Exercise 5 Sthavishtha Bhopalam Rajakumar November 28, 2017

1 Introduction

The objective of the current exercise is to implement Monte Carlo method to compute the mean distance between the hard spheres (or particles) in a box [1]. It is shown that this method greatly simplifies the computation of high dimensional integrals, which makes it reliable for such cases.

2 Algorithm Description

The algorithm for this implementation is illustrated here :

1. Choose the position of each particle randomly
2. Check the following conditions before proceeding (Else go back to Step 1) :
   - If the position of the particle lies in the range $[R, L - R]$
   - If the distance between each particle is more than $2R$ (incorporated by the `accept_chk` function in the code)
3. Repeat the above steps for M configurations and n particles

3 Results and Discussions

The Figure 1 appropriately depicts the variation of `d_{mean}` with the number of configurations M for a particular case (number of particles taken to be 10). It can be clearly seen that a large number of configurations (M) is necessary to attain the required convergence level. However, the minimum M to attain convergence diminishes as the number of particles increases (evident from Figure 2). In the Figure 2, the number n of the particles is varied along with the volume fraction [1]. It can also be seen that the average distance between the particles also decreases as the number of particles decreases (as seen from 3). This clearly shows that as the number of particles n increases (and the volume fraction subsequently), the dimensionality of the integral also improves, making Monte Carlo method to be accurate (as the accuracy of Monte Carlo method is inversely proportional to the square root of n).

References

[1] Hans Hermann. Lecture notes on introduction to computational physics. Institute for Building Materials, ETH Zürich, 2017.

[1] For the current case, the volume fraction has been limited only upto 0.00418. For larger volume fractions, a much efficient Monte Carlo algorithm is necessary due to excessive computational expenses.

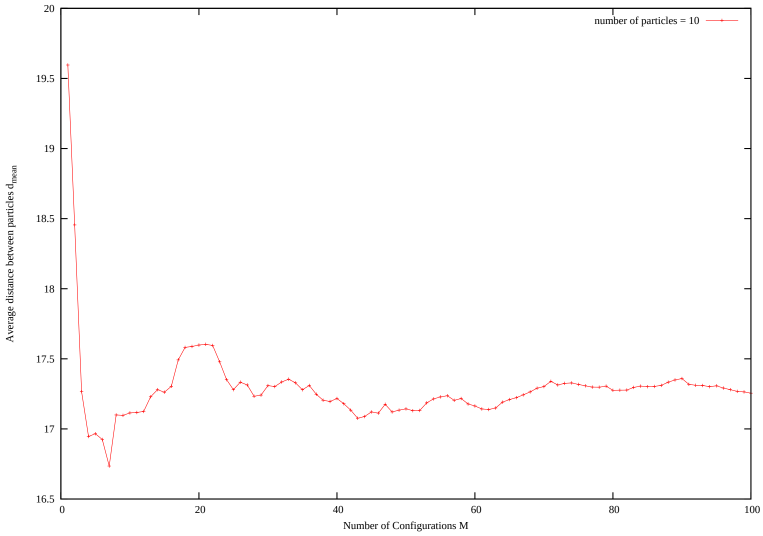

Figure 1: Mean diameter vs number of configurations for $n = 10$

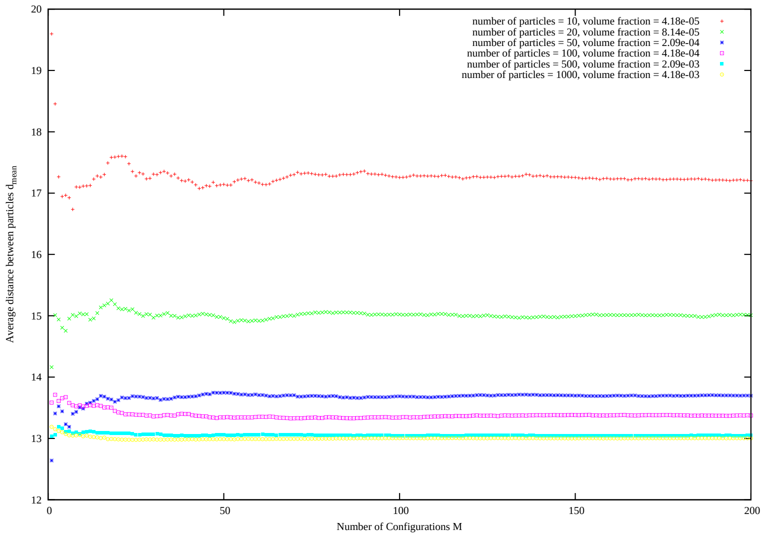

Figure 2: Mean diameter vs number of configurations for various volume fractions

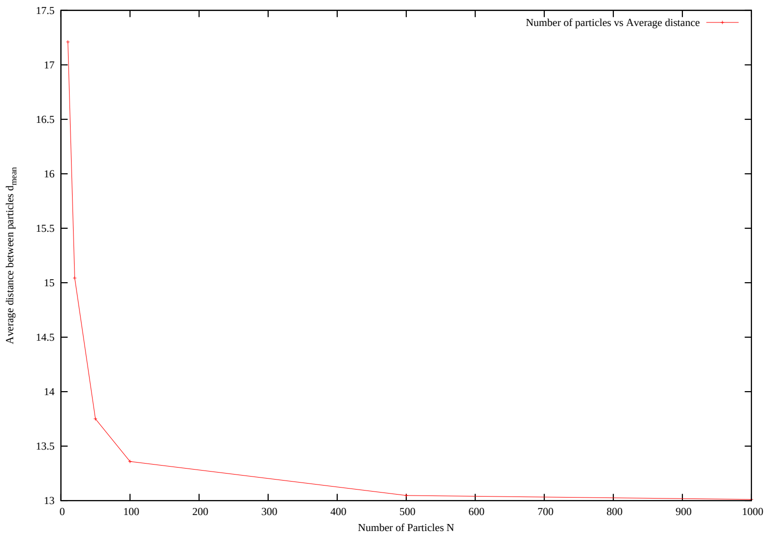

Figure 3: Mean diameter vs the number of particles