Numerical Analysis and Computational Physics PHN 311, 2022
Dept. of Physics, IIT Roorkee

Computational projects

Group A

1: Oscillation

This problem considers oscillatory motion which is not necessarily simple harmonic.

Consider the one-dimensional motion of a particle of mass m in a time independent potential $V(x)$. Since the energy E is conserved, one can integrate the equation of motion and obtain a solution in a closed form

$$t - C = \sqrt{\frac{m}{2}} \int_{x_i}^{x} \frac{dx}{\sqrt{E - V(x)}}. \tag{1}$$

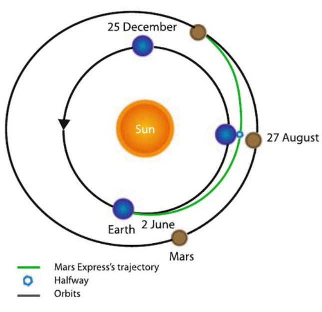
For the choice $C = 0$, the particle is at the position x_i at the time $t = 0$ and x refers to its position at any arbitrary time t. Consider a particular case where the particle is in bound motion between two points a and b where $V(x) = E$ for $x = a, b$ and $V(x) < E$ for $a < x < b$. The time period of the oscillation T is given by

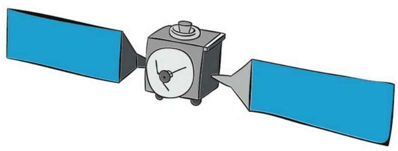
$$T = 2\sqrt{\frac{m}{2}} \int_{x_i}^{x} \frac{dx}{\sqrt{E - V(x)}} \tag{2}$$

(i) First consider a particle with $m = 1\ Kg$ in the potential $V(x) = 0.5\ \alpha x^2$ with $\alpha = 4\ Kg\ sec^{-2}$. Numerically calculate the time period of oscillation and check this against the expected value. Verify that the frequency does not depend on the amplitude of oscillation.
(ii) Next consider a potential $V(x) = e^{0.5\alpha x^{\wedge}2} - 1$. Numerically verify that for small amplitude oscillations you recover the same results as the simple harmonic oscillator.
(iii) The time period is expected to be different for large amplitude oscillations. How does the time period vary with the amplitude of oscillations? Show this graphically.

2. Mars Express and Kepler's laws

This problem is an example in learning physical laws from raw data analysis





The Mars Express probe was launched on June 2nd 2003 and reached Mars in December 2003. See the schematic motion diagram of the trajectory. The path of the MarsExpress from the earth the to mars is approximately given by the attached data set `marsExp_coarse.dat`. Each line has the following four columns

t_1	x_1	y_1	z_1

The time t is given in days, and the spatial coordinates (x,y,z) are in Km. Note the coordinates are measured with the sun at the origin.

a) Convert the distances into astronomical unit *AU*. *1 AU = 149598000 Km* = average distance of the earth from the sun.
b) Plot the trajectory in *X-Y* plane.
c) Compute the velocity and acceleration of the probe. Note that the given data has low resolution, i.e. the position of the probe are recorded approximately *30 days* intervales. So instantaneous velocities and accelerations can not be computed numerically in a reliable manner. Define your velocity and acceleration carefully.
d) Show the velocity and acceleration in the plot in (b)
e) Now use the attached dataset `marsExp_fine.dat` for the path, which has higher resolution. Plot the trajectory on *X-Y* plane.
f) Can you now compute instant velocities and accelerations reliably? Determine how the speed (in units of *AU/days*) and the magnitude of the acceleration (in units of AU/day^2) of the probe changes with time.
g) To build physical intuition about the speed, use a reference. Compute the average speed of the earth (v_E) and of the mars (v_M) in *AU/days*. Assume that the average distance of the mars from the sun = *1.5 days*. Look up one Martian year in earth days. Show v_E and v_M in the plot in (f).
h) Similarly compute the average acceleration of the earth a_E and the mars a_M and show in the plot in (f). In part (g)-(h) what assumptions do you make to model the orbit of the earth and the mars around the sun?
i) Use the high resolution data set to analyze how the acceleration a of the probe changes with the distance from the sun. What can you say about the force law that is causing the acceleration?
j) What can you say about the Kepler's laws of planetary motion from the data?

