Projects

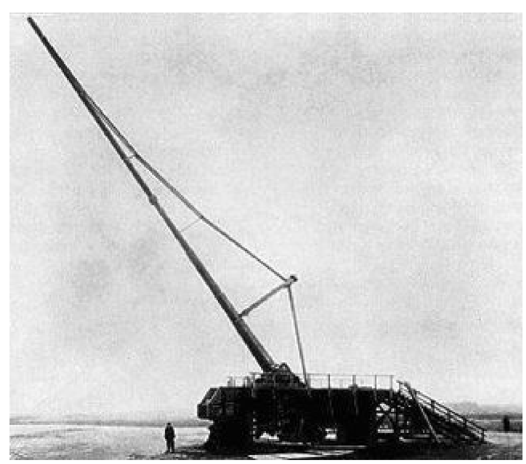
Structure of Project Reports:

1 Introduction. Briefly summarize the nature of the physical system.
2 Theory. Describe equations selected for the project. Discuss relevance and limitations of the equations.
3 Method. Describe briefly the algorithm and how it is implemented in the program.
4 Verification of a program. Confirm that your program is not incorrect by considering special cases and by giving at least one comparison to a hand calculation or known result.
5 Results. Show the results in graphical or tabular form. Additional runs can be included in an appendix. Discuss results.
6 Analysis. Summarize your results and explain them in simple physical terms whenever possible.
7 Critique. Summarize the important concepts for which you gained a better understanding and discuss the numerical or computer techniques you learned. Make specific comments on the assignment and your suggestions for improvements or alternatives.
8 Appendix. Give a typical listing of your program. The program should include your name and date, and be self-explanatory (comments, structure) as possible.

Project 1. Projectile motion with air resistance (Due on October 18, 2009 by 21:00)

Write a program that simulates the projectile motion with allowing for air resistance, varying air density and wind. The amplitude of air resistance force on an object moving with speed v can be approximated by $F_{drag}=-0.5C\rho_0 Av^2$, where ρ_0 stands for air density ($\rho_0=1.25$ kg/m^3 at sea level), and A is the cross section. The drag coefficient C depends on an object shape and for many objects it can be approximated by a value within 0.05 - 0.5. Use Runge-Kutta method as a primary method for solving a system of differential equations.

Application: Study the trajectory of shells of one of the largest cannons "Pariskanone" used during the First World War. Calculate effects of air resistance, varying air density and wind on the range, time of flight and max altitude of shells. Determine the angle (between 0 and 90 degrees) that gives the maximum range for such cannon. The range and time of flight have to be calculated numerically (using interpolation) by the program.



Some initial information: The shell mass - 94 kg., initial speed - 1600m/s, caliber - 210 mm, and the C coefficient is about 0.12. Approximate the density of the atmosphere as $\rho = \rho_0 * \exp(-y/y_0)$, where y is the current altitude, $y_0 = 1.0*10^4$m, and ρ_0 is air density at sea level (y=0).

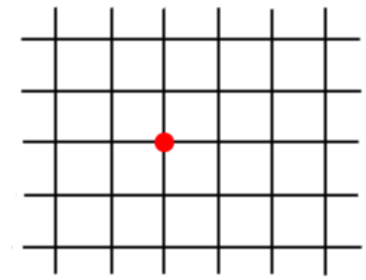
Discuss the accuracy of the "Pariskanone".

Extra credit: compare accuracy of Verlet method to Runge-Kutta.

Project 2: Random walks in two dimensions (Due on November 6, 2008 by 13:30)

Part 0. Study the quality of a built-in random number generator (in C++ or Fortran): evaluate 4th moment of the random number distribution, evaluate near-neighbor correlation, plot a 2D distribution for two random sequences x_i and y_i (a parking lot test), plot a 2D distribution for correlation (x_i, x_i+5).

Part 1: Diffusion (simple random walk). Write a program that simulates a random 2D walk with the same step size. Four directions are possible (N, E, S, W). Your program will involve two integers, K = the number of random walks to be taken and N = the maximum number of steps in a single walk. Run your program with at least K >= 1000. Find the average distance R to be from the origin point after N steps. Assume that R has the asymptotic dependence as $R \sim N^a$, and estimate the exponent a.



Part 2: Random walk on a 2D crystal. Consider a two dimension lattice of size L*L. Randomly place a "random walker" on the lattice and start walking (only four directions are possible: left, right, up, down). As soon as the “random walker” reaches a site outside the L*L area the random walk stops. Find the average number of steps S to get out of the crystal. Is there a connection between S and L?

Part 3: Random walk on a 2D lattice with traps. Consider the same two dimension lattice of size L*L. Now the lattice contains a trap. (An analogy would be a city with (L-1)*(L-1) blocks and a police patrol).

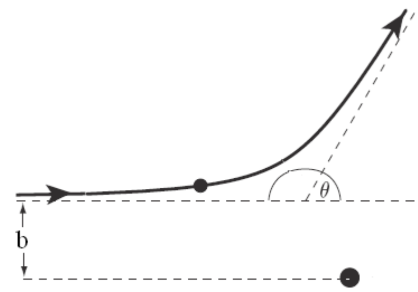
Randomly place a "random walker" on the lattice. When the walker arrives to the trap site, it can no longer move. So, the random walk stops when the walker either trapped or our of the L*L area. Find probabilities to get the walker trapped and get free. Find also the mean number of steps (“survival time”) before a trap site is reached, or the walker is out of the area, as a function of L or ρ.

