Analyzing The Impact of Mutations on Genetic Algorithms for Finding the Lowest Energy Structure of Atomic Clusters

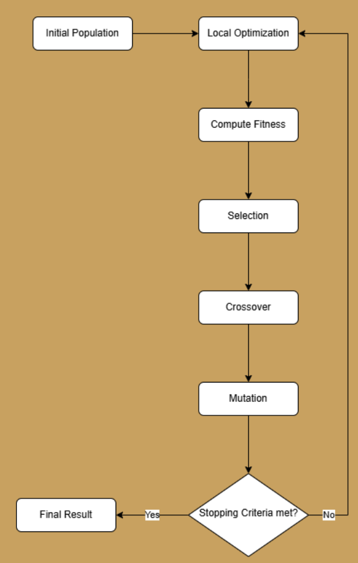
1. Introduction

- A cluster of atoms is a finite group of atoms bound together by physical or chemical forces.
- Based on the positions and types of these atoms we can compute the potential energy of a cluster
- Finding the lowest-energy structure of a cluster of atoms is a proven NP-Hard problem [1] that has important implications in the field of materials science
- An efficient way of solving this problem could help with discovering new materials with potential applications in areas such as biomedical imaging [2], semiconductor development [3], and aerospace engineering [4]
- Methods of solving: Simulated Annealing, Basin Hopping, **Genetic Algorithms (GA)**
- GA solutions are very varied and employ a multitude of different mutation operations
- We do not know the impact and effectiveness of each individual mutation

2. Research Question

"What is the best mutation operation for a genetic algorithm finding the lowest-energy structure of a cluster of atoms in terms of how often and how fast it finds the global minimum?"

3. Methodology



- Start from a simple implementation of a GA that can solve the problem on small clusters and experiment on different mutations
- Local Optimizer: BFGS
- Lennard-Jones Potential is used to compute the energy of the cluster (Fitness Function)
- Crossover: Cut-and-Splice
- Stopping criteria: global minimum reached / 100 iterations reached / no improvement in past 10 iterations

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

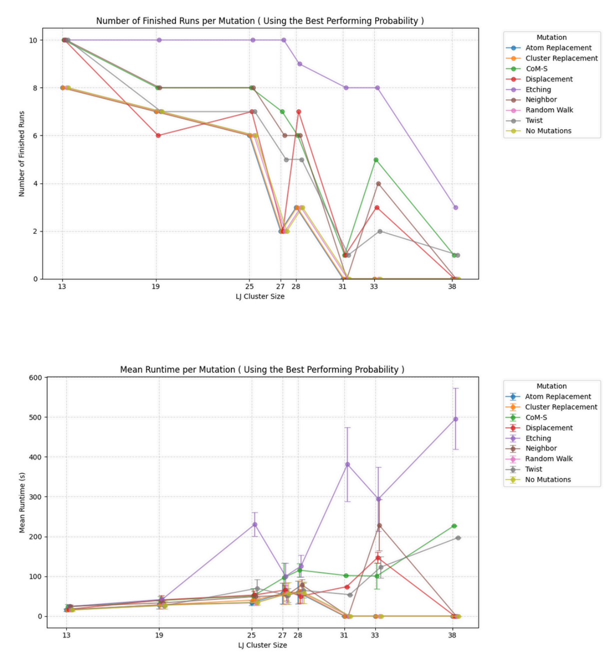
The following mutations have been compared:

- Atom Replacement
- Cluster Replacement
- Center of Mass Spherical (CoM-S)
- Random Displacement
- Etching
- Neighbor
- Random Walk
- Twist

- Mutations evaluated based on accuracy (number of finished runs finding global minimum) and speed (runtime)
- Each mutation is benchmarked with multiple probabilities ranging from 0.005 to 0.3
- Experiments are ran on clusters with 13, 19, 25, 27, 28, 31 and 38 atoms
- Experiments are ran using population sizes of 8, 15 and 20
- Each experiment is ran 10 times in order to get an average value of the time to converge

