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Master Thesis

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Abstract

A raw writing of hard sphere nucleation, a simulation to measure quantiteis, and a analysis of data generate by means of the simulation.

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1 Theory

1.1 Theory and Background

1.1.1 Hard sphere system

Explain the Hard sphere system and the first predictions of the phase transition

1.1.2 metastable fluid/ phase diagram

maybe include disperisty of radii

1.1.3 Classical nucleation theory :/

Estimate of r_{crit} by Δ_μ
SOmehow this wshould be doable ;)

1.1.4 Computer Precision

Explain a little about what numerics does, compared to the real world.
Maybe include the time evolution of minimal changes

1.1.5 Comparsion to Real world experiments

Compare, regadring the solvent. Esspeically with Hajos finding.

2 Simulation details

2.1 Simulation

2.1.1 Algorithm explanation

Explain the EDMD algorithm

2.1.2 Simulation

Add Details of for example FEL, and backupevent handling, double time precision, reset sim

2.1.3 Estimate of calculation times

GIve some profiling numbers of the simulation Also conclude that missing q6q6 O(N^2), broke the walltime.

2.1.4 Produced Data

Overview of produced data with visualized snapshot?

3 Data Analysis

3.1 Data analysis

This is the analysis part

3.1.1 Diffusion of the lqiuid

This contain analysis of diffusion in the liquid to prove the simulations accuray

3.1.2 Diffusion of the metastable liquid

This contains Diffusion constants to normalize the rates

3.1.3 Cluster growth

Cluster growth depending on density

3.1.4 ToG

Well only swamp here, but it can be shown to conclude the swamp.

3.1.5 ACF largest cluster?

Just in case anything can be seen here

3.1.6 Induction time dilemma

Evaluation of induction time. Prolem with accuracy and precision. Compare methods.

3.1.7 Induction time by exponential distribution

Obtain exp assumption and best estimator

3.1.8 Nucleation rate comparison

All Nucleation rates that can be found.-> mayhap ask Hajo.

3.1.9 Memory Kernels

Memory kernels of systems at various densities. Depends strongly on what is found here

4 Conclusion - Summary

4.1 Conclusion

.1 appendix a