Explore following scenarios:

1 A stationary trap located at the center of the area, i.e. with the coordinates (L/2,L/2)
2 A randomly placed stationary trap
3 A randomly moving trap – the trap “walks” randomly with the same speed (one block in a time). Since the trap can not leave the L*L are, use the periodic boundary conditions when needed.
4 **Extra credit (3 points)**. A persistent trap – the trap moves along a closed path (a box around the center with a side S<L – like a moving police patrol). Does the outcome depends on the S/L ratio?

Part 4: Extra credit (1 point): find examples in physics that can be related to the random walks in this project. Explain the relevance.

Project 3: Classical scattering (Due: November 20, 2009 by 13:30)



In classical scattering theory the differential scattering cross section is related to the impact parameter and the scattering angle as

$$\frac{d\sigma}{d\theta} = \frac{b}{\sin(\theta)}\left|\frac{db}{d\theta}\right|$$

Part 1: Rutherford scattering. Consider the elastic scattering of a projectile with mass M_1 and electric charge Z_1 with a target of mass M_2 and charge Z_2. The target is fixed in space. The projectile-target interaction (the Coulomb potential) can be written in atomic units as

$$V(R) = \frac{Z_1 Z_2}{R}$$

The analytic solution for the differential cross section is the Rutherford scattering formula.

$$\frac{d\sigma}{d\theta} = \left(\frac{Z_1 Z_2}{4E\sin^2(\theta/2)}\right)^2$$

Solve the problem of the Rutherford scattering numerically as an ODE initial value problem in the (x,y) plane. You initial conditions are the projectile velocity and the impact parameter. Calculate the differential cross section (use numerical differentiation) and compare your numerical result to the Rutherford scattering formula.

Part 2: Rutherford scattering (modified). The target is initially at rest, but may move during the collision due to the projectile-target interaction. Study the effect of the target motion on the differential scattering cross section. Now you have two moving objects. You should test your solutions by calculating the total energy and angular momentum of the system. Sure, the effect would depend on the ratio M_1/M_2.

Part 3: Yukawa potential (screened Coulomb potential). The long range Coulomb potential has been a serious problem in quantum scattering theory. Study numerically the elastic scattering of two particles interacting by the Yukawa potential

$$U(R) = \exp(-\alpha R)\frac{Z_1 Z_2}{R}$$

Test you results using conservation of the total energy and the total momentum for the two particles.

Extra credit (2 points): Compare you numerical results with the integral from classical mechanics

$$\theta = \pi - 2\int_{r\min}^{\infty} \frac{(b/r^2)}{\sqrt{1-(b/r)^2 - U(r)/E}}\,dr$$

but first, check conditions when the equation above is valid. Compare your results for the two potentials (Coulomb and Yukawa).

Part 4: Total cross sections: extra credit (1 points). Calculate the total cross section of the elastic scattering for the parts 1-3.

Comments: 1) It is much more convenient to work in the atomic system of units. 2) You need to use following numerical procedures: numerical solution of the ODE initial value problem, numerical derivatives, and numerical integration 3) Be reasonable selecting the initial conditions, as well as M_1, Z_1, M_2, Z_2, and α.

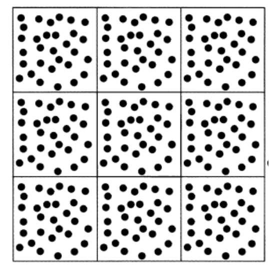
Project 4: A Simple Molecular Dynamics simulation (Due on November 20, 2009 by 13:30)

Part 1. 4 particles. Consider 4 particles on a (x,y) plane interacting via the Lennard-Jones potential. The initial conditions: the particles are on a square lattice, or placed randomly in L*L area, but no two particle are closer than 1.1225σ. Assign random initial velocities, but set the total momentum to zero, and rescale the velocities to correspond to an initial temperature of T.

Run the simulation. Check conservations of energy for steps h and h/2. Will the particles oscillate around some positions for very low temperatures?

Part 2. N particles. Increase the number of particles up to 100 (or as many as your computer can handle in reasonable time). For the initial conditions use either randomly placed particles, or placed on a lattice. Calculate average energy and temperature. What is the mean value of the temperature for the given total energy of the system?

Part 3. Periodic boundary conditions. Extra credit 2 points. Consider N particles with periodic boundary conditions (eight image cells around the primary cell). Calculate average energy, temperature and pressure as a function of time.



Helpful equations:

The Lennard-Jones potential

$$u(r) = 4a\left[\left(\frac{b}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6}\right]$$

The Störmer-Verlet method for solving a system of differential equations for N particles –

$$\begin{aligned} x(t+h) &= x(t) + hx'(t) + 0.5h^2 x''(t) \\ x'(t+h) &= x'(t) + 0.5h[x''(t+h) + x''(t)] \end{aligned}$$

The temperature at time t is defined by

$$kT(t) = \frac{2}{d}\frac{K(t)}{N}$$

where K is the total kinetic energy of the system, d is the spatial dimension, N is the number of particles.

The pressure at time t can be calculated from

$$P(t)V = NkT(t) + \frac{1}{d}\sum_{i<j} r_{ij} \cdot f_{ij}$$

where V is the volume for a 3D system (d=3) , and the surface for a 2D system (d=2)

For this project you may consider: m=1, a=1, b=1, k=1.