Parallel Genetic Algorithms for the Structural Characterisation of Nanoalloys

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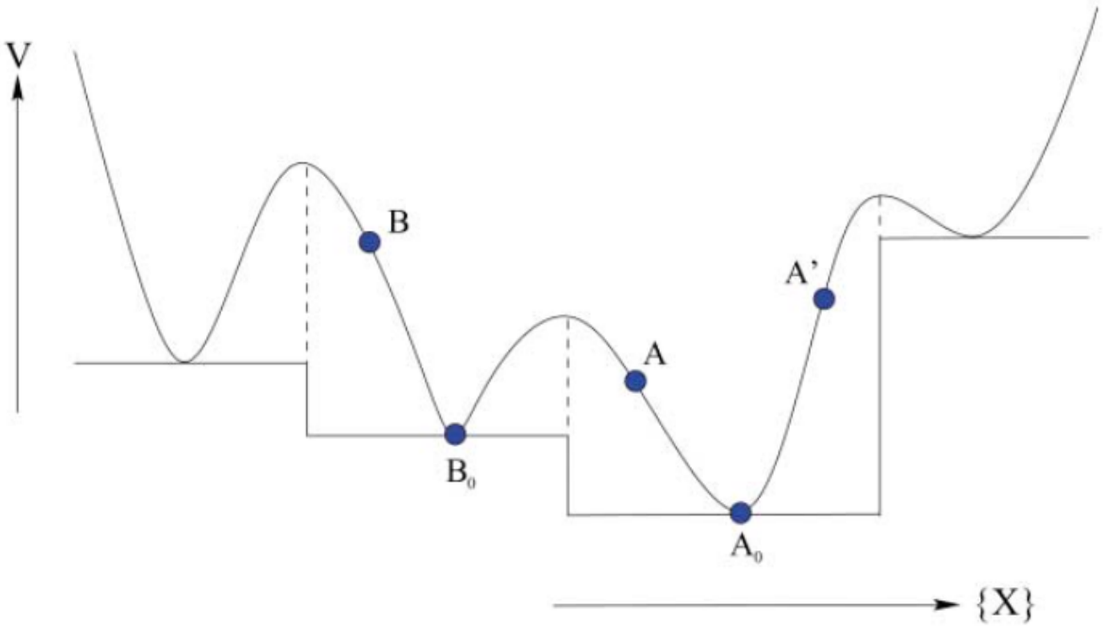
Birmingham Cluster Genetic Algorithm

- The Birmingham Cluster Genetic Algorithm (BCGA) is a genetic algorithm for the structural characterisation of nanoalloys.

- A GA is search method based on the principles of natural selection, sharing key terminology - Generation, Mutation, offspring etc.

- The BCGA includes local minimisation with each step - simplifying the search.



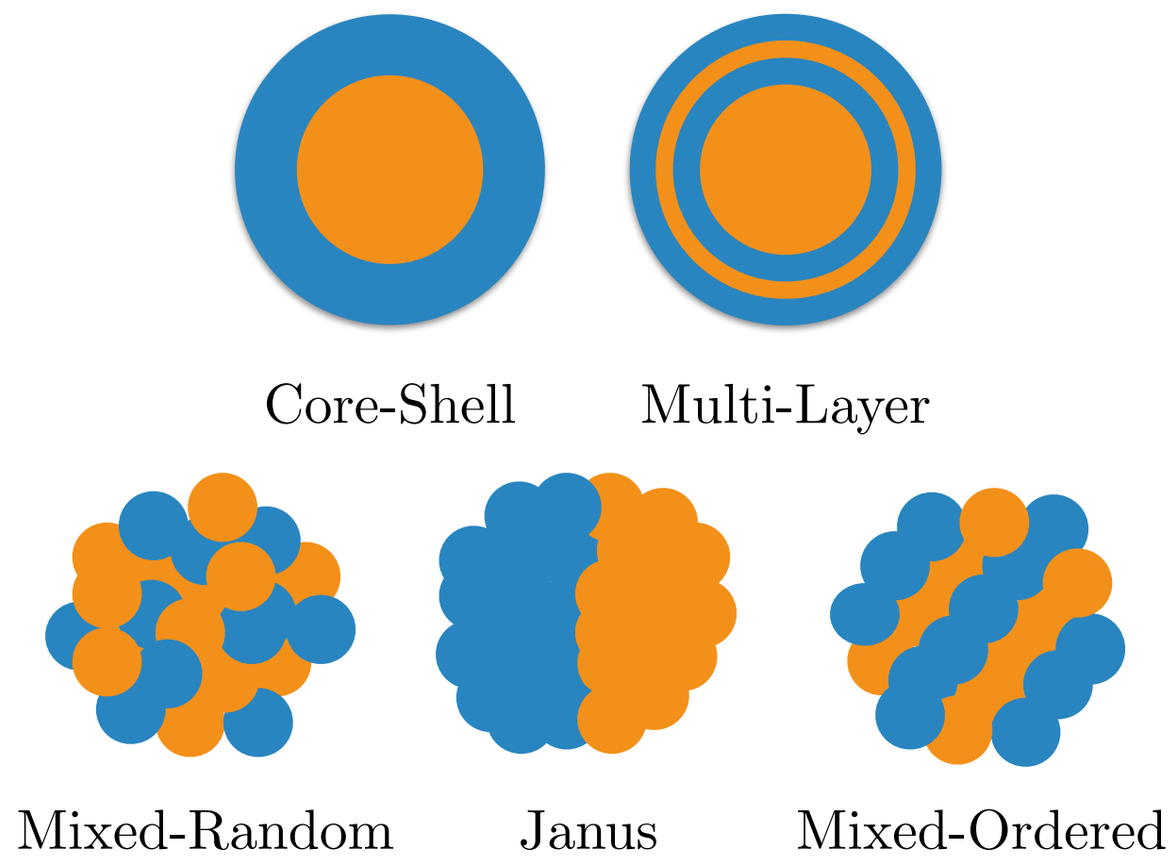
"Stepped Surface"

Nanoalloys

- Metallic nanoparticles composed of two or more metallic elements.

