = 0.$$

Since the force of an individual mass is determined only by the compression or expansion of the adjacent springs, the equation of motion for particle i is given by:

$$m\frac{d^2u_i}{dt^2} = -k_c(u_i - u_{i+1}) - k_c(u_i - u_{i-1}) \tag{46}$$
$$= -k_c(2u_i - u_{i+1} - u_{i-1}). \tag{47}$$

The equations for particles $i = 1$ and $i = N$ next to the walls are given by

$$m\frac{d^2u_1}{dt^2} = -k_c(u_1 - u_2) - ku_1, \tag{48}$$
$$m\frac{d^2u_N}{dt^2} = -k_c(u_N - u_{N-1}) - ku_N. \tag{49}$$

Note that for $k_c = 0$ all the equations will decouple and the motion of the particles become independent of their neighbors. The above equations describe longitudinal oscillations, *i. e.* motion along the direction of the chain. The equations for transverse motion are equivalent.

Exercise 5.1

Write a generalization of the program for one oscillator to describe the motion of N coupled linear oscillators.

Exercise 5.2: two coupled oscillators

1. Use the previous program with $N = 2$. Set the initial conditions $u_1 = 0.5$ an $u_2 = 0$ and compute the time dependence of the displacements for $k = 1, k_c = 0.8$ and $k = k_c = 1$. Remember that the mass of the particles has to be set to unity. Describe the qualitative behavior or the particles in each case. Is it possible to define a period of motion in the first case? What is the period in the second case?

2. Set $k = 1, k_c = 0.2$. Since $k_c < k$, we can describe the springs as being "weakly coupled". Observe the time dependence of the displacement of particle one. Can you identify two kinds of oscillations superimposed on upon each other? What is the time between the oscillations of the amplitude? What is the time between the zeroes of the displacement? Compute the corresponding angular frequency of each oscillation. How does the displacement of particle 2 correspond to that of particle 1?

Determine the qualitative changes in the frequencies of each oscillation for $k_c = 1$.

3. Choose the initial conditions $u_1 = u_2 = 0.5$ so that both particles have the same initial displacements, Set $k_c = 0.1$ and $k = 1$ and describe the motion. Compute the total energy of each particle as a function of time and describe its qualitative behavior. Does the period of motion depend on k_c? What if the dependence of the period on k?

4. Consider the initial conditions $u_1 = -u_2 = 0.5$ so that both particles have equal but opposite initial displacements. Is there a simple sinusoidal oscillation in this case? Compute the period T_1 for $k = 1, k_c = 1$, $k = 2, k_c = 1$, and $k = 1, k_c = 2$. Analyze your results for ω_1^2 and determine its dependence on k and k_c. What is the behavior of the energy of each particle as a function of time?

Exercise 5.3: response to an external force

Ass an external driving force $F(t) = F_0 \cos \omega t$ to particle 1. plot $u_1(t)$ and determine its maximum steady state amplitude $A(\omega)$ for each value of ω. Confirm that near a resonance $A(\omega)$ exhibits a rapid increase with ω, and $u_1(t)$ increases without bound at the resonant frequency. Determine the resonant frequencies for the pairs of k-values already considered in parts 2-4 in Exercise 5.2. How do these values of ω compare to those in the previous exercise?

Exercise 5.4: superposition of motion

The results of the previous exercises make plausible the assumption that an arbitrary motion of the system can be written as

$$u_1(t) = A_1 \cos(\omega_1 t + \delta_1) + A_2 \cos(\omega_2 t + \delta_2) \tag{50}$$

$$u_2(t) = A_1 \cos(\omega_1 t + \delta_1) - A_2 \cos(\omega_2 t + \delta_2) \tag{51}$$

The values of these constants can be expressed in terms of the initial values of the displacement and velocities of each particle. determine these constants for $u_1 = 0.5, u_2 = 0, v_1 = v_2 = 0$. Verify that the motion predicted by these equations is consistent with your measure values for u_1 and u_2 for

$k = 1$ and $k_c = 0.8$ in part 1 of Exercise 5.2. What is the periodicity of u_1 and u_2?

The effect of the spring k_c is to couple the motions of two particles so that they no longer move independently. For special initial conditions, only one frequency of oscillation appears. The resulting motion is called a "normal mode" of the system, and the corresponding frequency a "normal mode frequency". The higher frequency is given by $\omega_1^2 = (k + 2k_c)/m$. In this mode, the two particles oscillate exactly out of phase with the displacements of opposite directions. The motion at the lowest frequency $\omega_2^2 = k/m$ corresponds to the two particles oscillating exactly in phase.

The general motion is a superposition of the two normal modes. Unless there is a simple relation between the two frequencies, the general motion is a complicated function of time. However, if the coupling is small, ω_1 and ω_2 are nearly equal and u_1 and u_2 exhibit "beats". In this case the displacements oscillate rapidly at the angular frequency $1/2(\omega_1 + \omega_2)$ with an amplitude that varies sinusoidally at the beat frequency $1/2(\omega_1 - \omega_2)$.

We also found that if we drive the system by an external force applied to either particle (or both), the system is in resonance if the frequency of the force corresponds to either of the normal modes. We use this method for determining the normal mode frequencies in the following exercises.

Exercise 5.5: three coupled oscillators

1. Run the program with $N = 3$, $k_c = 0.2$ and $k = 1$ and arbitrary but nonzero initial displacements. Describe the time-dependence of the motion of the particles.

2. Consider the following initial conditions: $u_1 = u_2 = u_3 = 0.5$, $u_1 = 0.5, u_2 = -0.5, u_3 = 0.5$, $u_1 = 0.5, u_2 = 0, u_3 = -0.5$ (all the velocities are initially zero) If these initial conditions correspond to normal modes, determine the normal modes frequencies.

3. Add an external driving force to particle 1 and determine the normal mode frequencies. Compare your results with the frequencies you obtained in part 2. How many normal modes are there?

Exercise 5.6: N coupled oscillators

1. Choose $k_c = k = 1$ and $N = 10$. Find the normal modes by applying an external force to one of the particles and determine the resonant frequencies. Drive the system for several periods of the external force and compute the steady state amplitude of the displacement of each particle for each value of ω. Try values of ω in the range $0.2(k/m)^{1/2}$ to $3(k/m)^{1/2}$. If you think that you are close to a resonance, use several other values of ω to obtain a better estimate. How many normal modes are there?

2. Compare your results in part 1 with the analytic result

$$\omega_n^2 = \frac{4k}{m} \sin^2 \frac{n\pi}{2(N+1)},$$

where N is the number of particles and the mode index is $n = 1, 2, ..., N$.

Exercise 5.7: propagation speed in a linear chain

Another interesting property to analyze is the propagation of the energy. In this problem we'll disturb the system determine the time that takes for the disturbance to travel a given distance.

1. Consider a linear chain of coupled oscillators at rest with $k = k_c = 1$. Create a disturbance giving particle 1 an initial displacement $u_1 = 1$. Determine the time it takes for particles $N/2$ and N to satisfy the conditions $|u_{N/2}| \geq d$ and $u_N \geq d$. Choose $N = 10$ and $d = 0.3$ for your initial runs. Use your results to estimate v, the speed of propagation of the disturbance. Consider larger values of N to ensure that your value is independent of N.

2. Do you expect the speed of propagation to be an increasing or decreasing function of the spring constant k? Do a simulation and estimate v for different values of k.

3. Create a disturbance by applying an external force $F(t) = F_0 \cos \omega t$ to particle 1. Estimate the propagation speed of the disturbance as in part 1. Consider the value so $\omega = 0.1$ and $\omega = 1$. Explain why the propagation speed depends on ω. Can a disturbance propagate

for $\omega = 4$? In what way does the system act as a mechanical filter? Explain the "filtering" property of the system in terms of the frequency of the normal modes.

5.2 Fourier analysis

In the previous section we found that the displacement of a particle an be described as a linear combination of normal modes, *i.e.* a superposition of sinusoidal terms. This decomposition of the motion into various frequencies is more general. It can be shown that any arbitrary periodic function $f(x)$ of period T can be written as a Fourier series of sines and cosines:

$$f(t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}(a_n \cos n\omega t + b_n \sin n\omega t),$$

where ω_0 is the fundamental angular frequency given by

$$\omega_0 = \frac{2\pi}{T}.$$

The sine and cosine terms represent the harmonics. The Fourier coefficients a_n and b_n are given by

$$a_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t) \cos n\omega_0 t dt \tag{52}$$

$$b_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t) \sin n\omega_0 t dt \tag{53}$$

$$\tag{54}$$

The constant term $1/2a_0$ is the average value of $f(t)$. (all the oscillating contributions vanish in average)

In general, an infinite number of terms is needed to represent an arbitrary function $f(t)$. In practice, a good approximation can usually be obtained by including a relatively small number of terms.

Exercise 5.8: Fourier analysis

1. Consider the following series $f(t) = \frac{2}{\pi}\sum_{n=1}^{\infty} \sin nt$.Plot $f(t)$ retaining only the first 3 terms. Increase the number of terms until you are satisfied that you are converging to $f(t)$ with some arbitrary but sufficient accuracy. What is the function represented by the sum?

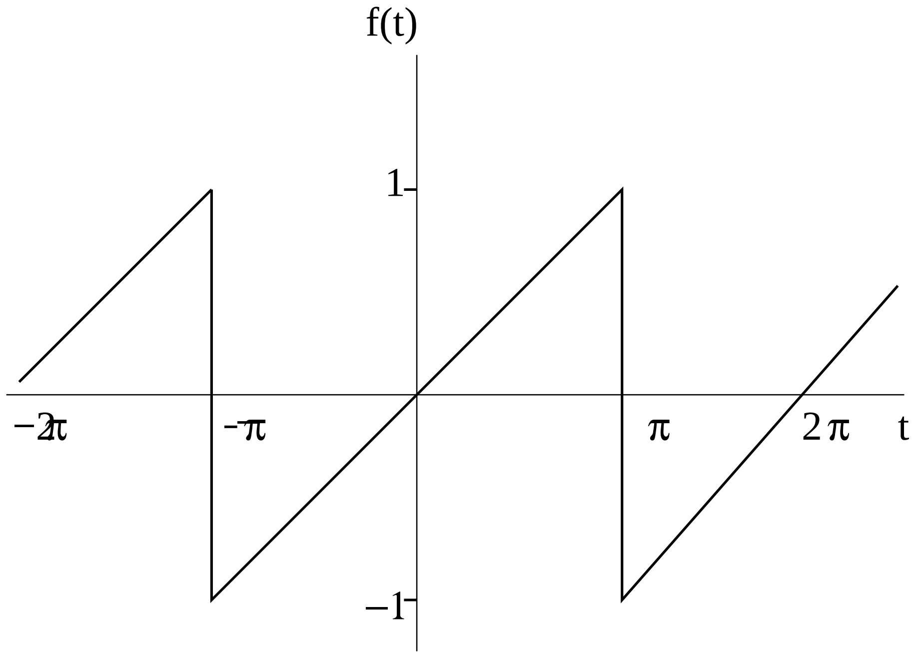

Figure 10: The “sawtooth” function studied in Exercise 5.8

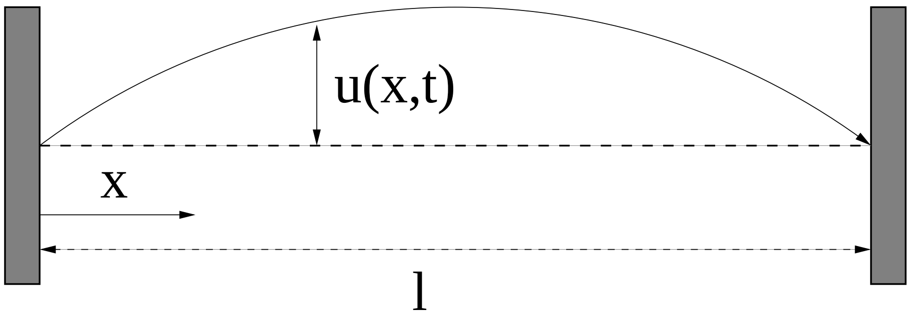

Figure 11: A stretched string of length l with the ends fixed.

2. Use the analytical expression for the Fourier coefficients and calculate the integrals using the "sawtooth" function depicted in Fig 5.2 to show that they are effectively given by $a_n = 0$ and $b_n = (1/n\pi)(-1)^{n-1}$

3. What function os represented by the Fourier series with coefficients $a_0 = 0$ and $a_n = b_n = 1/n^2$ for $n \neq 0$?

5.3 Waves on a string

The difference between waves and oscillatory motion is the scale. Waves are the "continuum" limit of the problem, or in the jargon "the long wavelength" limit. This is because in this limit, all the microscopic details are "washed out" and only the long distance behavior survives. In order to understand the transition between these two limits we have to perform a change of scale. The discrete equations of motion, as shown previously, can be written as:

$$\frac{d^2u}{dt^2} = -\frac{k}{m}(2u_i - u_{i+1} - u_{i-1}).$$

We consider the limits

$$N \to \infty, a \to 0.$$

with the length of the chain kept constant. The main result is that in this limit, the discrete equations of motion can me replaced by the continuous wave equation:

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{1}{v^2}\frac{\partial^2 u(x,t)}{\partial x^2}, \tag{55}$$

where v has the dimension of velocity and it is given by

$$v = \sqrt{k/\rho},$$

where k is the string tension and ρ is the linear density. Observe that the displacement u of the string is the dependent variable, and that the position along the string x and the time t are the independent variables. The existence of two independent variables makes this a Partial Differential Equation (PDE).

