

Internship Report

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1 Introduction

This report summarises in brief, the work that was carried out as a part of my summer internship at the *University of Luxembourg*, during May-July 2016.

The topic of the internship was the study of jamming in sphereocylinders with helical charge distribution, mainly the jamming density. A considerable amount of time was also dedicated to make the contemporary code bug-free and tweaking it so as to have a faster program.

For the most part during the internship, the parameters *pressure*, *charge per rod* and *salt concentration* were varied so as to study their impact on the jamming densities. The system used for these simulations consisted of 2116 rods, which was large enough to guarantee that there are enough rods (more than 2) along each dimension of the box, so that the assumed periodicity is valid.

2 Observations

For a given set of parameters, the system was compressed from the isotropic low density phase, until there was no appreciable increase in the density. At this point, the density was noted and plotted.

2.1 Pressure Variation

Five values of pressure were chosen, 50, 100, 200, 300, 500. The density curves are plotted below.

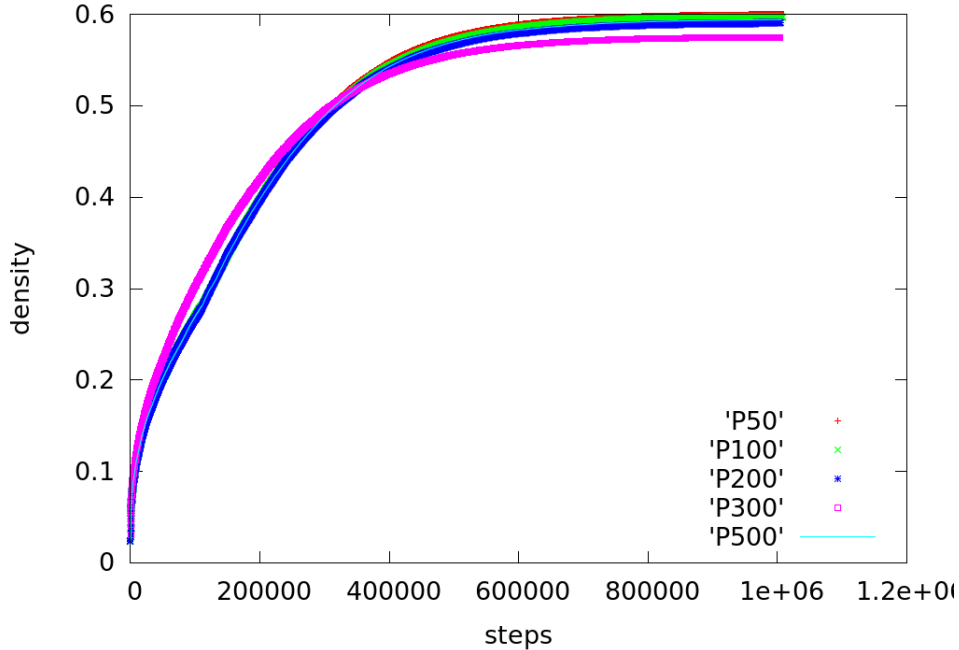


Figure 1: Variation of density with pressure

Z	SaltC	Pressure	Jamming density
300	0	50	0.59977
300	0	100	0.59734
300	0	200	0.59055
300	0	300	0.57495
300	0	500	0.59405

For a set of particular parameters above, 3 runs of simulations were made, but the deviation amongst these runs was high enough to demand a much larger number of runs. More runs were not made due to lack of time.

2.2 Charge per rod variation

Five values of charge per rod were chosen, 100, 200, 300, 400, 500. The density curves are plotted below.

