

Chem. 550  
Instructor: Nancy Makri

## MONTE CARLO – COMPUTER ASSIGNMENT 2

Write a symbolic algebra program that performs a Metropolis Monte Carlo random walk to evaluate integrals of the type

$$J = \int dx \rho(x) f(x)$$

where  $\rho$  is a *normalized* sampling function. Use your code to evaluate the integral

$$J = \int dx e^{-x^2} x^2 .$$

Note that you need to identify a normalized sampling function before proceeding. Report the results of your calculation for random walks of length  $10^3$ ,  $10^5$ ,  $10^7$  and compare to the analytical result.

The algorithm you developed can be used for any number integration variables.