There are many solutions to this equation. Examples are:

$$u(x,t) = A\cos\frac{2\pi}{\lambda}(x \pm vt), \tag{56}$$

$$u(x,t) = A\sin\frac{2\pi}{\lambda}(x \pm vt). \tag{57}$$

In fact, it is easy to show that any function of the form $f(x \pm vt)$ is a solution. Since the differential equation is a linear equation and hence satisfies the superposition principle, we can understand the behavior of a wave of arbitrary shape using the Fourier's theorem to represent its shape as a sum of sinusoidal waves.

Because both ends of the string are tied down, the boundary conditions are:

$$u(0,t) = u(l,t) = 0. \ \text{(boundary condition)}$$

Since this is a second order PDE, we still need to determine the initial distortion $u(x, t = 0)$ and velocity $\partial u/\partial t(x, t = 0)$. If the string is released from rest, this reduces to

$$u(x,t) = f(x), \quad \text{(initial condition 1)} \tag{58}$$

$$\frac{\partial u}{\partial t}(x,t = 0) = 0. \ \text{(initial condition 2)} \tag{59}$$

5.3.1 Numerical solution: finite differences

To solve the equation (55) as a function of position and time we need to discretize the (x,t) space in a rectangular grid (see Fig 12). In the present case, the horizontal axis represents the position x along the string, and the vertical axis represent time. We convert the equation to a finite difference equation expressing the second derivatives in terms of differences

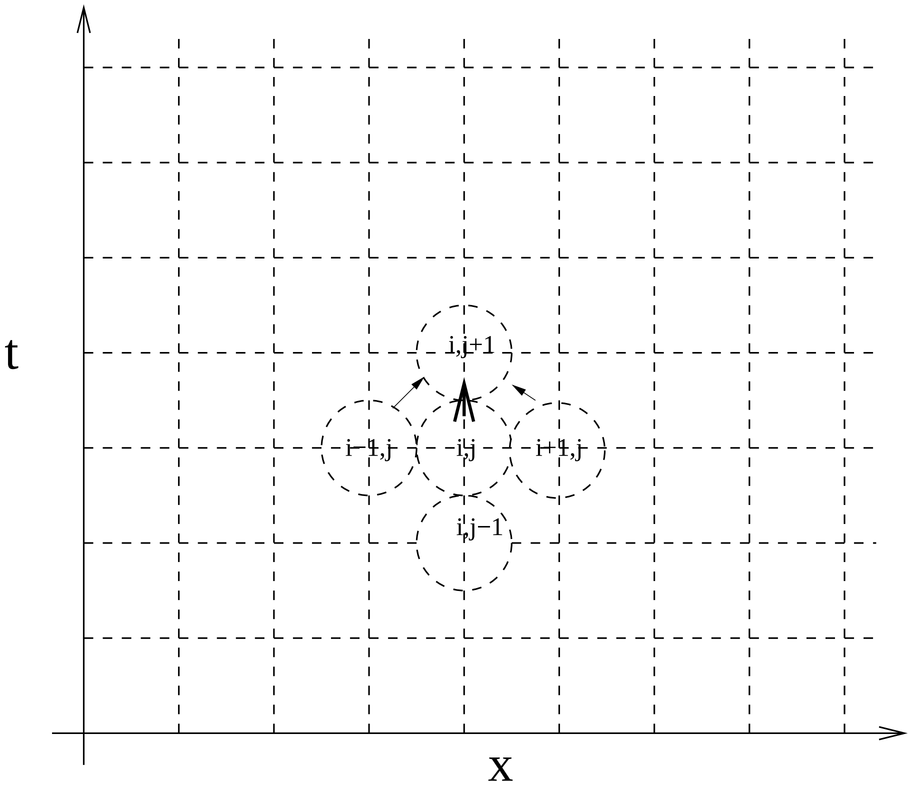

Figure 12: Finite differences grid for the vibrating string

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial t^2} &\simeq \frac{u(x,t+\Delta t)+u(x,t-\Delta t)-2u(x,t)}{(\Delta t)^2},\\ \frac{\partial^2 u(x,t)}{\partial t^2} &\simeq \frac{u(x+\Delta x,t)+u(x-\Delta x,t)-2u(x,t)}{(\Delta t)^2}.\end{aligned}$$

After substituting into (55) we obtain the discrete equations:

$$u(x,t+\Delta t) = 2u(x,t) - u(x,t-\Delta t) + \frac{v^2}{C^2}\left[u(x+\Delta x,t)+u(x-\Delta x,t)-2u(x,t)\right],$$

with $C = \Delta t/\Delta x$ is a constant with the dimension of velocity.

As shown in Fig. 12, this is a recurrence relation that propagates the wave from the two earlier times $t-\Delta t$ and t, and the three nearby positions

$x - \Delta x$, x, and $x + \Delta x$, to a later time $t + \Delta t$, and a single position x. We can see right a way that this is not a self starting algorithm, in the sense that we need to know the position fro two earlier times to start the iteration. However, we can use a simple trick to overcome this difficulty. Rewriting the initial conditions (58) and (59) in the finite differences form, we obtain:

$$\begin{aligned}\frac{\partial u(x,t=0)}{\partial t} &= 0 \Rightarrow \frac{u(x,\Delta t) - u(x,-\Delta t)}{2\Delta t} = 0, \\ &\Rightarrow u(x,-\Delta t) = u(x,\Delta t).\end{aligned}$$

Using this condition for the first iteration we obtain

$$u(x,t+\Delta t) = u(x,0) + \frac{1}{2}\frac{v^2}{C^2}\left[u(x+\Delta x,t) + u(x-\Delta x,t) - 2u(x,t)\right].$$

The success of this method depends on the relative sizes of the time and space steps. This stability criterion says that the finite difference algorithm is stable if

$$v \leq \frac{\Delta x}{\Delta t} = C. \tag{60}$$

This means that the solution gets better with smaller time steps, but worse with smaller space steps!

Exercise 5.9: Finite differences for the wave equation

Write a program to solve the wave equation using finite differences. Assume that the string has a length $l = 1$m, a linear density $\rho = 0.01$kg/m, and tension $k = 40$N.

1. Assume as initial conditions that the string is "plucked":

   $$u(x,t=0) = \begin{cases} 1.25x/l, & \text{for } x \leq 0.8l, \\ 5.0(1 - x/l), & \text{for } x > 0.8l, \end{cases}$$

   Plot the displacement u as a function of (x,t) using a space step $\Delta x = 0.01$m, and choosing the time step such that the solution is stable.

2. Explore the use of different steps Δx and Δt and determine at which values the solution becomes unstable. Does your assessment agree with the condition (60)?

3. Change the initial conditions to

$$u(x, t=0) = \begin{cases} x/l, & \text{for } 0 \leq x \leq 0.5, \\ -x/l, & \text{for } 0.5 \leq x \leq 0.1, \end{cases}$$

and compare results with the previous simulation.

4. Consider a string plucked at two points:

$$u(x, t=0)/0.005 = \begin{cases} 0, & 0.0 \leq x \leq 0.1, \\ 10x - 1, & 0.1 \leq x \leq 0.2, \\ -10x + 3, & 0.2 \leq x \leq 0.3, \\ 0, & 0.3 \leq x \leq 0.7, \\ 10x - 7, & 0.7 \leq x \leq 0.8, \\ -10x + 9, & 0.8 \leq x \leq 0.9, \\ 0 & 0.9 \leq x \leq 1.0. \end{cases}$$

Solve and observe wether the pulses move or oscillate up and down.

5. Explore what happens when the string is places in a "normal mode", for example:

$$u(x, t=0) = 0.001 \sin(2\pi x).$$

Try other modes. See if the sum of two modes gives "beating".

Exercise 5.10: String with friction

The effect of the friction on an element of string $(x, x + \Delta x)$ is to oppose its motion. Assume that the force of friction is proportional to the vertical velocity $\partial u/\partial t$ of the string element. This changes the wave equation to

$$\frac{\partial^2 u}{\partial t^2} + 2\kappa \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},$$

where the constant κ is proportional to the viscosity of the medium in which the string is vibrating, and is inversely proportional to the density of the string. Generalize the algorithm for the wave equation to include friction and observe the change in the wave behavior. Use the same parameters of the pervious example, with $\kappa = 5$.

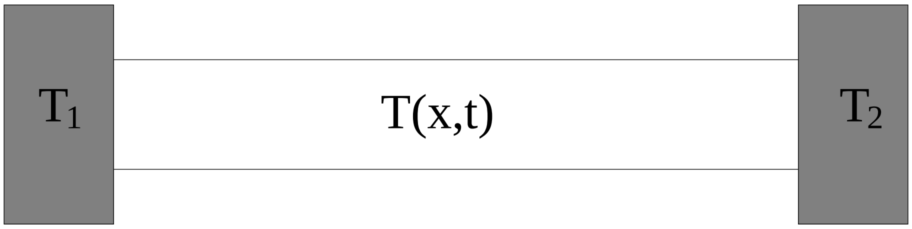

Figure 13: A bar with the ends in contact with heat reservoirs.

6 Heat Flow

The problems consiste in determining the temperature variation along a bar of length l at any instant of time, given the initial gradient of temperature.

The problem is described by the "Heat Equation" that can be derived as follows:

At any instant of time, the heat flow through the bar equals the variatioon of energy inside the bar:

$$\text{Heat Flow} = \text{Variation of internal energy}$$

or

$$\nabla \cdot Q = -\frac{dE}{dt}. \tag{61}$$

The variation of the internal energy is given by the body's ability to store heat by raising its temperature:

$$\frac{dE}{dt} = \rho c \frac{dT}{dt}, \tag{62}$$

where ρ is the density, and c is the specific heat of the material. Fourier's Law of heat conduction states that

$$Q = -K \nabla T, \tag{63}$$

where K is the thermal conductivity. Hence, we obtain

$$\nabla \cdot (K \nabla T) = \rho c \frac{dT}{dt}, \tag{64}$$

or

$$\frac{dT}{dt} = \alpha \nabla^2 T, \tag{65}$$

with $\alpha = K/(c\rho)$. In 1d this equation is written

$$\frac{\partial T(x,t)}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}. \tag{66}$$

We must solve this equation given the initial condition

$$T(x, t = 0) = f(x) \ \text{(initial condition)} \tag{67}$$

and the boundary condition

$$T(x = 0, t) = T_1, \tag{68}$$
$$T(x = l, t) = T_2. \tag{69}$$

6.1 Finite differences solution

The numerical solution is based on converting the differential equation into an approximate finite-diffence one. Following a derivation similar to the one we used for the wave equation we approximate the derivatives by finite differences:

$$\frac{\partial T}{\partial t} = \frac{T(x, t + \Delta t) - T(x,t)}{\Delta t}, \tag{70}$$
$$\frac{\partial^2 T}{\partial x^2} = \frac{T(x + \Delta x, t) + T(x - \Delta x, t) - 2T(x,t)}{(\Delta x)^2}. \tag{71}$$

Replacing in 66 we obtain the discrete equivalent:

$$T(x, t + \Delta t) = T(x,t) + \frac{\alpha}{C}\left[T(x + \delta x, t) + T(x - \Delta x, t) - 2T(x,t)\right], \tag{72}$$

with the constant $C = (\Delta x)^2/\Delta t$. We see in Fig. 14 that the temperature at the point $(x, t + \Delta t)$ is determined by the temperatures at three points of the previous time step. The boundary conditions impose fixed values along the perimeter. The initial condition 67 is used to generate the temperature gradient at time $t = \Delta t$, and the equation is used for the time evolution.

The stability condition for a numerical solution is iven by

$$\alpha \frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{4}. \tag{73}$$

This means that if we make the time step smaller we improve convergence, but if we decrease the space step without a simultaneous quadratic increase of the time step, we worsen it.

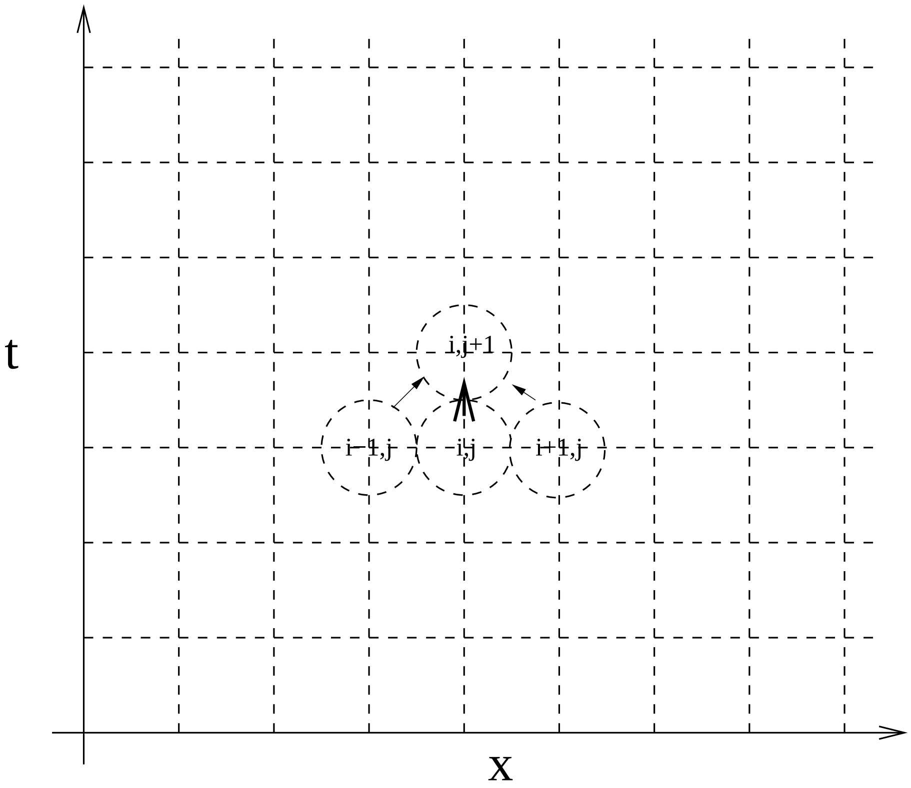

Figure 14: The finite differences algorithm for the heat equation.

