JT305 Advanced Computational Methods:
Monte Carlo Methods in Statistical Mechanics

Exercise 1

Calculation of π: *Consider a circle of diameter d surrounded by a square of length l ($l \geq d$). Random coordinates within the square are generated. The value of π can be calculated from the fraction of points that fall within the circle.*

1. *Write a program to implement the linear congruential pseudo random number generator,*

$$R_{i+1} = [a \times R_i + b](mod m)$$

where a, b and m are integers, and the recursion is initiated by an arbitrary integer R_0. (a) Explore how the choice of a, b and m affects the correlation between random numbers, defined as

$$C(i) = < R_k R_{k+i} >_k - < R >^2$$

where the averaging is done over a time series of random numbers generated. (b) Does the sequence of random numbers repeat itself? After how many steps? (c) How can you use the random number generator above, to produce real random numbers between 0 and 1? (d) Make normalized histograms of the random numbers for different numbers of random numbers generated. You should in principle get a uniform distribution. (e) Evaluate the deviation from a uniform distribution by calculating the squared difference of the obtained distribution from the expected distribution, for different numbers of random numbers generated. How does the deviation vary with the number of generated random numbers? Make a plot and analyze.

2. *How can π be calculated from the fraction of points that fall in the circle? Remark: the "exact" value of π can be computed numerically using $\pi = 4 \times arctan(1)$.*

3. *Write a small Monte Carlo program to calculate π using this method.*

4. *How does the accuracy of the result depend the number of generated coordinates? Make a plot of the squared difference between the estimated value and the exact value vs. number of coordinates generated after averaging the squared difference over a number of trial sequences.*

5. *Is this an efficient method for computing π accurately?*