3. Black Body Spectrum

This problem is an exercise in curve fitting.

Quantum mechanics began with Planck's fit to the spectrum of black body radiation:

$$\mathrm{I}(\nu,T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}}-1}.$$

Here $I(v,T)$ is the energy per unit time of radiation with frequency v emitted per unit area of emitting surface, per unit solid angle, and per unit frequency by a black body at temperature T. The parameter h is Planck's constant, c is the speed of light in vacuum, and k is Boltzmann constant. The COsmic Background Explorer (COBE) project measured the cosmic background radiation and obtained the results given in Table 6.1.

1. Plot the COBE data and see if it has a shape similar to the black body spectrum first explained by Planck.
2. Use these data to deduce the temperature T of the cosmic microwave background radiation.
3. Assess the accuracy of the fit by doing a χ^2 analysis.

Table 6.1. The energy spectrum of microwave radiation measured by COBE.

ν	$I(\nu, T)$	Error	ν	$I(\nu, T)$	Error	ν	$I(\nu, T)$	Error
1/cm	MJy/sr	kJy/sr	1/cm	MJy/sr	kJy/s	1/cm	MJy/sr	kJy/sr
2.27	200.723	14	2.72	249.508	19	3.18	293.024	25
3.63	327.770	23	4.08	354.081	22	4.54	372.079	21
4.99	381.493	18	5.45	383.478	18	5.90	378.901	16
6.35	368.833	14	6.81	354.063	13	7.26	336.278	12
7.71	316.076	11	8.17	293.924	10	8.62	271.432	11
9.08	248.239	12	9.53	225.940	14	9.98	204.327	16
10.44	183.262	18	10.89	163.830	22	11.34	145.750	22
11.80	128.835	23	12.25	113.568	23	12.71	99.451	23
13.16	87.036	22	13.61	75.876	21	14.07	65.766	20
14.52	57.008	19	14.97	49.223	19	15.43	42.267	19
15.88	36.352	21	16.34	31.062	23	16.79	26.580	26
17.24	22.644	28	17.70	19.255	30	18.15	16.391	32
18.61	13.811	33	19.06	11.716	35	19.51	9.921	41
19.97	8.364	55	20.42	7.087	88	20.87	5.801	155
21.33	4.523	282						

4. Radioactive decay

Consider a radioactive decay problem involving two types of nuclei, *A* and *B* with populations $N_A(t)$ and $N_B(t)$. Suppose that type *A* nuclei decay to form type *B* nuclei, which then also decay, according to the below differential equations:

$$\frac{dN_A}{dt} = -\frac{N_A}{\tau_A},$$

$$\frac{dN_B}{dt} = \frac{N_A}{\tau_A} - \frac{N_B}{\tau_B},$$

where τ_A and τ_B are the decay time constants for each type of nucleus. Use the 4th-order Runge-Kutta method to solve these coupled equations for N_A and N_B as functions of time. Obtain the analytical solutions for $N_A(t)$ and $N_B(t)$ and compare them with your numerical results. Also explore the behavior for different values of the ratio τ_A/τ_B. Interpret the short and long time behaviors for different values of this ratio.

5. Method of images

This problem considers computing and visualizing 2D electric field. Some textbooks for learning about the method of images – "Electricity and Magnetism" 3rd Ed. by E M Purcell and D J Morin, "Introduction to Electrodynamics" by D J Griffiths.

Given a problem with point charges and appropriate boundary conditions, the uniqueness theorem tells us that if we can insert an imaginary "image" charge external to the boundary that satisfies the boundary conditions, then we have solved the problem of finding the electric field. As an example, if the boundary conditions correspond to a conductor being present, then the field within the conductor would still be zero, even though we have placed an image charge there. Likewise, as a reflection of the symmetry of images, if the image charge is considered to be a real charge, and the real charge is considered to be an image, then we can solve for the electric field outside of the boundary. Some intuition is necessary to guess where to place the image charges, and that is helped along by the employment of visualization tools. Once the image charge is in place, solving for the field due to two charges is straightforward, and one visualizes the E_x and E_y components.