Exercise 6.1: Finite differences program

Solve the temperature distribution within an iron bar of length $l = 50$cm with the boundary conditions

$$T(x = 0, t) = T(x = l, t) = 0,$$

and initial conditions

$$T(x, t = 0) = 100°\text{C}.$$

The corresponding constants for iron are:

$$c = 0.113\text{cal}/(\text{g}°\text{C}),\ K = 0.12\text{cal}/(\text{sg}°\text{C}),\ \rho = 7.8\text{g}/\text{cc}.$$

1. Write the program to solve the heat flow equation using the finite differences method

2. Plot the temperature gradient along the bar at different instants of time. Use 100 space divissions for the calculation. Choose an appropiate time step such that the numerical solution is stable. Check that the temperature diverges with time is the constant c is made larger that 0.5.

3. Repeat the calculation for aluminum, $c = 0.217cal/(g°C)$, $K = 0.49cal/(g°C)$, $\rho = 2.7g/cc$. Note that the stability condition requires you to change the size of the time step.

4. Analize and compare the results for both materials. The shape of the curves may be the same but not the scale. Which bar cools faster and why?

5. Pick a sinusoidal initial gradient:

   $$T(x, t = 0) = \sin{(\pi x/l)}.$$

   Compare with the analytic solution

   $$T(x, t) = \sin{(\frac{\pi x}{l})}e^{\pi^2\alpha t/l^2}.$$

Exercise 6.2: Two bars in contact

Two identical bars, 25cm long each, are incontact. One bar is initially at $50°C$, and the other at $100°C$. The free ends are kept at $0°C$. Calculate and plot the temperature distribution as a function of time.

7 Electrostatic potentials

Suppouse that we are given the electrical potential in the boundaries of some region, and we want to find the potential $V(\mathbf{r})$ inside. Once we know V we can use the relation $\mathbf{E} = -\nabla V(\mathbf{r})$ to determine $\mathbf{E}$. This is a "boundary problem". We know from classical elctrodinamics (Gauss' Law) that the potential $V(x,y,z)$ satisfies Poisson's equation:

$$\nabla^2 V(x,y,z) = -\frac{\rho(x,y,z)}{\epsilon 0} \tag{74}$$

with

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2},$$

and ρ, the charge density inside the region; the constant ϵ_0 is the electrical permittivity of the vaccum. Besides satisfying, V has also to satify the boundary conditions. Since the shape of the region can be arbitrary, we need to use the computer to solve the problem. In the particular situation that there are no charges inside the region, the problem reduces to solving "Laplace's equation":

$$\nabla^2 V(x,y,z) = 0. \tag{75}$$

As we did in the previous examples of PDE's, we discretize the derivatives and we transform the equation to a finite difgferences problem. From now on we worry only about the two-dimensional case. We discretize the region in a grid with points (x,y) separated by intervals $(\Delta x, \Delta y)$. The second derivatives are approximated by:

$$\frac{\partial^2 V(x,y)}{\partial x^2} \simeq \frac{V(x+\Delta x,y) + V(x-\Delta xx,y) - 2V(x,y)}{(\Delta x)^2}, \tag{76}$$

$$\frac{\partial^2 V(x,y)}{\partial x^2} \simeq \frac{V(x,y+\Delta y) + V(x,y-\Delta xy) - 2V(x,y)}{(\Delta y)^2}. \tag{77}$$

Replacing these expressions in (75) and choosing $\Delta x = \Delta y = \Delta$ we obtain

$$V(x,y) \simeq \frac{1}{4}[V(x+\Delta,y) + V(x-\Delta,y) + V(x,y+\Delta) + V(x,y-\Delta)]. \tag{78}$$

That is, the value of $V(x,y)$ is given by the average of the values in the neighboring nodes in the grid.

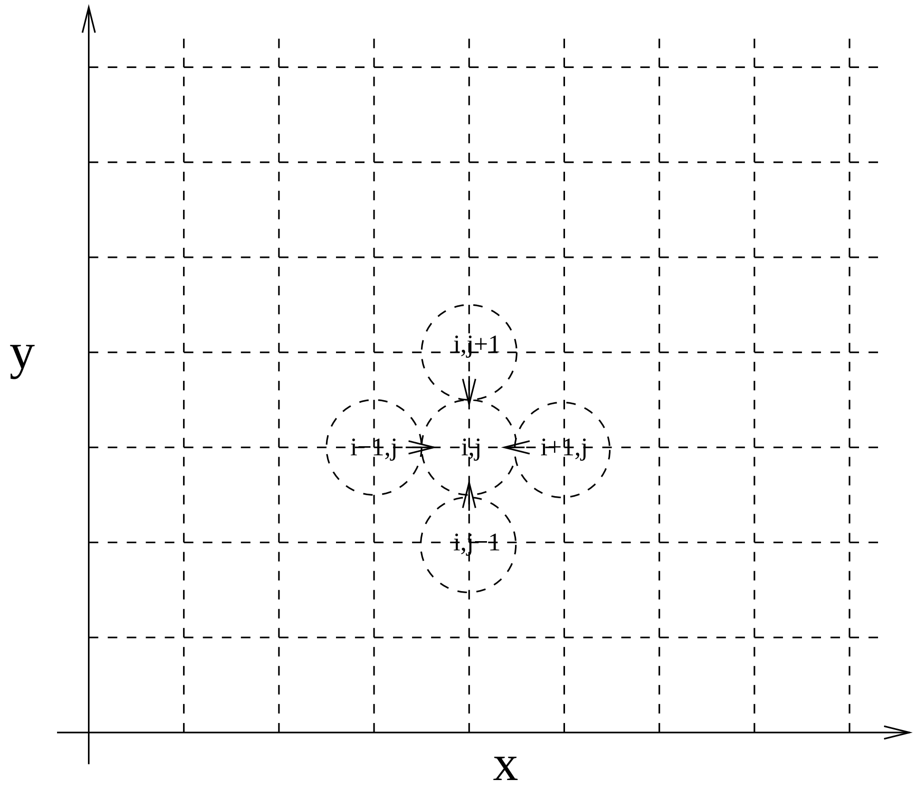

Figure 15: Finite differences for Laplace's equation. The value of the potential at one point is given by the average of the four neighboring points

7.1 Units

Notice that the charge of the electron is $e = 1.6\times10^{-19}C$. From a microscopic point of view, the Coulomb is a very large unit pof charge. Hence, we expect that for many simulatioons we will have to choose different units.

7.2 The finite differences algorithm

Suppouse that we are given the values of $V(x, y)$ in the boundaries of a rectangular area. If we divide the rectangle in a grid, we can the apply (78) to calculate the values of V inside. However, we notice right away that if we apply this equation in a point in the middle, we get zero as a result. So the first obvious observation is that the initial estimate for the method can not be a constant value. It is evident now that the procedure has to be iterative. We start from the bottom-left corner, and we sweep across the grid. As we obtain the first estimate for V, we repeat the sweep until the values of V do not change considerably, and we can say that we have converged with certain accuracy. Here we have started with the initial values $V(x, y)$ inside the grid that in principle can be any initial guess (exept a constant, as we have seen). The rate of convergence will be determined by the proximity of this guess to the actual solution.

The algorithm can be decribed as follows:

1. Divide the rgion of interest into a grid. The region must be enclosed by boundaries with known values of V.

2. Assingn to all points of the boundary the given values, and all interior cells an arbitrary potential (preferably a reasonable guess)

3. sweep the internal cells by rows or columns and calculate the new values of V as the average in the four neighboring points.

4. Repeat the sweep using the values obtained in the previous iteration, until the potential does not change within certain level of accuracy.

Exercise 7.1: Verification

1. Assume that the source of the potential is a point charge of $1\mu C$ at the origin. We know that the potential is going to be given by:

$$V(x, y) = \frac{1\mu C}{\sqrt{x^2 + y^2}} \tag{79}$$

Choose a reasonable value of Δ and compare the values of $V(x, y)$ given by (79) in the center of one, and the average of V in the four neighboring points (obtained also with Eq.(79)). Repeat for 5 different cells at different distances from the origin. Does the relative agreement depend on the distance of the cell to the origin?

2. Repeat part 1 with smaller values of Δ. Are the results in better agreement?

Exercise 7.2: Numerical solution inside a rectangular region

1. Determine the potential $V(x, y)$ inside a square region with linear dimension $L = 10cm$. The boundary of the square is at a fixed potential $V = 10V$. Before the computation, guess the exact form of the potential and set the values in the interior within 5the area of each cell to be 1cm^2. How many iteration do you need to achieve a 1

2. Consider the same situation, but with $V(5, 5) = 4$. Describe the evolution of the solution with the iterations. Does the potential distribution evolve o the correct solution? Are the final results independent of your initial guess? What is the effect of a poor initial guess? Note that if you pick a constant values as the intial guess, the result does not evolve toward a solution.

3. Set each side of the rectangle at a different potential 5,10,5,10, repectively. Do a contour plot and sketch the equipotential surfaces. What happens if the potential is 10V on three sides and 0 on the fourth? Start with a reasonable guess for the initial values of the potential of the interior points, and iterate until 1

4. Repeat the previous item with a twice the number of cells, and compare the results.

5. Modify your programs such the potential at each site is calculated sequentially rather than at the same time. How do your reults differ?

Exercise 7.3: Capacitance of concentric squares

1. Modify your code to treat a concentric square boundary, *i. e.*, a square centered inside a bigger square. The potential of the outer square is

10V and the inner square is set at 5V. The lineat dimensions of the two squares are $L_1 = 5$cm and $L_2 = 25$cm respectively. Choose a convenient grid. Plot the equipotential lines.

2. A system of two conductors with a charge Q and $-Q$ respectively has a capacitnce C which is defined by the formula:

$$C = \frac{Q}{\Delta V},$$

where ΔV is the potential difference between the two conductors. The charge can be determined by the expression:

$$\sigma = \frac{\mathbf{E} \cdot \mathbf{n}}{\epsilon_0} = \frac{E_n}{\epsilon_0}$$

where σ is the surface charge density, and E_n is the component of the electric field normal to the surface and can be approximated by

$$E_n = -\frac{\Delta V}{\Delta r},$$

where ΔV is the pottential difference between a boundary cell, and the adjacent interior at a distance Δr. Use the results of the previous part to calculate ΔV for each point next to the square surfaces. Use this information to obtain an estimate of E_n for the two surfaces, and teh charge per unit of length on each electrode. are the two charges equal and opposite in sign? Calculate the capacitance in Farads.

3. Move the inner square 1cm off center and repeat the calculations of parts 1. and 2. How do the equipotential surfaces change? Is there any qualitative difference if we set the center conductor potential to -5V instead of +5V?

Exercise 7.4: Poisson's equation

Laplace's equation holds for charge free regions. If there is a charge distribution inside the region we must use Poisson's equation (74) instead.

1. Generalize the difference equation for the Poisson's equation, and modify your program accordingly.

2. Consider a square of linear dimension $L = 25cm$ fixed at 10V. assume that each interior cell has a uniform charge density ρ such that $\frac{1}{4}A\rho/\epsilon_0 = 3V/cm^2$. Compute thte potential distribution for this case. Compare the equipotential lines with thos found in Exercise 7.3.

3. Find the potential distribution of the charge distribution of part 1. is restricted to a square of side $L = 5cm$ in the center.

8 Time dependent Schrödinger equation

We want to describe an electron wavefunction by a wavepacket $\psi(x,t)$ that is a function of position x and time t. We assume that the electron is initially localized around x_0, and model this by a Gaussian multiplying a plane wave:

$$\psi(x, t=0) = \exp\left[-\frac{1}{2}\left(\frac{x - x_0}{\sigma_0}\right)^2\right] e^{ik_0 x} \tag{80}$$

This wave function does not correspond to an electron with a well defined momentum. However, if the width of the Gaussian σ_0 is made very large, the electron gets spread over a sufficiently large region of space and can be considered as a plane wave with momentum k_0 with a slowly varying amplitude.

The behavior of this wave packet as a function of time is described by the time-dependent Schröedinger equation (here in 1d):

$$i\frac{\partial \psi}{\partial t} = H\psi(x, t). \tag{81}$$

H is the Hamiltonian operator:

$$H = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V(x), \tag{82}$$

where $V(x)$ is a time independent potential. The Hamiltonian is chosen to be real. we have picked teh energy units such that $\hbar = 1$, and from now on, we will pick mass units such that $m = 1$ to make equations simpler.

Schrödinger's equation is obviously a PDE, and we can use generalizations of the techniques learned in previous sections to solve it. The main observation is that this time we have to deal with complex numbers, and the function $\psi(x, y)$ has real and imaginary parts:

$$\psi(x, t) = R(x, t) + iI(x, t).$$

However, is this section we will present an alternative method that makes the quantum mechanical nature of this problem more transparent.

