Dynamic Mutation Rate Control for the Genetic Algorithm for Global Geometry Optimization

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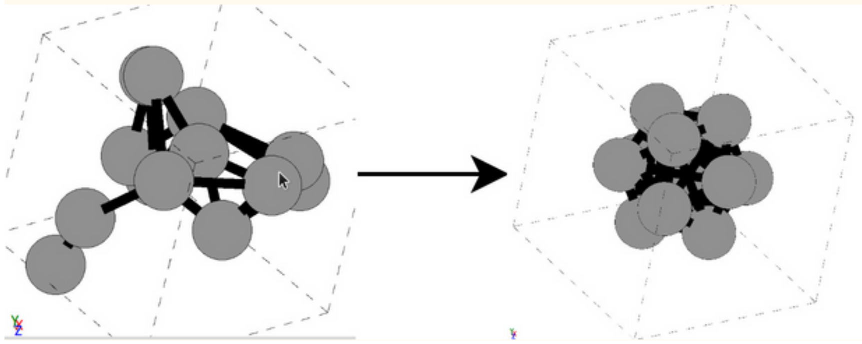
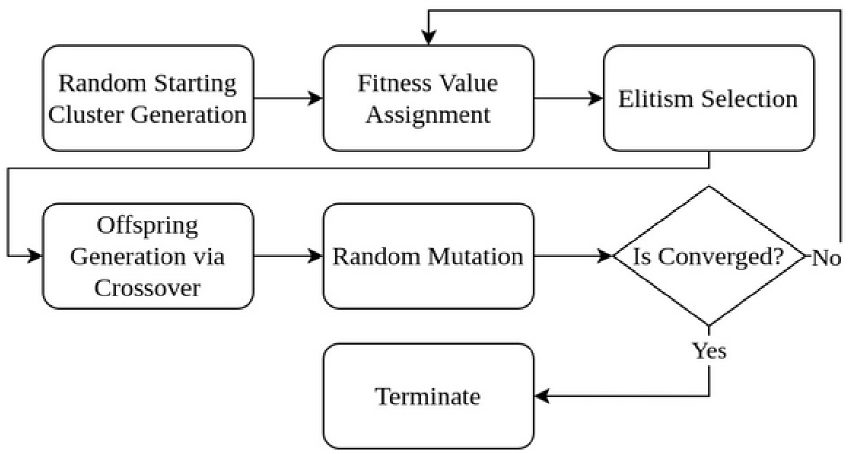
1. Global Geometry Optimization

Given a certain cluster of atoms this is the task of finding an arrangement of them that minimizes their interactions.
Modeled here using Lennard-Jones potential



2. Genetic Algorithm

Optimising a solution using genetic evolutionary principles. In this GA, local optimisation is applied to clusters after mutation. The algorithm used for this is BFGS



3. Adaptation Strategies

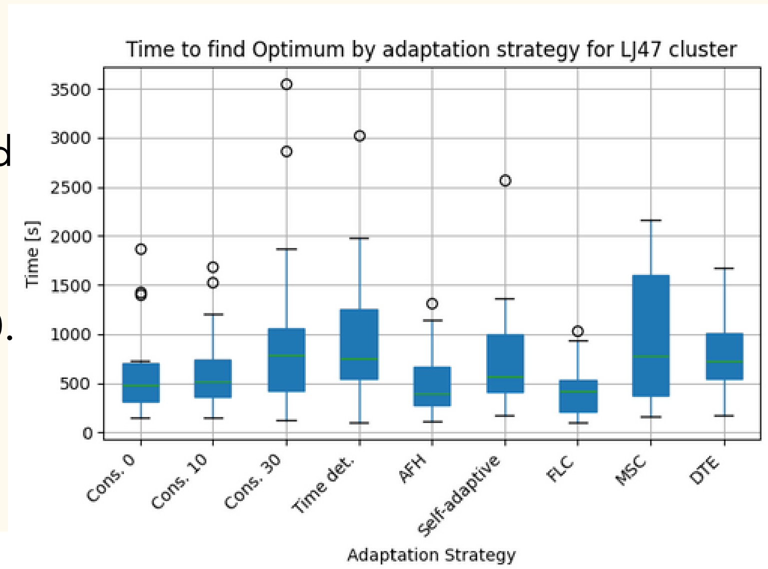
The mutation control strategies considered for this research were:

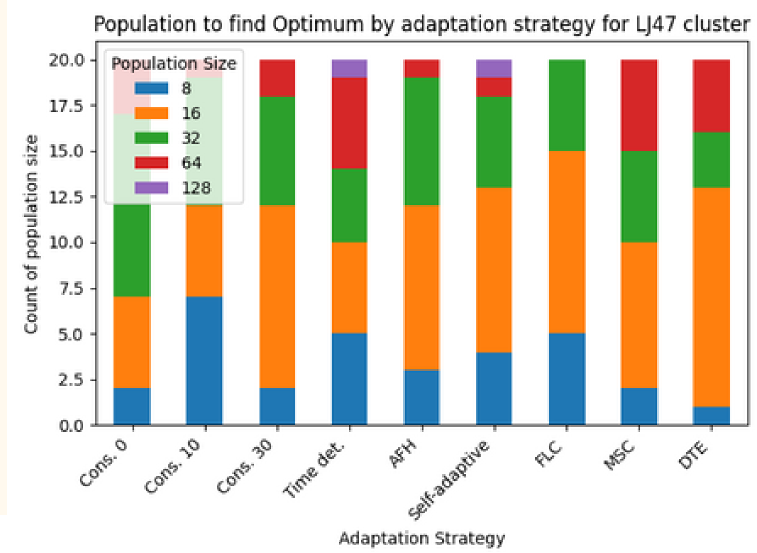
- Constant 0%
- Constant 10%
- Constant 30%
- Time Deterministic
- Average Frequency Heuristic (AFH)
- Self-adaptive
- Fuzzy-Logic Controller (FLC)
- Mutation Success Condition (MSC)
- Distance to Estimation (DTE)

4. Methodology and Results

Results presented here are for clusters of 47 carbon atoms. A run was done until the algorithm converged or found the globally optimum solution. If it didn't find the optimum, then the population was doubled and the experiment was repeated, up to a maximum population of 128. All experiments were run 20 times to reduce variance.

The best performing algorithm was AFH. AFH, self-adaptive and FLC usually outperformed both Const 10 and Const 30. Their average performance was better.





5. Conclusions and Future Work

Use of local optimisation makes results very varied and hard to draw statistically significant conclusions.
Future Work should could include:

- Investigating effects of local optimisation on performance
- Adapting other parameters
- Individually controlling mutation rates of different operators
- Developing real-world testing methodologies