(a) Use Matplotlib's built-in `streamplot` function to produce streamlines of a 2D vector field. Use this command to visualize the electric field due to (i) due to a point charge, (ii) due to two point charges (iii) due to an electric dipole.

(b) Use the method of images to determine and visualize the electric field due to a point charge above a grounded, infinite conducting plane.

Group B

1. Fraunhofer diffraction and Fourier transform: *The goal of this project is to learn how to compute diffration patterns and practice taking Fourier transform (FT) of a function numerically. Fourier transform is discussed in mathematical physics textbooks. Two brilliant books are: "Mathematical methods for Physicists" by G Arfken and H Weber, and "Mathematical methods for Physicists" by J Mathews and R L Walker. This project deals with application of FT in optics. The numerical methods of discrete and fast Fourier transforms are discussed in the course textbooks: "Computational Physics" by R H Landau, M J Paez and C C Bordeianu and "Computational Physics" by P O J Scherer.*

The Fraunhofer diffraction pattern from an aperture can be described by the Fourier transform of the aperture function. Using this information, numerically simulate the Fraunhoffer diffraction pattern for the following slits.

- Rectangular slit,
- Square slit,
- Circular slit.

2. Non-linear dynamics – predator-prey model

Most of the fundamental equations in Physics such as classical Newtonian laws of motion are linear. In the second half of the 20th century people discovered that non-linear laws of motion are also quite common in Nature. Population dynamics in biology and climate models are two important examples. Non-linear laws lead to an "chaos". The aim of this project is to study non-linear dynamics in a prototype example called predator-prey model. An excellent introduction to non-linear dynamics is "Nonlinear dynamics and Chaos" by S R Strogatz.

The predator-prey (foxes-rabbits) equation is given by

$$\frac{dr}{dt} = 2r - \alpha r f,$$

$$\frac{df}{dt} = -f + \alpha r f$$

Here $r(t)$ and $f(t)$ refer to the rabbit and fox population numbers respectively while α is the interaction coefficient. Calculate the phase plane trajectory for r(0) = 50, f(0) = 50 and α = 0.01. What are the maximum and minimum numbers to which the rabbit and fox population grow? Discuss the results.

3. Non-linear dynamics – logistic map

Most of the fundamental equations in Physics such as classical Newtonian laws of motion are linear. In the second half of the 20th century people discovered that non-linear laws of motion are also quite common in Nature. Population dynamics in biology and climate models are two important examples. Non-linear laws lead to an "chaos". The aim of this project is to study non-linear dynamics in a prototype example called predator-prey model. An excellent introduction to non-linear dynamics is "Nonlinear dynamics and Chaos" by S R Strogatz.

Consider the logistic map $x_{n+1} = Ax_n (1 - x_n)$ where x_n is the nth iteration for $0 \le x \le 1$. Here A is a constant. Vary the value of A from 0.89 to 3.995 in an interval of 0.0125 in each step.

(a) For each value of A, note the values of x_n for $15 < n < 200$. Then make a plot of x_n *versus* A and see the bifurcation and chaos.

(b) For $A = 4$, choose two points x and x' where $x' = x + 0.01$ and iterate. Plot $log(|x_n - x'_n|/0.01)$ as a function of n. See if it is approaching a straight line.

4. Real life projectile motion - effect of air resistance

Projectile motion in absence of drag force can not describe the fall of leaves from a tree and the swing of a cricket ball. Drag force must be condisered in many practical applications such as rocket motion through atmosphere. The aim of this project is how to go from an idealized textbookish model to a more real-life scenario in a systematic step by step manner.

(a) Neglect air resistance:

Find the trajectory of a projectile fired from a cannon shell located at the origin using the Runge-Kutta 4th-order method. Assume the initial projected speed to be *700 meter/s*, and using different firing angles starting from *20 degrees* to *60 degrees* with an interval of *5 degrees*. Neglect the effects of the air resistance. Plot the trajectories of the projectile for different firing angles. Also plot the range of the projectile against the firing angles and show numerically that the maximum range of the projectile corresponds to a firing angle of 45 degrees.