8.1 The time-evolution operator

The Schrödinger equation (81) can be integrated in a formal sense to obtain:

$$\psi(x, t) = U(t)\psi(x, t=0) = e^{-iHt}\psi(x, t=0). \tag{83}$$

From here we deduce that the wave function can be evolved forward in time by applying the time-evolution operator $U(t) = \exp(-iHt)$:

$$\psi(t + \Delta t) = e^{-iH\Delta t}\psi(t).$$

Likewise, the inverse of the time-evolution operator moves the wave function back in time:

$$\psi(t - \Delta t) = e^{iH\Delta t}\psi(t),$$

where we have use the property

$$U^{-1}(t) = U(-t).$$

Although it would be nice to have an algorithm based on the direct application of U, it has been shown that this is not stable. Hence, we apply the following relation:

$$\psi(t + \Delta t) = \psi(t - \Delta t) + \left[e^{-iH\Delta t} - e^{iH\Delta t}\right]\psi(t).$$

Now, the derivatives with recpect to x can be approximated by

$$\frac{\partial \psi}{\partial t} \sim \frac{\psi(x, t + \Delta t) - \psi(x, \Delta t)}{\Delta t}, \tag{84}$$

$$\frac{\partial^2 \psi}{\partial x^2} \sim \frac{\psi(x + \Delta x, t) + \psi(x - \Delta x, t) - 2\psi(x, t)}{(\Delta x)^2}. \tag{85}$$

The time evolution operator is approximated by:

$$U(\Delta t) = e^{-iH\Delta t} \sim 1 + iH\Delta t, \tag{86}$$

with an error of the order of $(\Delta t)^2$. Replacing the expression (82) for H, we obtain:

$$\psi(x, t + \Delta t) = \psi(x, t - \Delta t) - 2i[(4\alpha + \Delta t V(x))\psi(x, t) - \tag{87}$$

$$\alpha(\psi(x + \Delta x, t) + \psi(x - \Delta x, t))], \tag{88}$$

with $\alpha = \frac{\Delta t}{2(\Delta x)^2}$.

The probability of finding an electron at (x, t) is given by $|\psi(x, t)|^2$. This equations do no conserve this probability exactly, but the error is of the order of $(\Delta t)^2$. The convergence can be determined by using smaller steps.

Exercise 8.1: Single-slit diffraction

Young's single-slit experiment consists of a wave passing though a small slit, which causes the emerging wavelets to intefere with eachother forming a diffraction pattern. In quantum mechanics, where particles are represented by probabilities, and probabilities by wave packets, it means that the same phenomenon should occur when a particle (electron, neutron) passes though a small slit. Consider a wave packet of initial width 3 incident on a slit of width 5, and plot the probability density $|\psi^2|$ as the packet crosses the slit. Generalize the time-evolution equation (88), and the wave packet (80) for 2 dimensions (you need to use two coordinates x and y and the momentum will also have two components k_x and k_y). Model the slit with a potential wall:

$$V(x,y) = 100 \quad \text{for } x = 10, |y| \geq 2.5.$$

9 Random sequences

Imagine a bingo draw, where numbered balls are picked randomly. If you want to reproduce this process with a computer, you will find that it is not as easy as you might think. Computing is completely deterministic by nature, and reproducing or simulating naturally random processes is a particularly delicate matter.

The problem is how to use a computer to generate random numbers. In fact, this is impossible! We can program a computer to generate a sequence of numbers, following certain law. Although the output values of this sequence might look random (according to some rules that we will discuss in this section), the existence of a deterministic law behind them is telling us that precisely, these are not random numbers at all!

We define a sequence of numbers $\{r_1, r_2, ...r_n\}$ as "random" if there are no correlations among the numbers in the sequence. A random sequence can have a distribution, *i. e.* the probability of a number to appear in the sequence would correspond to some distribution. If the distribution is uniform, all numbers are equally probable to appear. Mathematically, the likehood of a number to occur is described by a distribution function $P(r)$. This means that the probability of finding r_i in the interval $[r, r+dr]$ is given by $P(r)dr$. The usual random number generators provided by compilers or libraries generate a uniform distribution between 0 and 1, that means $P(r) = 1$. Ideally this numbers have equal probability, and it is independent of the previous one.

The computer, the sequences are "pseudo-random" because knowing a number r_m and the preceeding r_i, we can predict the next one r_{m+1}. This is evident in the correlations. Some sophisticated psudo-random number generators do a good job hiding this fact from our eyes, although if you look hard enough, you will eventually figure it out.

9.1 Pseudo-random number generators

In this section we will simply review some possible alternatives for pseudo-random number generators. These go from the simplest "congruential" or "power residue" algorithm to more sophisticated ones that can be found in the literature. We will limit ourselves to understand this simple example. We want to generate a sequence $\{r_i\}$ over an interval $[0, M-1]$. You multiply the previous random number r_i by a constant a, add on another constant c, take the modulus by M, and then keep just the fractional part, the reminder, as the next rendom number r_{i+1}:

$$r_{i+1} = (ar_i + c)\mathrm{mod}M = \text{remainder}\left(\frac{ar_i + c}{M}\right).$$

The value r_1 has to be supplied by the user, and it is called the "seed" of the sequence. The sequence will be uniquely pre-determined by the seed.

As an example, let us pick $c = 1$,$a = 4$,$M = 9$ and $r_1 = 3$. We obtain the sequence:

$$\begin{aligned} r_1 &= 3, && (89)\\ r_2 &= (4 \times 3 + 1)\mathrm{mod}9 = 4, && (90)\\ r_3 &= (4 \times 4 + 1)\mathrm{mod}9 = 8, && (91)\\ r_4 &= (4 \times 8 + 1)\mathrm{mod}9 = 6, && (92)\\ &, 7, 2, 0, 1, 5, 3, ... && (93) \end{aligned}$$

We get a sequence of length $M = 9$ after which the entire sequence repeats. This means that the "period" of the sequence is $M - 1$. If we want the numbers in the range $[0, 1]$ we would divide these values by M. This algorithm is extremely simple and portable, and it's particularly suitable for simple applications. As we have seen, the longer the M, the longer the "period" of the sequence. Using large integer raises the problem of protability. Most processors use 32-bit representation for integers (some 64). This limits the largest possible integer that can be used. However, there are ways to work around this issue.

The C++ Standard Library provides a psuedo-random number generator. It provides a function to initialize the seed of the sequence:

srand(size_t seed); and the actual call to retrieve a new random number rand();

The generator provides a sequence between 0 and RAND_MAX, which is a large integer that deppends on the implementation. A common way to generate independent sequences is to use the internal clock of the computer to generate a relatively random seed.

For more on random number generators read Knuth, Numerical Recipes.

9.2 Testing for randomness and uniformity

Since the random numbers are generated according to a deterministic rule, the numbers in the sequence must be correlated in a certain way. This can affect a simulation that assumes random events.Therefore it is wise to test a generator before you use it.

9.2.1 Moments

The $k-th$ moment of a distribution is defined as:

$$\langle x^k \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i^k. \tag{94}$$

If the numbers are distributed with a uniform probability distribution $P(x)$, then (94) must correspond to the moment of P:

$$\int_0^1 x^k P(x) dx \sim \frac{1}{k+1}.$$

If this holds for your generator, then you know that the distribution is uniform. If the deviation from this varies as $1/\sqrt{N}$, then you also know that the distribution is random.

9.2.2 Autocorrelation

Another simple test determines the near-neighbor correlation in your random sequence by taking the sume of products at a "distance" m:

$$C(m) = \langle x_i x_{i+m} \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i x_{i+m}. \tag{95}$$

If your random numbers are distributed with a joint probability distribution $P(x_i, x_{i+m})$ and are independent and uniform, then (95) must compare to the integral:

$$\int_0^1 dx \int_0^1 dy P(x,y) xy.$$

9.2.3 Visual test

If you plot the points (r_{2i}, r_{2i+1}) and you notice some sort of regularity, the sequence is not random. If the points are random, they should uniformly fill a square with no discernible pattern.

9.2.4 Statistical errors

If you run a simulation using a pesudo-random generator, you may expect your measurements (of some quantity, and observable for instance) to be distributed according to some statistics. If your results do not satisfy these statistics, then you should pick another generator. If you know a good random-number generator (you usually try to avoid this kind because they are time-consumming), it is a good idea to compare your results for a short run, to see is they agree or not.

9.3 Non-uniform random distributions

In th eprevious section we learned how to generate random deviates with a uniform probability distribution in an interval $[a, b]$. This distributioon is normalized, so that

$$\int_a^b P(x)dx = 1.$$

Hence, $P(x) = 1/(b - a)$.

Now, suppose that we generate a sequence $\{x_i\}$ and we take some function of it to generate $\{y(x_i)\} = \{y_i\}$. This new sequence is going to be distributed according to some probaility density $P(y)$, such that

$$P(y)dy = P(x)dx$$

or

$$P(y) = P(x)\frac{dx}{dy}.$$

If we want to generate a desired normalized distribution $P(y)$, we need to solve the differential equation:

$$\frac{dy}{dy} = P(y).$$

But the solution of this is

$$x = \int_0^y P(y')dy' = F(y).$$

Therefore,

$$y(x) = F^{-1}(x), \tag{96}$$

where F^{-1} is the inverse of F.

9.3.1 Exponential distribution

As an example, let us take $y(x) = -\ln(x)$ with $P(x)$ representing a uniform distribution in the interval $[0,1]$. Then

$$P(y) = \frac{dx}{dy} = e^{-y},$$

which is distributed exponentially. This distribution occurs frequantly in real problems such as the readioactive decay of nuclei. You can also see that the quantity y/λ has the distribution $\lambda e^{-\lambda y}$.

9.4 von Neumann rejection

A simple and ingenious method for generating random points with a probability distribution $P(x)$ was deduced by von Neumann. Draw a plot with you probability distribution, and on the same graph, plot another curve $f(x)$ which has finite area and lies everywhere above your original distribution. We will call $f(x)$ the "comparison function". Generate random pairs (x_i, y_i) with uniform distribution inside $f(x)$. Whenever the point lies inside the area of the original probability, we accept it, otherwise, we reject it. All the accepted points will be uniformly distributed within the original area, and therefore will have the desired distribution. The fraction of points accepted/rejected will deppend on the ratio between the two areas. The closer the comparison function $f(x)$ resembles $P(x)$, the more points will be accepted. Ideally, for $P(x) = f(x)$, all the points will be accepted, and none rejected. However, in practice, this is not always possible, but we can try to pick $f(x)$ such that we minimize the fraction of rejected points.

It only remains how to pick a number with probability $f(x)$. For this purpose, we utilize the method shown in the previous section, using a function whose indefinite intergral is know analitically, and is also analitically invertible. We then pick a random number x and retrieve the corresponding $y(x)$ according to (96). Then, we generate a second random number and we use the rejection criterion.

An equivalent procedure consists of picking the second number between 0 and 1 and accept or reject according to wether is it respectively less than or greater than the ratio $P(x)/f(x)$

9.5 Random walk methods: the Metropolis algorithm

Suppose that we want to generate random variables according to an arbitrary probability density $P(x)$. The Metropolis algorithm produces a "random walk" of points $\{x_i\}$ whose asymptotic probability approaches $P(x)$ after a large number of steps. The random walk is defined by a "transition probability" $w(x_i \to x_j)$ for one value x_i to another x_j in order that the distribution of points x_0, x_1, x_2, ... converges to $P(x)$. In can be shown that it is sufficient (but not necessary) to satisfy the "detailed balance" condition

$$p(x_i)w(x_i \to x_j) = p(x_j)w(x_j \to x_i). \tag{97}$$

This relation dos not specify $w(x_i \to x_j$ uniquely. A simple choice is

$$w(x_i \to x_j) = \min\left[1, \frac{P(x_j)}{P(x_i)}\right]. \tag{98}$$

This choice can be described by the following steps. Suppose that the "random walker" is a position x_n. To generate x_{n+1} we

1. choose a trial position $x_t = x_n + \delta_n$, where the δ_n is a random number in the interval $[-\delta, \delta]$.
2. Calculate $w = P(x_t)/P(x_n)$.
3. If $w \geq 1$ we accept the change and let $x_{n+1} = x_t$.
4. If $w \leq 1$, generate a random number r.
5. If $r \leq w$, accept the change and let $x_{n+1} = x_t$.
6. If the trial change is not accepted, the let $x_{n+1} = x_n$.

It is necessary to sample a number of points of the random walk before the asymptotic probability $P(x)$ is attained. How do we choose the "step size" δ? If δ is too large, only a small fraction of changes will be accepted and the sampling will be inefficient. If δ is too small, a large number will be accepted, but it would take too long to sample $P(x)$ over the whole interval of interest. Ideally, we want at least 1/3-1/2 of the trial steps to be accepted. We also want to choose x_0 such that the distribution $\{x_i\}$ converges to $P(x)$ as quickly as possible. An obvious choice is to begin the random walk at the point where $P(x)$ is maximum.

9.5.1 Exercise 9.1: The Gaussian distribution

1. Use the Metropolis algorithm to generate a Gaussian distribution $P(x) = A \exp\left(-x^2/2\sigma^2\right)$. Is the numerical value of the normalization constant A relevant? Determine the qualitative dependence of the acceptance ratio and the equilibrium time on the maximum step size δ. One possible criterion for equilibrium is that $\langle x^2 \rangle \approx \sigma^2$. For $\sigma = 1$, what is a reasonable choice of δ? (choose $x_0 = 0$.)

2. Plot the asymptotic probability distribution generated by the Metropolis algorithm.

10 Monte Carlo integration

Imagine that we want to measure the area of a pond with arbitrary shape. Suppose that this pond is in the middle of a field with known area A. If we throw N stones randomly, such that they land within the boundaries of the field, and we count the number of stones that fall in the pond N_{in}, the area of the pond will be approximately proportional to the fraction of stones that make a splash, multiplied by A:

$$A_{pond} = \frac{N_{in}}{N} A.$$

This simple procedure is an example of the "hit and miss" "Monte Carlo" method.