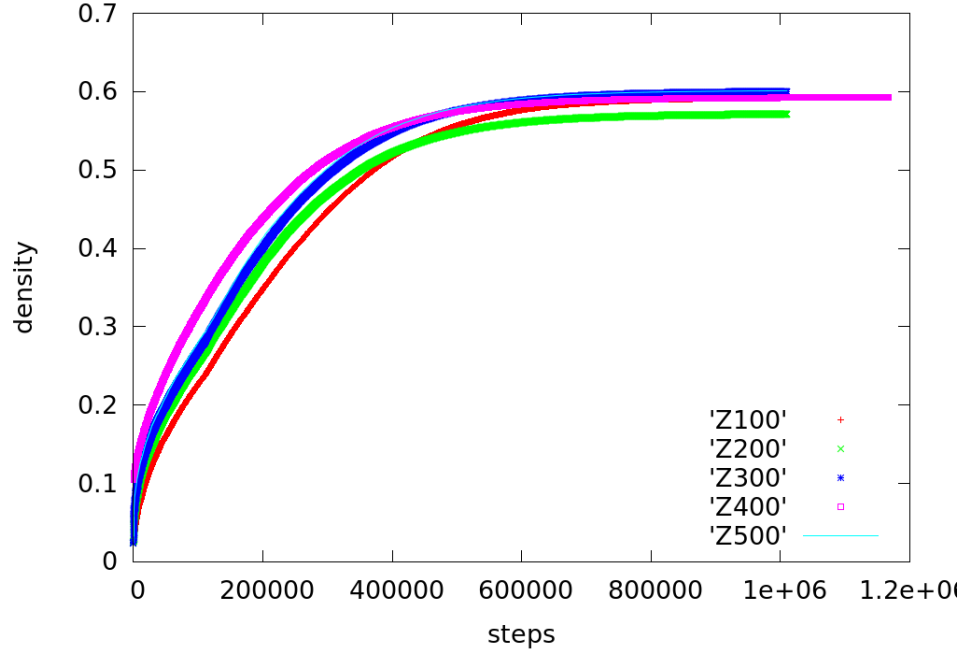


Figure 2: Variation of density with charge per rod

Z	SaltC	Pressure	Jamming density
100	0	50	0.592389
200	0	50	0.57108
300	0	50	0.599766
400	0	50	0.592584
500	0	50	0.60117

For a set of particular parameters above, 3 runs of simulations were made, but the deviation amongst these runs was high enough to demand a much larger number of runs. More runs were not made due to lack of time.

2.3 Salt concentration variation

Five values of salt concentration were used, 0.0, 2.0, 4.0, 6.0, 8.0. The density curves are plotted below.

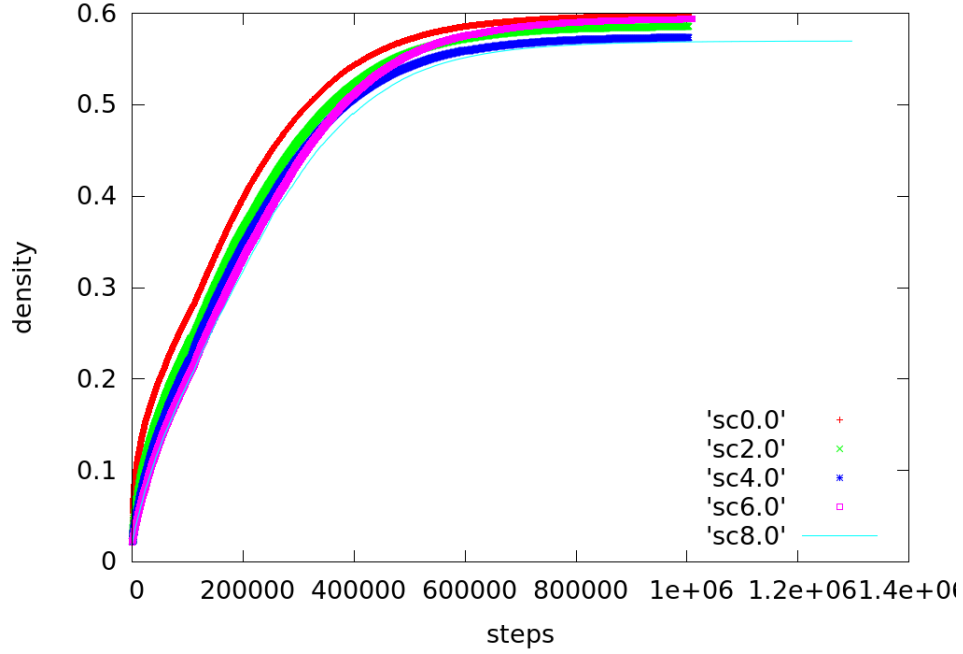


Figure 3: Variation of density with salt concentration

Z	SaltC	Pressure	Jamming density
300	0.0	100	0.59734
300	2.0	100	0.58559
300	4.0	100	0.57337
300	6.0	100	0.59354
300	8.0	100	0.56959