(b) Uniform air resistance:

Extend the above problem to include the effect of constant air resistance by assuming a value of $B/m = 4 \times 10^{-5}$ meter^{-1}. Plot the trajectories for a given firing angle for the case of no air resistance and with air resistance. Repeat this for different firing angles. Also plot the range of the projectile against the different firing angles and find numerically the firing angle which corresponds to the maximum range of the projectile.

(c) Air resistance varying with height:

Now consider that the air resistance is not uniform. Consider the air density varies as e^{-y/y_0}, where $y_0 = 104$ *meters*. Plot the trajectories for a given firing angle without air resistance, with constant air resistance and with varying air resistance as given above. Repeat this for different firing angles. Also plot the range of the projectile against the different firing angles and find numerically the firing angle which corresponds to the maximum range of the projectile.

5. Random walk

Random walk is an ubiquitous mathematical model. It arises in all areas of physics from Astronomy (e.g. how a photon generated in the core of the sun reaches the surface of the sun) to Condensed matter (e.g. how does a pollen grain moves through a liquid), as well as in many fields outside physics such as stock markets and biology. The aim of this project is to simulate a random walk and learn its statistical properties.

It is late night and a drunkard is walking along a very long street. The drunkard is not sure which is the way home, so he randomly takes steps of length *1.0 m* forward or backward – with equal probability. He takes one step every second continuously for *1 hr*. This resultant trajectory of the drunkard is an example of a *3600 step* random walk in *1 dimension*.

(a) Simulation of an *N*-step random walk:

Write a routine to generate an *N-step* random walk in *d dimensions*, with each step uniformly distributed in the range $(-1/2, 1/2)$ in each dimension (arbitrary units). You should use a random number generator. Generate 100 different realizations of the random sequence of steps by using a different seed each time.

(i) Take $d=1$. Plot the location of the walker at time step t, x_t versus t for a few *10000-step* random walks.

(ii) Take $d=2$. Plot x versus y for a few two-dimensional random walks, with $N = 10, 1000,$ and 100000. Try to keep the aspect ratio of the *XY* plot equal to one. Does multiplying the number of steps by one hundred roughly increase the net distance by ten?

(b) Emergent symmetry:

Each random walk is different and unpredictable, but the ensemble of random walks has elegant, predictable properties. Write a routine to calculate the endpoints of *W* random walks with *N* steps each in d dimensions. Do a scatter plot of the endpoints of *10000* random walks with $N = 1$ and *10*,

$d=2$, superimposed on the same plot. Notice that the longer random walks are distributed in a circularly symmetric pattern, even though the single step random walk $N = 1$ has a square probability distribution. This is an emergent symmetry; even though the walker steps longer distances along the diagonals of a square, a random walk several steps long has nearly perfect rotational symmetry.

(c) Central limit theorem:
The most useful property of random walks is the central limit theorem. The endpoints of an ensemble of N step one-dimensional random walks with root-mean-square (RMS) step-size a has a Gaussian or normal probability distribution as $N \to \infty$,

$$\rho(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-x^2/2\sigma^2), \text{ where } \sigma = a\sqrt{N}$$

Calculate the RMS step-size a for one dimensional steps uniformly distributed in $(-1/2, 1/2)$. Write a programme that plots a histogram of the endpoints of W one dimensional random walks with N steps and *50 bins*, along with the prediction of the above eqn. for x in $(-3\sigma, 3\sigma)$. Do a histogram with $W = 10000$ and $N = 1,2,3$, and 5. How quickly does the Gaussian distribution become a good approximation to the random walk?

6. Ising model in 2D and phase transition

One of the great problems in statistical physics is to describe phases and phase transition. The Lenz-Ising model is a simple but famous model of ferromagnetic materials. This model is particularly easy to simulate using Monte Carlo methods. In dimensions d>=2, at high temperature it displays a paramagnetic phase and below a characteristic temperature T_c, the system shows ferromagnetism. The aim of this project is to simulate Ising model in 2D and demonstrate the phase transition as temperature is gradually decreased.