10.1 Simple Monte Carlo integration

Imagine a rectangle of height H in the integration interval $[a, b]$, such that the function $f(x)$ is within its boundaries. Compute n pairs of random numbers (x_i, y_i) such that they are uniformly distributed inside this rectangle. The fraction of points that fall within the area contained below $f(x)$, *i. e.*, that satisfy $y_i \leq f(x_i)$ is an estimate of the ratio o fthe integral of $f(x)$ and the area of the rectangle. Hence, the estimate of the integral will be given by:

$$\int_a^b f(x)dx \simeq I(N) = \frac{N_{in}}{N} H(b-a). \tag{99}$$

Another Monte Carlo procedure is based on the definition:

$$\langle f \rangle = \frac{1}{(b-a)} \int_a^b f(x)dx. \tag{100}$$

In order to determine this average, we sample the value of $f(x)$:

$$\langle f \rangle \simeq \frac{1}{N} \sum_{i=1}^{N} f(x_i),$$

where the N values x_i are distributed unformly in the interval $[a, b]$. The integral will be given by

$$I(N) = (b-a)\langle f \rangle.$$

10.2 Monte Carlo error analysis

The Monte Carlo method clearly yields approximate results. The accuracy deppends on the number of values N that we use for the average. A possible measure of the error is the "variance" σ^2 defined by:

$$\sigma^2 = \langle f^2 \rangle - \langle f \rangle^2, \tag{101}$$

where

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

and

$$\langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)^2.$$

The "standard deviation" is σ. However, we should expect that the error decreases with the number of points N, and the quantity σ defines by (101) does not. Hence, this cannot be a good measure of the error.

Imagine that we perform several measurements of the integral, each of them yielding a result I_n. These values have been obtained with different sequences of N random numbers. According to the central limit theorem, these values whould be normally dstributed around a mean $\langle I \rangle$. Suppouse that we have a set of M of such measurements I_n. A convenient measure of the differences of these measurements is the "standard deviation of the means" σ_M:

$$\sigma_M^2 = \langle I^2 \rangle - \langle I \rangle^2, \tag{102}$$

where

$$\langle I \rangle = \frac{1}{M} \sum_{n=1}^{M} I_n$$

and

$$\langle I^2 \rangle = \frac{1}{M} \sum_{n=1}^{M} I_n^2.$$

Although σ_M gives us an estimate of the actual error, making additional meaurements is not practical. instead, it can be proven that

$$\sigma_M \approx \sigma/\sqrt{N}. \tag{103}$$

This relation becomes exact in the limit of a very large number of measurements. Note that this expression implies that the error decreases with the square root of the number of trials, meaning that if we want to reduce the error by a factor 10, we need 100 times more points for the average.

Exercise 10.1: One dimensional integration

1. Write a program that implements the "hit and miss" Monte Carlo integration algorithm. Find the estimate $I(N)$ for the integral of
$$f(x) = 4\sqrt{1-x^2}$$
as a function of N, in the interval $(0, 1)$. Choose $H = 1$, and sample only the x-dependent part $\sqrt{1-x^2}$, and multiply the result by 4. Calculate the difference between $I(N)$ and the exact result π. This difference is a measure of the error associated with the Monte Carlo estimate. Make a log-log plot of the error as a function of N. What is the approximate functional deppendece of the error on N for large N?

2. Estimate the integral of $f(x)$ using the simple Monte Carlo integration by averaging over N points, using (100), and compute the error as a function of N, for N upt to 10,000. Determine the approximate functional deppendence of the error on N for large N. How many trials are necessary to determine I_N to two decimal places?

3. Perform 10 measurements $I_n(N)$, with $N = 10,000$ using different random sequences. Show in a table the values of I_n and σ according to (100) and (101). Use (102) to estimate the standard deviation of the means, and compare to the values obtained from (103) using the 100,000 values.

4. To verify that your result for the error is independent of the number of sets you used to divide your data, repeat the previous item grouping your results in 20 groups of 5,000 points each.

Exercise 10.2: Importance of randomness

To examine the effects of a poor random number generator, modify your program to use the linear congruential random number generator using the parameters $a = 5$, $c = 0$, $M = 32$, and the seed $x_1 = 1$. Repeat the integral of the previous exercise and compare your results.

10.3 Variance reduction

If the function being integrated does not fluctuate too much in the interval of integration, and does not differ much from the average value, then the standard Monte Carlo mean-value method should work well with a reasonable number of points. Otherwise, we will find that the variance is very large, meaning that some points will make small contributions, while others will make large contributions to the integral. If this is the case, the algorithm will be very inefficient. The method can be improves by splitting the function $f(x)$ in two $f(x) = f_1(x) + f_2(x)$, such that the integral of $f_1(x)$ is known, and $f_2(x)$ as a small variance. The "variance reduction" technique, consists then in evaluating the integral of $f_2(x)$ to obtain:

$$\int_a^b f(x)dx = \int_a^b f_1(x)dx + \int_a^b f_2(x)dx = \int_a^b f_1(x)dx + J.$$

10.4 Importance Sampling

Imagine that we want to sample the function $f(x) = e^{-x^2}$ in the interval $[0, 1]$. It is evident that most of our points will fall in the region where the value of $f(x)$ is very small, and therefore we will need a large number of values to achieve a decent accuracy. A way to improve the measurement by reducing the variance is obtained by "importance sampling". As the name says, the idea is to sample the regions with larger contributions to the integral. For this goal, we introduce a probability distribution $P(x)$ normalized in the interval of integration

$$\int_a^b P(x)dx = 1.$$

Then, we can rewrite the integral of $f(x)$ as

$$I = \int_a^b \frac{f(x)}{P(x)} P(x)dx \tag{104}$$

We can evaluate this integral, by sampling according to the probability distribution $P(x)$ and evaluating the sum

$$I(N) = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{P(x_i)}. \tag{105}$$

Note that for the uniform case $P(x) = 1/(b-a)$, the expression reduces to (100).

We are free to choose $P(x)$ now. We wish to do it in a way to reduce and minimize the variance of the integrand $f(x)/P(x)$. The way to to this is picking a $P(x)$ that mimics $f(x)$ where $f(x)$ is large. if we are able to determine an apropiate $p(x)$, the integrand will be slowly varying, and hence the variance will be reduced. Another consideration is that the generation of points according to the distribution $P(x)$ should be a simple task. As an example, let us consider again the integral

$$I = \int_0^1 e^{-x^2} dx.$$

A reasonable choice for a weigh function is $P(x) = Ae^{-x}$, where A is a normalization constant.

Notice that for $P(x) = f(x)$ the variance is zero! This is known as the zero variance property.

Exercise 10.3: Importance sampling

1. Choose the weight function $P(x) = e^{-x}$ and evaluate the integral:

$$\int_0^\infty x^{3/2} e^{-x} dx.$$

2. Choose $P(x) = e^{-ax}$ and estimate the integral

$$\int_0^\pi \frac{dx}{x^2 + \cos^2 x}.$$

   Determine the value of a that minimizes the variance of the integral.

Exercise 10.4: The Metropolis algorithm

Use the Metropolis algorithm to sample points according to a ditribution and estimate the integral

$$\int_0^4 x^2 e^{-x} dx,$$

with $P(x) = x^2 e^{-x}$ for $0 \leq x \leq 4$. Plot the number of times the walker is at points x_0, x_1, x_2, ... Is the integrand sampled uniformly? If not, what is the approximate region of x where the integrand is sampled more often?

11 Random walks

Imagine the following problem: a drunkard starts walking from a lampost taking N steps of equal length in random directions: how far will the drunkard be from the lampost? This is the original formulation of the "random walk" problem, that can be generalized to more complex problems is physics, biology, chemistry and social sciences. We have seen an application to one dimensional integration in the previous section. Here we are going to study them in a more general context.

11.1 A one-dimensional random walk

Let us reformulate the previous problem in terms of diffusion of a molecule in a dilute gas. Suppose that the molecule travels a distance l between collisions with other molecules. If we assume that the successive displacements of the molecule between collisions are statistically independent, then its motion is identical to the motion of the drunk. At each step he molecule has a probability p to move to the right, and a probability $q = 1 - p$ to move to the left. If n_{right} is the number of steps to the right, and n_{left} the number of steps to the left, the total number of steps is going to be $N = n_{right} + n_{left}$, and the net displacement after N steps will be $x = (n_{right} - n_{left})l$, with $-Nl \leq x \leq Nl$. The main quantity of interest will be the probability $P_N(x)$ for the molecule to be in position x after N steps. The mean net displacement $\langle x_N \rangle$ and the variance $\langle \Delta x_N^2 \rangle$ are going to be given by

$$\langle x_N \rangle = \sum_{x=-Nl}^{Nl} x P_N(x)$$

and

$$\langle \Delta x_N^2 \rangle = \langle x_N^2 \rangle - \langle x_N \rangle^2$$

with

$$\langle x_N^2 \rangle = \sum_{x=-Nl}^{Nl} x^2 P_N(x).$$

all the averages are over all possible walks of N steps. The analytical result can be obtained exactly for this case and the result is:

$$\langle x_N \rangle = (p - q)Nl$$

and

$$\langle \Delta x_N^2 \rangle = 4pqNl^2$$

Note that for the symmetrical case with $p = q = 1/2$, the results is $\langle x_N \rangle = 0$. Now, let us identify these quantities for the case of the diffusion of the molecule. If l is the mean free path, and τ the time between collisions, at a time t, the molecule would suffer $N = t/\tau$ collisions, obtaining

$$\langle \Delta x^2 \rangle = 4pql^2(t/\tau).$$

Since we know that the diffusion is characterize by the linear relation

$$\langle \Delta R(t)^2 \rangle = 2Dt,$$

where D is the "self-diffusion constant", we obtain

$$D = 2pql^2/\tau.$$

This is a very particular case that can be solved exactly. We need to develop a method to solve the general problem numerically. Two important approaches are exact enumeration and Monte Carlo methods.

11.1.1 Exact enumeration

in this approach, the number and probability of all walks for a given N and x are determined explicitly. Imagine that we represent by bits 0 and 1 as step to the right or left, respectively. The number of possible walks with a given N is going to be equivalent to the number of combinations of N bits, that is, 2^N. The value of x for each configuration of ones and zeroes is going to be given by the difference between the number of ones and the number of zeroes. If n is the number of ones, this is $x = n - (N - n) = 2n - N$. From here we obtain that $n = (x + N)/2$. The probability $P_N(x)$ for each configuration will be given by $p^n q^{N-n}$. Since the number of configurations with a given x or n is $N_{conf}(n) = \frac{N!}{/}n!(N-n)!$, we obtain:

$$P_N(x) = \frac{N!}{n!(N-n)!} p^n q^{N-n}.$$

11.1.2 Monte Carlo

The Monte Carlo method generates walks with different N using the correct probabilities to ensure that the sampled walks are representative of the total population of possible walks. Clearly, the more walks we use, the close we will come to the exact result. In practice, we obtain the desired accuracy by comparing our results to the increasing number of trials until the results do not appear to vary within a tolerance.

The walker performs a steps to the right with probability p, and a step to the left with probability $q = (1 - p)$. To simulate this, we pick a random number r between 0 and 1. If $r \leq p$, we move one step to the right, otherwise, we move one step to the left. We repeat this operation N times to obtain the net displacement x, and we accumulate the result to calculate the averages.

The pseudocode to generate a random configuration of N steps would look like this:

1. Start from $x = 0$. Let $nstep = 0$.
2. Pick a random number r between 0 and 1.
3. If $r \leq p$, then $x = x + 1$, else $x = x - 1$.
4. Let $nstep = nstep + 1$. If $nstep < N$, repeat from step 2.

In order to determine the probability $P_N(x)$ we need to perform many trials and record the fraction of times that a walker is at position x after N steps. All the other quantities can be calculated at the end using the values we obtained for $P_N(x)$.

Exercise 11.1: Random walks in 1d

1. Implement a program to calculate the probabilities $P_N(x)$ for a given N.
2. Determine $P_N(x)$, $\langle x_N \rangle$, and $\langle \Delta x_N^2 \rangle$ for $p = 0.5$, and $N = 8, 16, 32, 64$. Compare your results to the exact answers.
3. Plot $P_N(x)$ versus x for the above values of N. Is x a continuous function? What is the value of $P_N(x)$ at its maximum for each value of N? What is the approximate "width" of $P_N(x)$ in each case?

4. Show from your previous plot that for sufficiently large N, the computed distribution can be approximated by the Gaussian

$$P(x) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left[-(x - \langle x \rangle)^2/2\sigma^2\right]$$

where $\sigma^2 = \langle \Delta x^2 \rangle$. Does the fit work equally well for all x?

5. Suppose that $p = 0.7$. Compute $\langle x_N \rangle$ and $\langle \Delta x_N^2 \rangle$ for the same values of N used in part 2. What is the interpretation of $\langle x_N \rangle$ in this case?

6. Make a log-log plot of $\langle \Delta x_N^2 \rangle$ vs. N and analyze the behavior for large.

Many applications of random walk models make use of asymptotic behavior for large N. For example in many random walk models,

$$\langle \Delta x_N^2 \rangle \sim N^{2\eta} \quad (N \gg 1).$$

This is an example of a "scaling law". That is, if the number of steps is doubled, the net mean square displacement increases by a factor 2^η. For one-dimensional random walks we find from the exact solution described above that $\eta = 1/2$. If this kind of scaling law exists, its exponent depends on the geometry of the lattice, as well as the nature of the walk.

