

COMPUTATIONAL PHYSICS

Bonus: HOMEWORK #7

Numerical Methods for Physics , chapters 10 & 11

1. Perform the following integration (appears in the *Voigt* profile calculation)

$$I = \int_a^b \frac{e^{-y^2}}{c + y^2} dy$$

for $a = -10$, $b = 10$ and $c = 10^{-3}$. Use the trapezoidal method with bins of decreasing sizes $h_n = (b - a)/2^n$, and calculate $I(h_n)$. Plot $I(h_n)$ vs. n . How large does n needs to be for the integral to converge? Explain the reason for this value of n . Now use the Romberg integration method. How large is the required n with this method, in order to reach the same accuracy?

2. A Monte-Carlo calculation of π . Use a random number generator to generate N points which are randomly scattered in the $X - Y$ plain between 0 and 1, in both axis. Count the number of points which satisfy $x^2 + y^2 < 1$, and use this fraction to estimate π . Make a plot of the log of the absolute value of the relative error in the derived value of π versus $\log N$. Use $N = 10^n$, for $n = 1, 2, 3, 4, 5, 6$. Explain the slope you find. Repeat the above calculation of π , now use evenly spaced points in both axis. Say $x_i = (i - 0.5) \times 1/M$ and $y_j = (j - 0.5) \times 1/M$, for $i, j = 1 - M$, i.e. using $N = M^2$ points. Again, make a similar plot of the error vs. N . Compare the accuracy of the two methods. Explain the results.
3. A numerical experiment derivation of the Maxwell-Boltzmann distribution. Select N particles. Assume all particles have the same initial velocity $v = 1$. Use a random number generator to assign a random direction for \vec{v} of each particle. Assume an even distribution over a sphere, i.e. $\phi = 0 - 2\pi$ and $\cos \theta = -1 - 1$. Pick randomly two particles with \vec{v}_i , \vec{v}_j from the N particles you prepared. Find their centre of mass velocity v_{CM} . Transform their velocities to the CM frame, and assume the velocities are conserved in magnitude, but redirected randomly following a collision, i.e pick a new random direction for the velocity of one of the particles (the other particles goes in the opposite direction, to keep a total momentum of zero). Transform the new velocities back to the lab frame, and update the velocities of the two particles. Repeat the collisions M times, and make a histogram of the the derived velocity distribution. Increase M until the distribution appears to reach a steady state. Compare to the Maxwell-Boltzmann distribution.

Please include a listing of your code.

Please submit in writing by February 15th, 2018.

Behatzlacha!