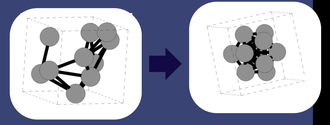
EVALUATING DIFFERENT CROSSOVER, INITIALIZATION STRATEGIES FOR GENETIC ALGORITHMS OPTIMIZING LENNARD JONES CLUSTERS

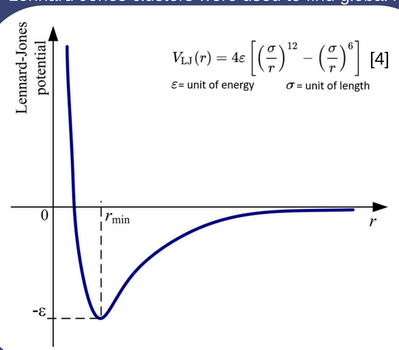
AUTHOR

Student: Emīls Dzintars
Supervisors: Peter A.N. Bosman, Anton Bouter, Vanessa Volz

INTRODUCTION

- Finding stable materials in material science provides big breakthroughs and helps advance other fields further, but it is proven to be NP-Hard problem
- Lennard Jones clusters were used to find global minimum





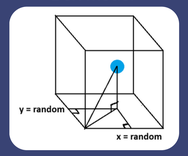
- All the experiments were done in python using Atomic Simulation Environment library

RESEARCH QUESTION

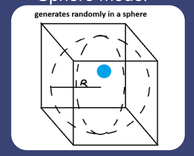
What is the difference in run time between genetic algorithms with different crossover, initialization strategies optimizing lennard jones clusters?

INITIALIZATION METHODS

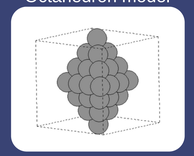
Box model



Sphere model

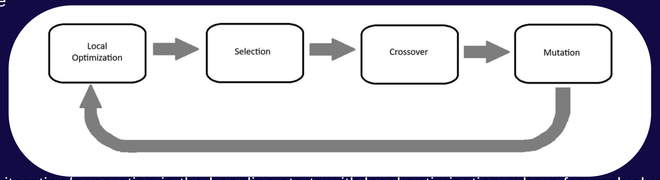


Octahedron model



BASELINE GENETIC ALGORITHM

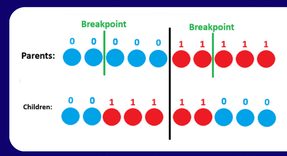
Our group collaborated to create baseline genetic algorithm and later on our own compare the results of our individual changes to baseline



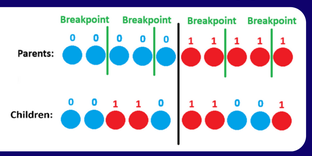
- Every iteration/generation in the baseline starts with local optimization, where for each cluster algorithm finds local minimum.
- In selection algorithm selects two parents with best fitness function
- Using two parents we create new generation using plane cut splice crossover
- After crossover each cluster has chance to mutate (twist mutation (20%), displacement(10%), etching(5%))
- At the end of the current itaration algorithm checks if stopping criteria is not satisfied and moves to the next iteration

CROSSOVER METHODS

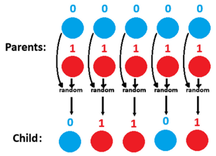
One point Crossover[1]



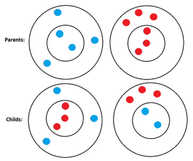
Two point Crossover[5]



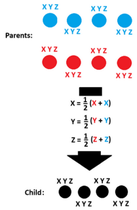
Uniform Crossover[3]



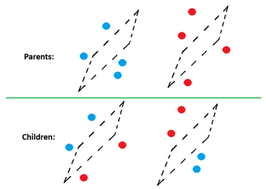
Sphere cut Crossover[3]



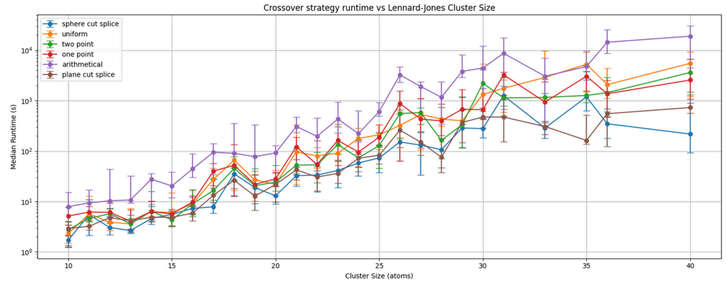
Arithmetical Crossover[3]

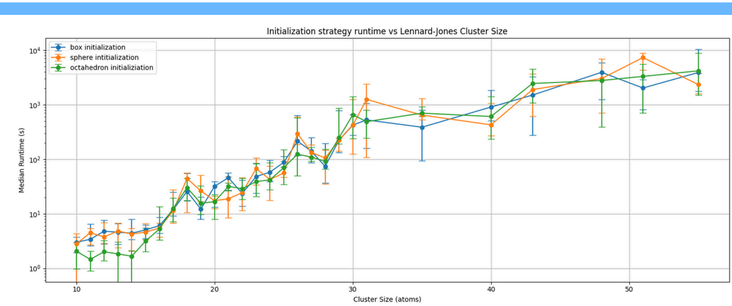


Plane cut Crossover[3]



RESULTS





CONCLUSION

- Arithmetical crossover performed the worst.
- It is inconclusive, which crossover was the best.
- Octahedron Initialization was the best choice for clusters 10-14.
- Possible improvements: introduce multi-threading, not skipping clusters, increasing amount of runs per configuration, using more powerful hardware, study more variables (population size, mutation, selection strategies , etc.)

[1] David E. Goldberg. Genetic Algorithms in Search,Optimization, and Machine Learning. Addison-Wesley, Reading, Massachusetts, 1989.
[2] Roy L. Johnston. Evolving better nanoparticles:Genetic algorithms for optimising cluster geometries. Dalton Transactions, pages 4193–4207,2003. Received 21st May 2003, Accepted 15th August 2003, First published online 1st September 2003.
[3] Frederico T. Silva, Mateus X. Silva, and Jadson C. Belchior. A new genetic algorithm approach ap-plied to atomic and molecular cluster studies. Frontiers in Chemistry, 7:707, 2019. Published: 05 November 2019.
[4] LibreTexts. Lennard-jones potential. Accessed: 2025-05-22.