Exercise 11.2: Random walk with steps of variable length

1. Consider a 1d random walk with jumps of all lengths allowed. The probability that the length of a single step is l is denoted $p(l)$. If the form of $p(l)$ is given by $p(l) = e^{-l}$, what is the form of $P_N(x)$? Suggestions: Use the inverse transform method explained in the previous chapter to generate steps of length l according to $p(l)$. Then generate a walk of N steps and determine the net displacement x. Generate many such walks and determine $P_N(x)$. Plot $P_N(x)$ vs. x and confirm that the form of $P_N(x)$ is consistent with a Gaussian distribution.

2. Consider the step probability $p(l) = A/l^2$. Determine the normalization constant A using:

$$\sum_{l=1}^{\infty} \frac{1}{l^2} = \frac{\pi^2}{6}$$

and the requirement that $p(l)$ be normalized to unity. Perform a Monte Carlo simulation as in part 1 and verify that the from of $P_N(x)$ is given by

$$P_N(x) \sim \frac{bN}{x^2 + b^2N^2}.$$

What is the magnitude of the constant b? Does the variance of $P_N(x)$ exist?

The "central limit theorem" states that the probability distribution of a large number of measurements will be a Gaussian centered at the mean. The only requirement is that the probability $p(x)$ has finite first and seconds moments, that the measurements are statistically independent, and that N is large. In part 2 of the previous exercise, the probability distribution has no second moment, and that explains the result.

11.2 The continuum limit

Let us consider the continuum limit of the 1d random walk. If there is an equal probability of taking a step to the right or left, the random walk can be described by a simple "master equation"

$$P_n(i) = \frac{1}{2}P_{n-1}(i+1) + \frac{1}{2}P_{n-1}(i-1) \tag{106}$$

where $P_n(i)$ is the probability that the walker is at site i after n steps. In order to obtain a differential equation for the probability density $P(x,t)$, we set $t = n\tau$, $x = ia$, and $P_n(i) = aP(x,t)$, where τ is the time between steps, and a is the lattice spacing. Now we can rewrite (106) as

$$P(x,t) = \frac{1}{2}P(x+a,t-\tau) + \frac{1}{2}P(x-a,t-\tau). \tag{107}$$

We substract $P(x,t-\tau)$ from both sides, we divide by τ, and rewrite (107) as:

$$\frac{P(x,t) - P(x,t-\tau)]}{\tau} = \frac{a^2}{2\tau}\frac{[P(x+a,t-\tau) - 2P(x,t-\tau) + P(x-a,t-\tau)]}{a^2}. \tag{108}$$

Talking the limit $a \rightarrow 0$ and $\tau \rightarrow 0$ with the ratio $D = a^2/2\tau$ finite, we obtain the diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2} \tag{109}$$

The generalization to three dimensions is

$$\frac{\partial P(\mathbf{r},t)}{\partial t} = D\nabla^2 P(\mathbf{r},t). \tag{110}$$

This is the "diffusion equation" or "Fokker-Planck equation" and is frequently used to describe the dynamics of fluid molecules. The solution in free space can be shown to be a Gaussian

$$P(x,t) = \sqrt{\frac{1}{2\pi Dt}} e^{-x^2/4Dt}$$

where $P(x,t)$ is the probability of finding a particle at position x at time t if is started from $x = 0$ at $t = 0$. From this equation we can obtain:

$$\langle x(t) \rangle = \int_{-\infty}^{\infty} dx\, x P(x,t) = 0,$$

and

$$\langle x^2(t) \rangle = \int_{-\infty}^{\infty} dx\, x^2 P(x,t) = 2Dt$$

The generalization to d dimensions is $\langle R^2(t) \rangle = 2dDt$, where R^2 is the square of the displacement of the particle.

11.3 Two and three dimensional random walks

The algorithms and methods explained in the previous sections can be easily generalized to more dimensions. Consider a discrete lattice, either rectangular or triangular. The difference is the coordination number z, the number of nearest neighbor sites. In the rectangular lattice, we can move to $z = 4$ different sites, while in the triangular, we can move to $z = 6$ different sites. We can define the "root mean square displacement" (rms) as

$$R_N \equiv \sqrt{\langle \Delta R_N^2}.$$

Exercise 11.3: A random walk in two dimensions

Consider a collection of "bees" which are initially localized in a circle of unit radius centered about the origin. At each time step, each bee moves at random with equal probability to one of four possible directions north, south, east, or west.

1. Implement a program to simulate the motion of the bees, and describe the qualitative nature of their motion.

2. Suppose that each bee is placed at random within a circle of unit radius and is given an initial velocity in one of the four directions. This means that at each time interval, a bee takes an additional step in the direction of the original velocity. Is the motion of the bees changes from part 1?

3. Compute $\langle x_N \rangle$, $\langle y_N \rangle$, $\langle \Delta x_N^2 \rangle$ and $\langle \Delta y_N^2 \rangle$ as a function of the number of steps N. The average is over all the M bees. Also compute the mean square displacement defined as

$$\langle \Delta R_N^2 \rangle = \langle x_N^2 \rangle + \langle y_N^2 \rangle - \langle x_N \rangle^2 - \langle y_N \rangle^2.$$

What is the qualitative dependence of these quantities on the number of steps? Compute the N-dependence of R_{max}^2, the maximum displacement of the bees as step N. Is the behavior of R_{max}^2 qualitatively different that $\langle \Delta R_N^2 \rangle$ for all N?

Exercise 11.4: Individual particle diffusion in a lattice gas

Consider a nonzero concentration of ρ random walkers (particle) on a square lattice. Each particle moves at random to empty nearest-neighbor sites but double occupancy of a site is forbidden; otherwise, the particles are non-interacting. Such model is an example of a "lattice gas". Note that the motion of an individual particle is correlated with the motion of the other particles. The physical motivation of this model arises from metal physics where diffusion is caused by thermal vacancies with a concentration that depends on the temperature. The main quantity of interest is the self-diffusion constant D of an individual particle. The algorithm for a Mont Carlo simulation can be stated as follows:

1. Occupy the lattice sites at random with a concentration of rho particles. We have to follow the motion of each particle individually, so we identify them as the elements of some array.

2. At each step, pick a particle at random, and choose a neighboring site. if the neighboring site is empty, the particle is moved to this site, otherwise, the particle remains in the present position.

The measure of time in this context is arbitrary. The usual definition is that one unit of time corresponds to one Monte Carlo step per particle. During each of these steps, each particle attempts one jump on the average. The diffusion constant D is obtained as the limit $t \to \infty$ of $D(t)$, where $D(t)$ is given by

$$D(t) = \frac{1}{2dt}\langle \Delta R(t)^2 \rangle$$

and $\langle \Delta R(t)^2 \rangle$ is the net mean-square displacement per particle after t units of time.

11.4 Restricted random walks

This corresponds to a random walk in the presence of a boundary. Here we list some examples:

- Traps: Consider a 1d lattice which has "traps" at sites $x = 0$ and $x = l$. A random walker starts a site x_0 somewhere in the center $(0 < x_0 < l)$ and steps to a neighboring site with equal probability. It can be shown that the mean "fist passage time" τ for a particle to be trapped is given by

  $$\tau = \frac{1}{2D} x_0 (l - x_0)$$

  where D is the self-diffusion constant in the absence of the traps, and the average is over all possible walks.

- Reflecting boundaries: Consider the case of reflecting sites at $x = 0$ and $x = l$. If a walker reaches a boundary, it is reflected back to the previous site. What is the probability of finding a walker in site x after N steps?

- "Gambler's ruin": Suppose that two gamblers are given \$10 and on each throw of a dice, one gambler must win \$1 and the other must loose \$1. How long can they play in average until the capital of the loser is exhausted?

11.5 Self-avoiding walks

Imagine a solution of polymers. A good solvent allows the polymer chains to move freely and adopt different configurations. A fundamental geometrical property that can be used to characterize a polymer is the rms end-to-end distance R_N, where N is the number of monomers.

A simple model to describe the global features of a polymer in a solution consists of same-size straight segments joined toghether at random angles. The most important feature of a polymer is that two monomers cannot occupy the same spatial position. This is precisely the property that defines the self-avoiding walk (SAW), a walk that starts from a point, subject to the global constraint that cannot visit the same site of the lattice more than once during the walk.

11.5.1 Monte Carlo simulation of the SAW in 2d

It is convinient to represent the lattice as a two-dimensional array to record the sites that have been already visited. Choose an arbitrary site as the origin and assume that the first step is "north" (the other directions are equivalent by symmetry) We label the four possible directions from 0 to 3. Next, we generate a random integer to choose one of the three possible directions. If a step leads to an intersection, *i. e.* a site that has already been visited, the walk is terminated and we start again from the origin.

11.6 The traveling salesman

The traveling salesman problem, or TSP for short, is this: given a finite number of "cities" along with the cost of travel between each pair of them, find the cheapest way of visiting all the cities and returning to your starting point. (Here, we consider just the symmetric TSP, where traveling from city X to city Y costs the same as traveling from Y to X; the "way of visiting all the cities" is simply the order in which the cities are visited.) To put it differently, in terms of "graph theory" the data consist of integer weights assigned to the edges of a finite complete graph; the objective is to find a hamiltonian cycle (that is, a cycle passing through all the vertices) of the minimum total weight. In this context, hamiltonian cycles are commonly called tours.

This is a problem in discrete or combinatorial optimization. It is a prominent illustration of a class of problems in computational complexity theory which are hard to solve.

12 The Microcanonical Ensemble

In this chapter we apply Monte Carlo methods to the simulation of the equilibrium properties of systems with many degrees of freedom. This application will allow us to explore the methodology of statistical mechanics and to introduce important concepts.

We first discuss as closed system of fixed number of particles N, volume V, and total energy E. We also assume that the system is isolated, *i.e.* that the influence of external parameters such as gravitational and magnetic fields can be ignored. We know that in general a closed macroscopic system tends to a time-independent equilibrium stat of maximum randomness or entropy. The macrostate of the system is the specified by the values of N, V and E. At a microscopic level there are in general a large number of different ways or *configurations* in which a microstate (N, V, E) can be realized. A particular configuration or "microstate" is "accessible" if its properties are consistent with the specified macrostate.

Since in principle we don not have a reason to prefer a microstate over another, it is reasonable to postulate that at any given time, the system is equally likely to be on any one of its accessible microstates. This can be formulated through a probability P_s of finding the system in a microstate s

$$P_s = 1/\Omega, \quad \text{if } s \text{ is accessible.} \tag{111}$$

The sum of P_s over all the Ω states is equal to unity.

To estimate the average of a physical quantity it is convenient to formulate statistical averages at a fixed instant of time. Imagine a collection or "ensemble" of systems which are mental replicas characterized by the same macrostate. The number of systems equals the number of possible microstates. An ensemble of such systems specified by E, N, V which is described by the probability distribution (111) is called a "microcanonical ensemble".

Supouse that a physical quantity A has the value A_s when the system is in the state s. Then, the ensemble average of A is given by

$$\langle A \rangle = \sum_s A_s P_s. \tag{112}$$

12.1 Enumeration

Consider a model in which the particles are distinguishable, non-interacting, and have only two possible velocities v_0 and $-v_0$. Since the particles are non-interacting, the size of the system and the positions of the particles are irrelevant. Consider a system of $N = 4$ of such particles and fixed energy $E = 2v_0^2$. (the mass of the particles is taken to be unity) The number of possible microstates with these constraints is $2^N = 16$. The enumeration of these configuration allows us to calculate the ensemble averages for the physical quantities of the system. The enumeration procedure is equivalent to the one used to enumerate 1D random walks. If we fix the number n_R of particles moving to the right, the number of configurations for a given n are 1, 4, 6, 4, 1 for $N = 0, 1, 2, 3, 4$, respectively, and the corresponding probabilities P_n are 1/16, 4/16, 6/16, 4/16, 1/16. Hence, the mean number of particles moving to the right is

$$\langle n \rangle = \sum nP_n = (0 \times 1 + 1 \times 4 + 2 \times 6 + 3 \times 4 + 4 \times 1)/16 = 2.$$

12.2 Monte Carlo simulation

As we have seen in a previous chapter, the motion of a system of N particles with fixed N, E, V can be simulated integrating the equations of motion performing a MD simulation and time averaging the quantities of interest. How can we do an ensemble average? One way would enumerating all the microstates, but this approach is not practical since the number of configurations is generally too large. In the spirit of Monte Carlo, we wish to develop a practical method to obtain representative sample of the total number of microstates. An obvious procedure is to fix N and V, change the positions and velocities of individual particles at random, and retain the configuration of it has the desired total energy. However, this procedure is very inefficient, since in general most configuration will not have the desired total energy and must be discarded.

Imagine a macroscopic system which is divided into two "subsystems": the original system of interest, referred to as the *system*, and a *subsystem* which has one element. For historical reasons this extra degree of freedom is called a "demon". The demon travels about the system transferring energy as it attempts to change the dynamical variables of the system. If the demon has sufficient energy in its sack, it gives energy to any element of the system who requires energy to make the desired change. Conversely if the desired change lowers the energy of the system, the excess energy is given to the demon. The only limitation on the demon is that it cannot have negative energy. The algorithm is summarized in the following:

1. choose a particle at random and make a trial change of its coordinates;

2. compute the change in the energy of the system due to the change in coordinates;

3. if the trial change decreases the energy of the system, the system gives its energy to the demon, and the new configuration is accepted;

4. if the trial change increases the energy of the system, the new configuration is accepted if the demon has sufficient energy to give to the system. Otherwise, the new configuration is rejected and the particle retains its old coordinates;

5. if the trial change does not change the energy of the system, the new coordinate is accepted.