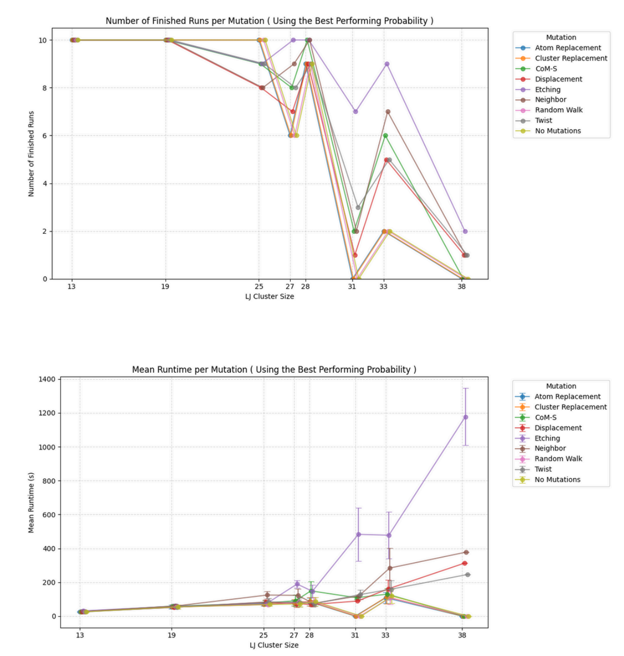
4. Results

- **Population 8**



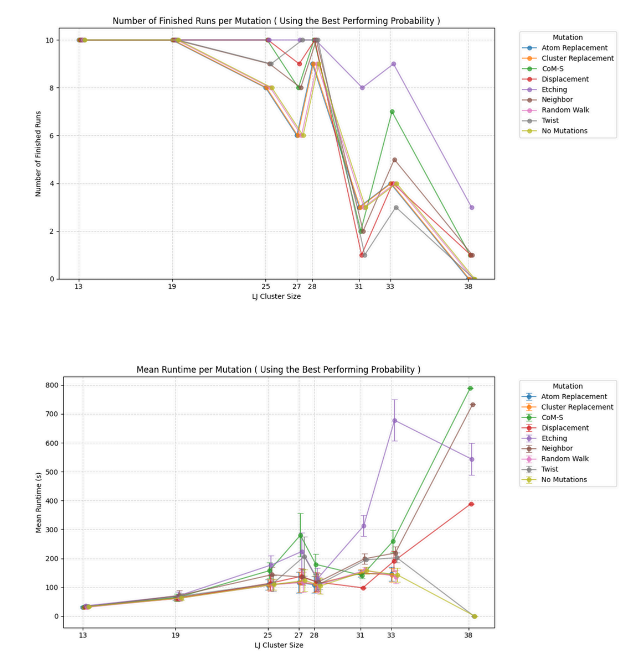
- Etching performs best in terms of finding global minimum, but is the slowest
- CoM-S and Neighbor have slightly lower accuracy
- Random Displacement and Twist even lower accuracy
- CoM-S, Neighbor, Random Displacement and Twist perform similarly in terms of runtime
- Atom / Cluster Replacement and Random Walk perform the same as using no mutations

- **Population 15**



- Etching still the best performer in terms of accuracy
- CoM-S, Neighbor, Random Displacement and Twist have very similar accuracy and runtimes
- Random Displacement and Twist seem to have more stable runtimes

- **Population 20**



- Random Displacement seems to benefit from higher populations
- Runtime of Etching appears much closer to the others

5. Conclusions

- **Atom Replacement, Cluster Replacement and Random Walk do not bring any improvements to the GA**
- **Etching performs best in terms of accuracy**
- **Random Displacement and Twist perform best in terms of convergence time**
- **CoM-S and Neighbor also fast, but more unstable**
- **It is suggested that future GA's use a combination of Etching and other fast converging mutations**

6. Future Work

- **Can Etching be improved with a different local optimizer?**
- **Do our results translate to larger clusters / population sizes or different fitness functions?**
- **How well do hybrid mutations strategies (containing multiple types of mutations) perform?**

References

[1] L. T. Wille and J. Vennik. "Computational complexity of the ground-state determination of atomic clusters". In: Journal of Physics A: Mathematical and General 18.8 (1985), pp. L419–L422.
[2] Sanne M. van de Looij et al. "Gold Nanoclusters: Imaging, Therapy, and Theranostic Roles in Biomedical Applications". In: Bioconjugate Chemistry 33.1 (2022). PMID: 34894666, pp. 4–23.
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[4] Abhishek K. Pathak and Sanjay R. Dhakate. "Carbon Nanomaterial-Carbon Fiber Hybrid Composite for Lightweight Structural Composites in the Aerospace Industry: Synthesis, Processing, and Properties". In: Advanced Composites in Aerospace Engineering Applications. Ed. by Norkhairunnisa Mazlan, S.M. Sapuan, and R.A. Ilyas. Cham: Springer International Publishing, 2022, pp. 445–470.

Authors Stefan Bud sbud@tudelft.nl

Responsible Professors Peter Bosman, Anton Bouter, Vanessa Volz

TU Delft