For a set of particular parameters above, 3 runs of simulations were made, but the deviation amongst these runs was high enough to demand a much larger number of runs. More runs were not made due to lack of time.

3 Study of clusters

In the simulations that were carried out, it was almost always observed that the final jammed configuration of rods comes in the form of clusters of rods, with rods of same cluster pointing in the same direction. A sample snapshot is added below. An effort was made to tweak the program so that it calculates the cluster sizes. In the infile, I have introduced two parameters, namely *Distance* and *MinScalPro*.

Distance is the minimum distance at which two rods have to be, to be called as neighbours and *MinScalPro* is the minimum dot product of the orientations of the two rods, above which they will be counted as having the same orientation (ranges from 0 to 1).

It turns out that the number of clusters counted, and the cluster size distribution is very sensitive to the parameters *Distance* and *MinScalPro*. These parameters should be changed according to the definition of the user's perception of a cluster.

Since its difficult to tell whether the outcome of the program is correct or not just by looking at a snapshot of rods, further work in this field was not carried out, due to lack to time. Though it would be really great if one can find out the correct set of values for the parameters *Distance* and *MinScalPro* to get correct cluster size distributions.

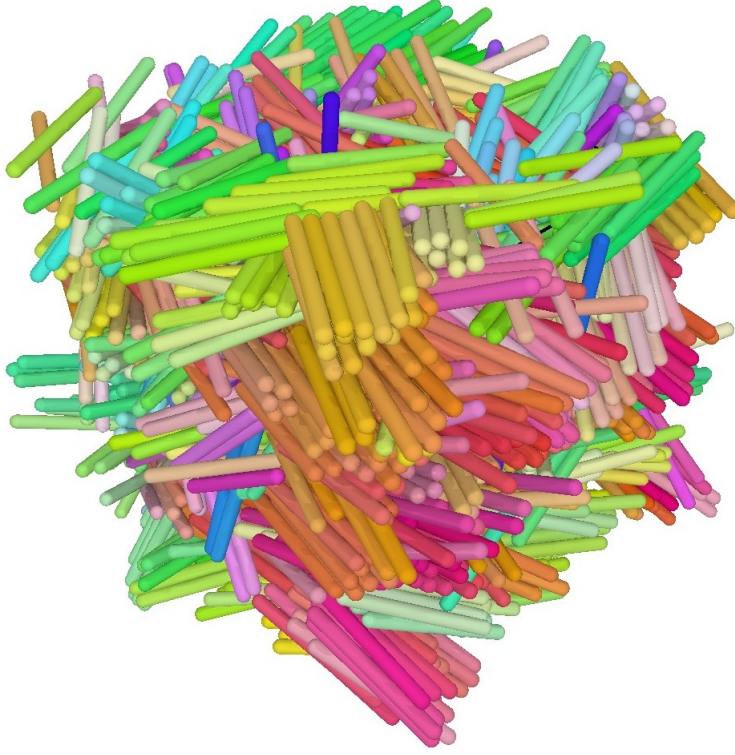


Figure 4: Formation of clusters in the jammed phase.

4 Conclusion

As far as the results of this project are concerned, we can see that there doesn't appear to be much impact on the final jamming density by the variation of *pressure*, *salt concentration* or *charge per rod*. Then again, to be completely sure, more amount of runs must be simulated so as to have a clear statistical picture.

As far as the study of clusters is concerned, due to the very sensitive nature of the program to the parameters *Distance* and *MinScalPro*, one needs to try out various sets of these parameters and determine the appropriate values of both these parameters.