The above procedure is repeated until a representative sample of states is obtained. After a period of time for equilibration, the demon and the system will reach a compromise and agree on an average energy for each. The total energy remains constant, and since the demon is only one degree of freedom in comparison to the many degrees of freedom of the system, we expect that the energy fluctuations of the system will be small.

How do we know that his Monte Carlo simulation of the microcanonical ensemble will yield results equivalent to the time-average results of MD simulations? The assumption that the two averages yield equivalent results is called the "ergodic hypothesis" (or more accurately the quasi-ergodic hypothesis) Although these two averages cannot be shown to be identical in general, they have been found to yield equivalent results in all cases of practical interest.

12.3 One-dimensional Classical Ideal Gas

In this case, the particle velocities are continuous and unbounded. The energy of the configuration is independent of the position of the particles, and is the sum of the kinetic energies of the individual particles. Hence, for and ideal gas, the only coordinates of interest are the velocities. In order to change a configuration, we choose a particle at random and change its velocity by a random amount. For simplicity we consider only the one-dimensional case.

We do not need to use the demon algorithm for an ideal gas, since a reduction in the energy of one particle can be easily compensated by the corresponding increase in the energy of another particle. However, in order to illustrate the more general case, we will use the demon anyway.

Exercise 12.1: MC simulation of the 1D ideal gas

1. Write a program to simulate a 1D ideal gas using the demon algorithm.

2. Use the initial condition that all particles have the same velocity v_0. The mass of the particles is set to unity. Choose $N = 20$, total energy $E = 10$, a maximum velocity change $\Delta v = 2$, and 50 steps for the simulation. Increase the number of MC steps per particle until the desired averages are constant within a desired range.

3. What is the initial mean velocity per particle? What is the equilibrium mean velocity per particle?

4. Compute the mean energy of the demon and the mean system energy per particle. Do your results in parts 3 and 4 depend on whether the particles are chosen randomly or sequentially?

5. Choose $E = 20$ and find the value of the maximum velocity change Δv that yields an acceptance rate of 50%. Compute the mean demon energy and mean system energy per particle after equilibrium has been established. Then consider $E = 40$ and obtain an approximate relation between the mean demon energy and the mean system energy per particle.

6. The MC simulation in the microcanonical ensemble is done at a fixed total energy with no reference to temperature. Determine the temperature by the relation
$$\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_B T.$$
Set the Boltzamann's constant to unity. Use this relation to obtain T. Is T related to the mean demon energy?

7. What is the meaning of the "acceptance ratio"? What is the empirical relation between the acceptance ratio and $\Delta v/v_0$?

12.4 Temperature and the Canonical Ensemble

Let us consider the more realistic case in which our system is in thermal contact with the environment, allowing energy to be exchanged in the form of heat. This situation corresponds to a system in a heat reservoir or heat bath. Now consider that the total energy of the environment and the system is fixed and constant, but the energy of the system can vary. Imagine a large number of copies of the composite system+reservoir, and we consider that this composite supersystem is isolated and can be described by the microcanonical ensemble. However, since we are only interested in the physical properties of the system without the reservoir, we need to know the probability P_s of finding the laboratory system in the state s with energy E_s. The ensemble which describes the probability distribution of a system in thermal equilibrium with a heat bath is known as the "canonical ensemble".

An example of such a system is our demon, immersed in the heat bath of the other N particles. The microstate of the demon is defined by its energy E_d.

Our strategy for finding the form of the probability distribution of the canonical ensemble is to do a computer simulation of a demon which can exchange energy with an ideal gas of N particles. The ideal gas will serve as the heat bath and we will determine the probability $P(E_d)$ that the demon has energy E_d. The exact form of this probability distribution is given by

$$P(E_d) = \frac{1}{Z} e^{-E_d/k_B T} \tag{113}$$

where Z is the normalization constant such that the sum over all states of the demon is unity. The parameter T in (113) is called the "absolute temperature". If T is measured in Kelvin, $k_B = 1.38 \times 10^{-}16 erg\ deg^{-1}$. The probability distribution (113) is called the "Boltzmann" or "canonical" distribution.

Note that the Boltzmann distribution is specified by the temperature. If we assume that the form (113) is applicable to any system in thermal equilibrium with a heat bath, we see that the macrostate in the canonical ensemble is specified by T, N and V. In contrast, a macrostate in the microcanonical ensemble is specified by E, N and V.

The form (113) of the Boltzmann distribution provides a simple way of computing T from the mean energy $\langle E_d \rangle$ of the demon. Since $\langle E_d \rangle$ is given by

$$\langle E_d \rangle \frac{\int dE\, E\, e^{-E/k_B T}}{\int dE\, e^{-E/k_B T}} = k_B T, \tag{114}$$

we see that T is simply the average demon energy divided by k_B. Note that the result $\langle E_d \rangle = k_B T$ holds only if the energy of the demon can take continuous values.

Exercise 12.2: The Boltzmann distribution

1. Add a subroutine to your program to compute the probability distribution $P(E_d)$ of finding the demon with a particular energy. Plot the logarithm of $P(E_d)$ vs. E_d and verify the form (113) for the Boltzmann distribution. What is the slope of the plot? Choose units such that $k_B = 1$ and estimate the corresponding magnitude of T. Choose the same parameters that were used in the previous exercise.

2. Determine the magnitude of T from the relation (114). Are the two estimates consistent?

3. Compare the value of T obtained in the previous two parts with the value of T found in Exercise 12.1 using the kinetic definition of the temperature. Is the demon in thermal equilibrium with its heat bath?

12.5 The Ising model

Consider a lattice with N sites, where each site i can assume two possible states $s_i = +1, -1$, or spin "up" and spin "down". A particular configuration or microstate of the lattice is specified by the set of variables $\{s_1, s_2, ...s_N\}$ for all lattice sites.

Now we need to know the dependence of the energy E of a given microstate, according to the configuration of spins. The total energy in the presence of a uniform magnetic field is given by the "Ising model":

$$E = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_{i=1}^{N} s_i, \tag{115}$$

where the first summation is over all nearest neighbor pairs and the second summation is over all the spins of the lattice. The "exchange constant" J is a measure of the strength of the interaction between nearest neighbor spins. If $J > 0$, the states with the spins aligned $\uparrow\uparrow$ and $\downarrow\downarrow$ are energetically favored, while for $J < 0$ the configurations with the spins antiparallel $\uparrow downarrow$ and $\downarrow\uparrow$ are the ones that are preferred. In the first case, we expect that the state with lower energy is "ferromagnetic", while in the second case, we expect it to be "antiferromagnetic". If we subject the system to a uniform magnetic field h directed upward, the spins $\uparrow$ and $\downarrow$ possess and additional energy $-h$ and $+h$ respectively. Note that we chose the units of h such that the magnetic moment per spin is unity.

Instead of obeying Newton's laws, the dynamics of the Ising model corresponds to "spin flip" processes: a spin is chosen randomly, and the trial change corresponds to a flip of the spin $\uparrow\rightarrow\downarrow$ or $\downarrow\rightarrow\uparrow$.

12.5.1 Boundary conditions

Since we are interested in the properties of an infinite system, we have to consider the boundary conditions. The simplest case corresponds to "free boundary condition", where the spins at sites 1 and N are open ends and have one interaction each. In general a better choice is periodic boundary conditions, where sites 1 and N interact with each other closing a loop. In this situation, the chain has the topology of a ring, and all the spins have the same number of interactions. We also say that there is translational invariance, since the origin can be picked arbitrarily.

12.5.2 Physical quantities

The net magnetic moment or "magnetization' M is given by

$$M = \sum_{i=1}^{N} s_i. \tag{116}$$

Usually we are interested in the average $\langle M \rangle$ and the fluctuations $\langle M^2 \rangle - \langle M \rangle^2$ as a function of the temperature of the system and the applied magnetic field. We can determine the temperature as a function of the energy of the system in two ways. One way is to measure the probability that the demon has an energy E_d. An easier way to determine the temperature is to measure the mean demon energy. However, since the values of the demon energy are not continuous for the Ising model, the temperature is not proportional to the mean demon energy as it is for the ideal gas. It can be shown that in the limit of an infinite system, the temperature for $h = 0$ is related to E_d by

$$k_B T/J = \frac{4}{\ln(1 + 4J/E_d)}. \tag{117}$$

This results is obtained by replacing the integrals by sums over all the possible demon energies. Note that in the limit $|J/E_d| \ll 1$, this reduces to $k_B T = E_d$ as expected.

12.6 Monte Carlo simulation of the Ising model

We now apply the demon algorithm to the simulation of the Ising model in the microcanonical ensemble. In the one-dimensional Ising model the demon must chose the spins randomly in order to avoid configurations periodically repeating themselves.

We pick a spin randomly, we try a spin inversion, and we accept the move if the change in energy is lower or equal than E_d.

Note that for $h = 0$, the change in energy due to a spin flip is either 0 or $\pm 4J$. Hence the initial energy of the system plus the demon must be an integer multiple of $4J$. Since the spins are interacting, it is difficult to choose an initial configuration of spins with precisely the desired energy. We can start the simulation from a configuration with all the spins pointing "up". The advantage of picking this configuration is that the total energy can be easily computed. The demon energy is then chosen so that the total energy of the system plus the demon is equal to the desired multiple of $4J$.

Exercise 12.3: MC simulation of the Ising model in 1D

1. Write a program to simulate the Ising model in the microcanonical ensemble in 1D. Use $N = 100$, $J = 1$, $h = 0$, and a desired total energy $Eini = -20$. The physical quantities drift as the demon's energy is distributed over the N spins. Compute a running average o the demon energy and M as a function of the number of Monte Carlo steps per spin (our measure of "time"). Note that the data is taken after every attempts rather than after every Monte Carlo step per spin. What is the approximate time necessary for these quantities to approach their equilibrium values? Modify the program so that you only start taking

averages after some warmup time, leaving out the nonequilibrium configurations. What are the equilibrium values of $\langle E_d \rangle$, $\langle M \rangle$, and $\langle M^2 \rangle$? A choice of 1000 MC steps gives good results within 5% accuracy.

2. Use the relation (117) to obtain the equilibrium temperature T for the system parameters considered in part 1. Measure E in units of J. What is the corresponding energy of the system?

3. Compute T and E for the three cases $N = 100$, $J = 1$ and $Eini = -40, -60, -80$. Compare your results to the exact results for an infinite one-dimensional lattice $E/N = -\tanh(J/k_B T)$. How do your results for E/N depend on the number of spins N and the number of Monte Carlo steps per spin?

4. Use the same runs to compute $\langle M^2 \rangle$ as a function of T. Does $\langle M^2 \rangle$ increase or decrease with T?

13 The Canonical Ensemble

Most physical systems are not isolated, bu exchange energy with the environment. Since the system is very small compared to the environment, we consider that the environment acts effectively as a heat reservoir or heat bath at a fixed temperature T. If a small system is put in thermal contact with the heat bath, it will reach thermal equilibrium exchanging energy until the system attains the temperature of the bath.

Imagine an infinitely large number of mental copies of the system and the heat bath. The probability P_s that the system is found in a microstate s with energy s is given by:

$$P_s = \frac{1}{Z} e^{-E_s/k_B T}, \tag{118}$$

where Z is the normalization constant. This corresponds to the canonical ensemble. Since $\sum P_s = 1$, we have

$$Z = \sum_s e^{-E_s/k_B T}, \tag{119}$$

where the sum is over all the possible microstates of the system. This equation defines the "partition function" of the system.

We can use (118) to obtain the ensemble average of physical quantities of interest. For instance, the mean energy is given by:

$$\langle E \rangle = \sum_s E_s \, P_s = \frac{1}{Z} \sum_s E_s \, e^{-\beta E_s},$$

with $\beta = 1/k_B T$.

13.1 The Metropolis algorithm

we wan to obtain an estimate for the mean value of an observable A:

$$\langle A \rangle = \sum_s A_s e^{-\beta E_s} / \sum_s e^{-\beta E_s},$$

where E_s and A_s are the values of the energy and the quantity A in the configuration s. The idea of using Monte Carlo consists in sampling a subset of configuration and approximating the average by the mean over the sample:

$$\langle A \rangle \simeq \sum_s^m A_s e^{-\beta E_s} / \sum_s^m e^{-\beta E_s},$$

where the sampling is over m configurations.

A crude Monte Carlo procedure is to generate a configuration at random, calculate E_s and A_s, and the contributions of this configuration to the sums. This is equivalent to the "hit and miss" Monte Carlo method for evaluating integrals. We have seen that this approach is very inefficient, because the configurations generated would likely be very improbable and contribute very little to the sum. Instead, we want to generate a sample of configurations that are *important*, *i. e.* have large contributions to the sums. This is precisely the equivalent to "importance sampling". Hence, we need to generate the configurations according to a probability distribution. In this case, the most convenient one is not other than the Boltzmann probability itself P_s (118). Since we will average over the m configurations generated with this probability, we must use the expression:

$$\langle A \rangle \simeq \sum_s^m \frac{A_s}{P_s} e^{-\beta E_s} / \sum_s^m \frac{1}{P_s} e^{-\beta E_s} = \frac{1}{m} \sum_s^m A_s$$

The idea of the Monte Carlo algorithm consists in performing a random walk over the space of configurations. The walker "hops" from a configuration i to another j using the "transition probability"

$$W = \min \left(1, \frac{P_j}{P_j} \right).$$

Replacing by the corresponding expression, we obtain:

$$W = \min \left(1, e^{-\beta(E_j - E_i)} \right).$$

Since we are only interested in the ratio P_j/P_j, it is not necessary to know the normalization constant Z. Although we have picked this expression for the transition probability W, is not the only choice. It can be shown that the only requirement is that W satisfies the "detailed balance" condition:

$$W(i \to j) e^{-\beta E_i} = W(2 \to j) e^{-\beta E_j}.$$

Another comon choice in the literature is given by:

$$W(i \to j) = \frac{1}{e^{-\beta(E_j - E_i)} + 1}.$$

Note that if $\Delta E = 0$, then $W = 1/2$ and the trial configuration has an equal probability of being accepted.