Consider the two-dimensional Ising model on a square lattice involving classical spins

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_{zi} S_{zj},$$

where $J=1$ is the exchange constant, <> represents the nearest-neighbor sites, and the spin moments can take values $S_{zi} = \pm 1$.
(a) Use classical Monte Carlo simulated annealing with Metropolis energy minimization algorithm to obtain the the spin configuration at different temperatures T. Plot the average moment as a function of T.
(b) Use this model to study phase transition. Make a movie of configurations to show paramagnetic to ferromagnetic phase transition as the temperature is decreased from a high temperature $T_h > T_c$ to a low temperature $T=0$. Here T_c is the transition (Curie) temperature.

7. Hard disk liquid in 2D and phase transition

One of the great problems in statistical physics is to describe phases and phase transition. The most common phase transition we encounter is perhaps the fluid-solid phase transition. The aim of this project is to simulate a simple model liquid to understand the liquid state of matter and demonstrate the crystallization as density is gradually increased.

The probem is taken from "Statistical and Thermal Physics" by H Gould and J Tobochnik and is described here. You may also go to this webpage and look up "STP Hard disks Metropolis documentation".

The goal of this project is to simulate the liquid state of matter using a simple model of N hard disks in 2D and Metropolis algorithm. See equation 1 and section III Algorithm of the documentation.

Answer the questions 1-4 in the documentation.

8. Orbit of a body in a gravitational field

Planetary orbits is one of the oldest mechanics problem in physics. The aim of this project is to numerically compute the trajectory of a particle in a gravitation field.

(a) Two body problem:
Use Newton's law of gravitation to simulate the two-body motion of two stellar objects with masses M_1 and M_2. Plot the trajectory of the motion. What kind of trajectory is expected if a satellite (in geocentric orbit) comes in proximity to the Earth and the Moon?

(b) Three body problem: one planet, two suns
The three-body problem in which three particles move via pairwise interactions can be complicated and chaotic. Here we ask you to examine a simple version in which two heavy stars 1 and 2 are kept at a fixed separation along the *x* axis, while a lighter planet moves about them. We use natural units $G=1$ to keep the calculations simpler, and treat all bodies as point particles. It is best to view the output as animations so that you can actually see the planet pass through a number of orbits. A characteristic of this kind of chaotic system is that there are periods with smooth precessions followed by chaotic behavior, and then smooth precession again. This means that we on earth are lucky having only one sun as this makes the year of reliably constant length.

(i) Start with $M_1 = M_2 = 1$ and the planet at $(x, y)_0 = (0.4, 0.5)$ with $(v_x , v_y)_0 = (0, -1)$.
(ii) Set $M_2 = 2$ and see if the planet remains in a stable orbit about sun 2.
(iii) Return to the equal mass case and investigate the effect of differing initial velocities.
(iv) Make M_1 progressively smaller until it acts as just a perturbation on the motion around planet 2, and see if the year now becomes of constant length.
(v) What might be the difficulty of having life develop and survive in a two sun system?
(vi) Explore the effect on the planet of permitting one of the suns to move.

9. Schrodinger equation:

The aim of this project is to solve Schrodinger's equation of motion in some toy 1D models to compute the energy levels of an electron.

Numerically solve the Schroedinger's equation for a simple harmonic potential and the Lennard-Jonnes potential. Plot the wave functions for the ground state and first two excited states. For both cases, compare the results with the analytical results.

10. [Top algrorithms of the 20th century:]

The aim of this project is to do a self-study of a few important algorithms that is not part of the syllabus, but is useful for many applications.

Consider the following list of influential algorithms for computation:

- Singular value decomposition of a matrix
- Krylov subspace methods for solving Ax=b
- Optimization – steepest descent and conjugate gradient
- JPEG – Joint Photographic Experts Group image compression algorithm

Do a self study and prepare a write-up on <u>any one</u> of the above.