Heinrich-Heine-Universität Düsseldorf Institut für Theoretische Physik II Computational Physics Wintersemester 2018/2019 Prof. Dr. J. Horbach M. Eshraghi (mojtaba.eshraghi@hhu.de) M. Golkia (mehrdad.golkia@hhu.de) Blatt 9 vom 11.12.2018 Abgabe bis 16:00 Uhr am 18.12.2018

## Problem 9.1: Monte-Carlo Integration

Integrals can be computed using the Monte-Carlo method. Here in this exercise we calculate the area of a circle in 2D. Consider a circle of radius r=0.5 embedded in a square of length l=1. The constant  $\pi$  is equal to the ratio between the area of the circle  $A_c$  and the area of the square  $A_c$ 

$$\frac{A_c}{A_s} = \frac{\pi}{4} \tag{1}$$

The ratio in Eq. (1) can be approximated by sampling uniformly distributed random points (x, y) in the square,  $x \in [-0.5, 0.5]$  and  $y \in [-0.5, 0.5]$ , using the equation

$$\frac{A_c}{A_s} = \frac{N_c}{N} \,, \tag{2}$$

where N and  $N_c$  correspond to the total number of sampling points and the number of points inside the circle, respectively. A trial point contribute to  $N_c$  if  $x^2 + y^2 < r^2$  with r = 0.5.

- a) Plot the value of the estimated  $\pi$  as a function of N; try  $N=10,\ N=100,\ N=1000,$  and N=10000.
- b) Repeat a), but now using the Markov chain sampling.
- c) Find the optimum value of the maximum number displacement  $\delta$ , i.e. the value of  $\delta$  for which the convergence is faster (see lecture for a definition of  $\delta$ ).

<u>Hints</u>: To generate uniform random numbers  $u_n \in [0,1]$  can use the recursive equation

$$x_n = \operatorname{mod}(a \cdot x_{n-1}, b)$$
$$u_n = \frac{x_n}{c} ,$$

with a = 16807, b = 2147483648, c = b + 1 and  $x_0 \in [0, 1]$ .

## <u>Problem 9.2</u>: The volume of a hyper-sphere

The shape of a circle (defined in 2D by  $x^2 + y^2 < R^2$ ) can be generalized to three dimensions by  $x^2 + y^2 + z^2 < R^2$  (referred to as sphere). One can continue the generalization to higher dimensions although they are difficult to imagine.

- a) Find, in the literature, the general definition of a sphere in n-dimensions.
- b) By extending your code Exercise 9.1, find the volume of a sphere in 5 dimensions.