The pseudocode for a Monte Carlo simulation can be outlined as follows:

1. Establish an initial configuration.
2. Make a random trial change in the configuration. For example, choose a spin at random and try to flip it. Or choose a particle at random and attempt to displace it a random distance.
3. Compute the change in the energy of the system ΔE due to the trial change.
4. If $\Delta e \leq 0$, accept the new configuration and go to step 8.
5. If ΔE is positive, compute the "transition probability" $W = e^{-\beta \Delta E}$.
6. Generate a random number r in the interval $[0, 1]$.
7. If $r \leq W$, accept the new configuration; otherwise retain the previous configuration.
8. Repeat steps (2) to (8) to obtain a sufficient number of configurations or "trials".
9. Compute averages over configurations which are statistically independent of each other.

Exercise 13.1: Classical gas in 1D

1. simulate an ideal gas of N particles in 1D. Choose $N = 20$, $T = 100$ and 200 MC steps. Give all the particles the same initial velocity $v_0 = 10$. Determine the value of the maximum velocity change Δv so that the acceptance ratio is approximately 50%. What is the mean kinetic energy and mean velocity of the particles?
2. We might expect that the total energy of an ideal gas to remain constant since the particles do not interact with each other and hence they cannot exchange energy directly. What is the initial value of the energy of the system? Does it remain constant? If it does not, explain how the energy changes. Explain why the measured mean particle velocity is zero even though the initial particle velocities are not zero.
3. What is a simple criterion for "thermal equilibrium"? Estimate the number of Monte Carlo steps per particle necessary for the system to

reach thermal equilibrium. What choice of the initial velocities allows the system to reach thermal equilibrium at temperature T as quickly as possible?

4. Compute the mean energy per particle for $T = 10$, 100 and 400. In order to compute the averages after the system has reached thermal equilibrium, start measuring only after equilibrium has been achieved. Increase the number of Monte Carlo steps until the desired averages do not change appreciably. What is the approximate number of warmup steps for $N = 10$ and $T = 100$, and for $N = 40$ and $T = 100$? If the number of warmup steps is different in the two cases, explain the reason for this difference.

5. Compute the probability $P(E)dE$ for the system of N particles to have a total energy between E and $E + dE$. Do you expect $P(E)$ to be proportional to $e^{-\beta E}$? Plot $P(E)$ as a function of E and describe the qualitative behavior of $P(E)$. Doe s the plot of $\ln(P(E))$ yield a straight line?

6. Compute the mean energy for $T = 10$, 20, 30, 90, 100 and 110 and estimate the heat capacity.

7. Compute the mean square energy fluctuations $\langle \Delta E^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2$ for $T = 10$ and $T = 40$. Compare the magnitude of the ratio $\langle \Delta E^2 \rangle / T^2$ with the heat capacity determined in the previous item.

Exercise 13.2: One-dimensional Ising model

1. Choose $N = 20$, $T = 1.0$, and all the spins initially pointing "up" as the initial state. Calculate the energy after each step, and estimate the number of steps for the system to reach equilibrium.

2. Pick all the spins initially poiting randomly. Estimate the time that takes for the system to reach equilibrium.

3. Choose $N = 20$ and equilibrate the system for 100 MC steps. Use at least 200 MC steps to determine the mean energy $\langle E \rangle$ and magnetization $\langle M \rangle$ as a function of T in the range $T = 0.5$ to 5.0. Plot $\langle E \rangle$

as a function of T ans discuss its qualitative features. Compare your computed results for the mean energy to the exact values:

$$\langle E \rangle = -N \tanh\left(\frac{J}{k_B T}\right).$$

What are yout results for $\langle M \rangle$? Do they depend on the initial configuration?

4. Is the acceptance ratio and increasing or decreasing function of T? Does the Metropolis algorithm become more or less efficient at low temperatures?

13.2 Simulation of the 2D Ising model

One of the most interesting phenomena in nature is ferromagnetism. A FM material exhibits a non-zero spontaneous magnetization in the absence of an applied magnetic field. This occurs below a well-defined critical temperature T_c known as the Curie temperature. For $T > T_c$ the magnetization vanishes. Hence T_c separates two phases, a disordered one for $T > T_c$, and a ferromagnetic one for $T < T_c$.

Although the Ising model is too simple, it already contains much of the physics of the FM phase transition. In order to explore the properties of this model, we need to calculate some physical quantities of interest, including the mean energy $\langle E \rangle$, the mean magnetization $\langle M \rangle$, the heat capacity C, and the magnetic susceptibility χ.

13.2.1 The heat capacity

One way to measure the heat capacity at constant external field id from the definition:

$$C = \frac{\partial \langle E \rangle}{\partial T}.$$

Another way is to use the statistical fluctuations for the total energy in the canonical ensemble:

$$C = \frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right).$$

13.2.2 The magnetic susceptibility

The magnetic susceptibility χ is an example of a "response function ", since it measures the ability of a spin to "respond" or flip with a change in the external magnetic field. The zero isothermal magnetic susceptibility is defined by the thermodynamic derivative

$$\chi = \lim_{H \to 0} \frac{\partial \langle M \rangle}{\partial H}.$$

The zero field susceptibility can be related to the magnetization fluctuations in the system:

$$\chi = \frac{1}{k_B T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right),$$

where $\langle M^2 \rangle$ and $\langle M \rangle^2$ are zero field values.

13.3 Metropolis algorithm

13.3.1 Boundary conditions

As discussed earlier, the use of PBC minimizes the finite size effects. However, a disadvantage is that they reduce the minimum separation between two spins to half the length of the system.

13.3.2 Initial conditions and equilibration

We can pick a random initial configuration. However, as we shall see, in some simulations the equilibration process can account for a substantial fraction of the total computer time. The most practical choice of an initial condition is an "equilibrium" configuration of a previous run which is at a temperature close to the desired temperature.

13.3.3 Tricks

It is convenient that we store all the transition probabilities in lookup tables, so we do not have to calculate them at each step. Another trick consists of storing all the positions of the spins and their neighbors to avoid calculating many random numbers. If you need to perform several runs for different values of the temperature T, you can do it at the same time using the same random numbers.

Exercise 13.3: Equilibration of the 2D Ising model

1. Run your simulation with $L = 8$ and $T = 2$ and choose the initial spins to be all up. Plot the variation of the energy and the magnetization with time. How much time is necessary for the system to reach equilibrium?

2. Visually inspect several "equilibrium" configurations. Is the system ordered or disordered?

3. Run the program with $T = 1.5$ and chose the same initial configuration with all the spins up. How long does it take for the system to reach equilibrium?

4. Visually inspect several equilibrium configurations with $T = 1.5$. Are they more or less ordered than those in part 2?

13.4 Measuring observables

Note that after reaching equilibrium we wish to compute the mean values of several physical quantities of interest. In general this is quite time consuming and hence we do not want to calculate their values more that necessary. After a single spin flip of one spin, the values of the observables in the two configurations will not differ much, and will be almost the same. Ideally, we wish to compute the observables for configurations that are statistically independent. This means that we have to run the simulation severals steps in between measurements. This number of steps is a typical quantity that depends on the physics of the model, the parameters used, the temperature, and in particular, the "update dynamics" used in the algorithm, as we shall see below. This "correlation time" is not known *a priori*, and we have to estimate it with a preliminar test run.

One way to determine the time intervals over which configurations are correlated is to compute the time-dependent autocorrelation functions defined by:

$$C_M(t) = \langle M(t)M(0)\rangle - \langle M\rangle^2$$

and

$$C_E(t) = \langle E(t)E(0)\rangle - \langle E\rangle^2.$$

Note that at $t = 0$, C_M is proportional to the susceptibility, and C_E is proportional to the heat capacity. For sufficient large t, $M(t)$ and $M(0)$ will become uncorrelated, and

$$\langle M(t)M(0)\rangle \rightarrow \langle M(t)\rangle\langle M(0)\rangle = \langle M\rangle^2$$

, and the same will occur with C_E. Hence C_M and C_E should vanish for $t \rightarrow \infty$. In general, we expect these quantities to decay exponentially with time. The time is takes $C(t)$ to decay to $1/e$ of its value at $t = 0$ is an estimate of the autocorrelation time τ. Since configurations separated by times less that τ are statistically correlated, we will compute the desired physical quantities for times intervals of the order of τ rather than after each MC step.

Exercise 13.4: The correlation time

Consider $L = 8$ and $T = 3.0$ (high T) and $T = 2.3$, and $T = 1.5$ (low T). Estimate the correlation time τ for the energy and the magnetization fluctuations. Are the values comparable for the two fluctuations? How do your estimates for τ compare with your estimates for the relaxation time found in the previous problem?

13.4.1 Exercise 13.5: Comparison with exact results

1. Generate all the possible configurations of spins for $L = 4$.

2. Calculate the mean value of the energy, magnetization, susceptibility, and heat capacity as a function of the temperature. For calculating the magnetization use $|m|$ instead of m.

3. Use your MC program to compute the same quantities and compare with the exact results. Use the necessary MC steps to obtain an accuracy of 1% for the energy.

13.5 The Ising phase transition

We have seen that at $T = T_c$, the magnetization vanishes. This happens continuously with increasing temperature and hence, it is a "2nd order" phase transition. In 1st order phase transition the magnetization, vanishes abruptly. A way to characterize phase transition is though studying the

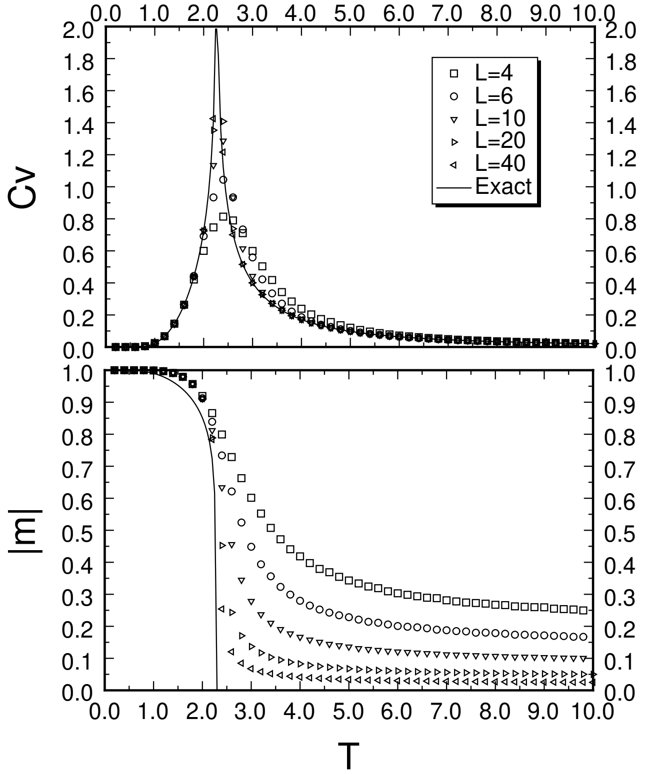

Figure 16: Comparison between exact results for small lattices and the exact solution in the thermodynamic limit

"critical behavior" of the system. First, we have to define a quantity called "order parameter" which vanishes above the critical temperature, and is finite below it. We clearly see that the magnetization satisfies this criterion, and is a suitable candidate. The critical behavior of the system is determined by the functional form of the order parameter near the phase transition. In this region, physical quantities show a power law behavior

$$m(T) \sim (T - T_c)^\beta,$$

where β is the "critical exponent". Although M vanishes with T, thermodynamic derivatives such as the heat capacity and sucseptibility diverge at T_c:

$$\chi \sim |T - T_c|^{-\gamma}$$

and

$$C \sim |T - T_c|^{-\alpha}.$$

We have assumed that the exponent is the same on both sides of the transition.

Another measure of the magnetic fluctuations is the linear dimension $\xi(T)$ of a typical magnetic domain. We expect that this "correlation length" to be the order of the lattice spacing for $T \gg T_c$. Since the alignment of the spins will become more correlated as T approaches T_c from above, ξ will increase. We can characterize the divergent behavior of $\xi(T)$ near T_c by a critical exponent η

$$\xi(T) \sim |T - T_c|^{-\eta}$$

A finite system cannot observe a true phase transition. Nevertheless we expect that if the correlation length is less than the linear dimension L of the system, then a finite system will be an accurate representation of the infinite system. In other words, our simulations would yield accurate results comparable to an infinite system is T is not too close to T_c.

Exercise 13.6: Qualitative behavior of the 2D Ising model

Calculate $\langle E \rangle$, C, χ and m as a function of temperature for $L = 4$, $L = 8$ and $L = 16$. Plot the results and describe their qualitative behavior. Do you see any evidence of a phase transition?

Exercise 13.7: Critical slowing down

1. Consider the 2D Ising model on a square lattice with $L = 16$. Compute the correlation time τ for $T = 1.5$, 2.4, and 2.3. Show that τ increases as the critical temperature is approached, a physical effect known as "critical slowing down".

   The magnitude of τ depend in part on our choice of "dynamics". Although we generate trial configurations attempting a single spin flip, it is possible to simultaneously flip two or more spins, even an entire cluster. This other update strategies are more efficient and lead to smaller correlation times.