Homework 1; due on Sunday, March 23

PHY336, Computational Physics, Spring 2025

Department of Physics, SUSTech

1. MONTE CARLO INTEGRATION

A sphere of radius r_1 consists of two different materials, with densities ρ_1 and ρ_2. The material with density ρ_2 is located within a cylinder of radius r_2, as illustrated in Fig. 1, and the material of density ρ_1 fills up the rest of the sphere. Write a program that calculates the two moments of inertia of this sphere corresponding to rotation about the z and x axis. The inner cylinder is centered around the z-axis, as also shown in the figure.

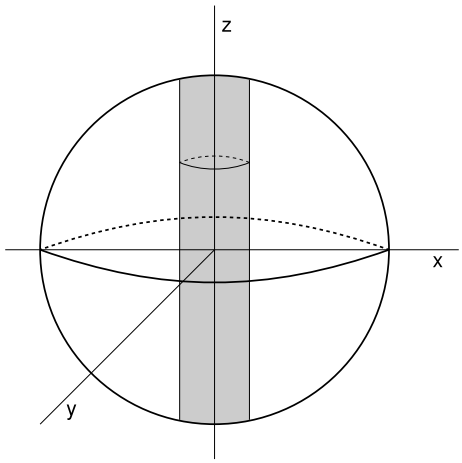

Figure 1: A solid sphere of radius r_1 with an inner solid cylinder of radius r_2. The cylinder consists of a material with density ρ_2; the rest of the sphere consists of a material with density ρ_1.

Carry out the calculation using Monte Carlo sampling of the moment of inertia integral

$$I = \int dx \int dy \int dz \rho(x,y,z) r_\perp^2(x,y,z), \tag{1}$$

where $r_\perp(x,y,z)$ is the perpendicular distance of the point (x,y,z) from the axis of rotation (here the x or z axis, giving I_x and I_z). Enclose the sphere in a box with side $L = 2r_1$ in order to easily do the calculation using (x,y,z) points.

The program should read the following input from a file `read.in`:

```
r1,r2,rho1,rho2,npt,nbi
```

where `r1,r2` are the two radii (in m), `rho1,rho2` are the densities (in kg/m^3), `npt` is the number of random points generated per "bin" (for which bin averages are computed) and `nbi` is the number of bins (on the basis of which the final average and statistical error are computed).

Bin averages should be computed for both the I_z and I_x moments of inertia and these should be written to a file `bin.dat` containing `nbi` lines, each with the bin number followed by the I_z and I_x values (write these averages to the file after each bin is completed; it is not necessary to store the data in the program). The final average and error bar (standard deviation of the mean) computed using the bin averages should be written to a file `res.dat`.

As a specific case, do the calculation for a copper (8930 kg/m^3) sphere of radius 5 cm with an inner gold (19320 kg/m^3) cylinder of radius 1 cm. Use 10^6 points per bin (`npt`) and do the calculation for `nbi=50,500,5000`. For the final case, construct a histogram of the bin averages (with the width of the histogram bins chosen in a reasonable way to get of the order tens of histogram bins with significant weight). The report on this problem needs to contain only the final numerical results (averages and standard deviations) for the three runs and the histogram for the last run. Comment on the shape of the histogram.

2. Evaluate the 10 dimensional integral

$$I = \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 \cdots \int_0^1 \mathrm{d}x_{10} \left(x_1 + x_2 + \cdots + x_{10}\right)^2 .$$

Check your numerical answer against the analytic one, 155/16.

(1) Conduct 16 trials and take the average as your answer.

(2) Try sample sizes of N=1, 4, 8, ..., 8192.

(3) Plot the relative error vs. 1/sqrt(N) and see if linear behavior occurs.

(4) What is your estimate for the accuracy of the integration.