- Potential optical, electronic and catalytic applications.

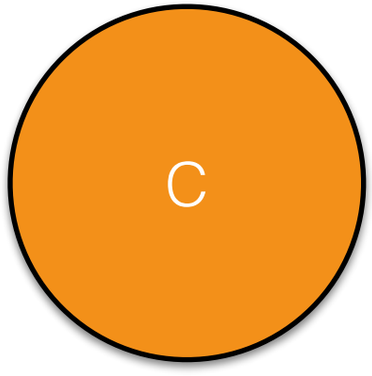
- Structural characterisation is an essential step towards understanding these properties.



Operations

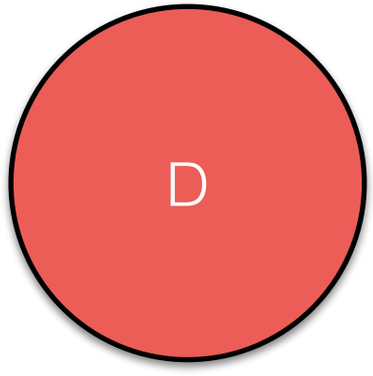
Daven and Ho Crossover

Mutation



Random new geometry

Atom Swap



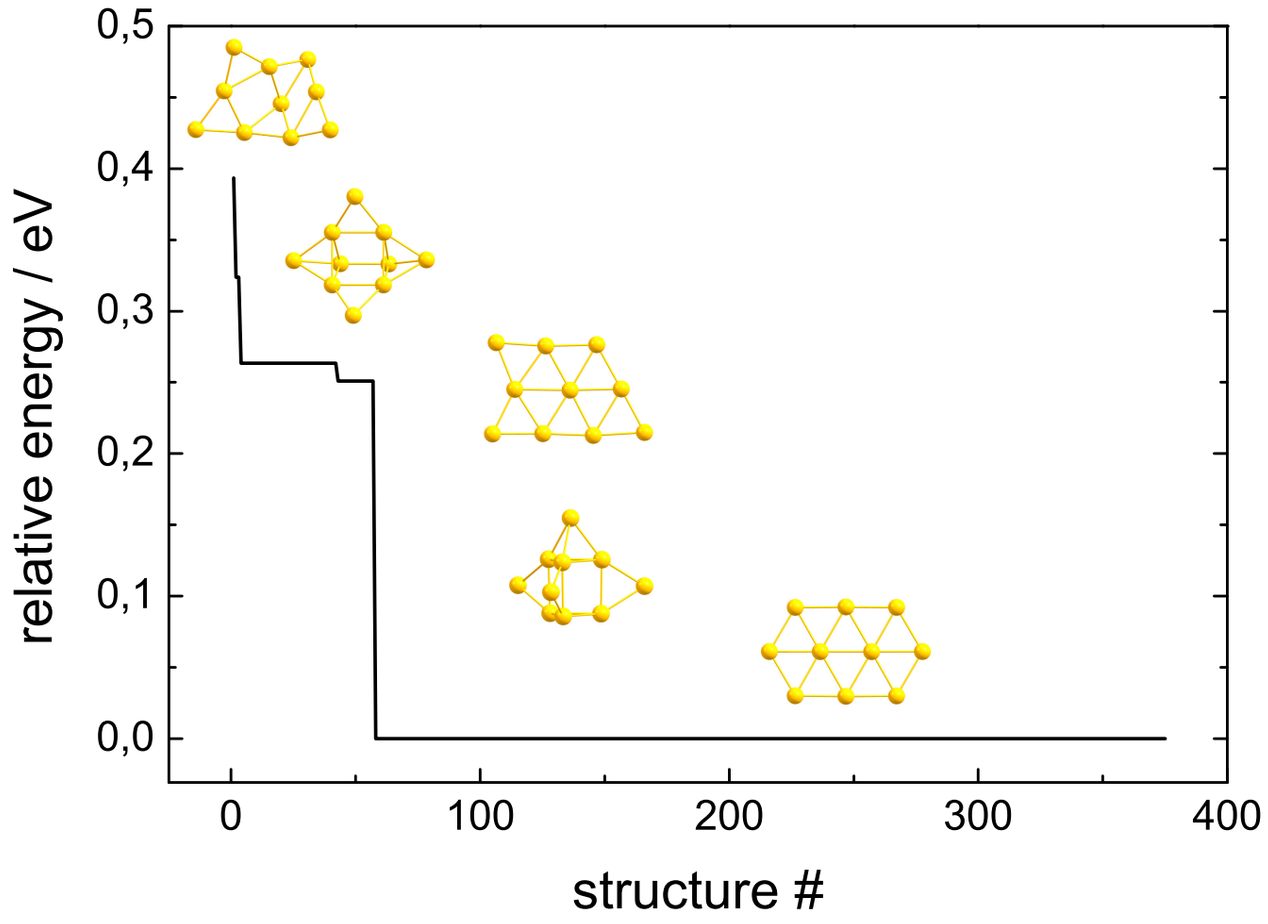
Displace

BCGA-DFT

- Local minimisation carried out directly at the density functional theory level.

- Allows the BCGA to capture size-specific effects commonly seen in small clusters, otherwise missed with potentials.

- Hugely expensive, only possibly for 10 atom or less sized clusters.



Parallelisation

- How can we study larger clusters?

- The BCGA is intrinsically parallelisable as local minimisations have no interdependence.

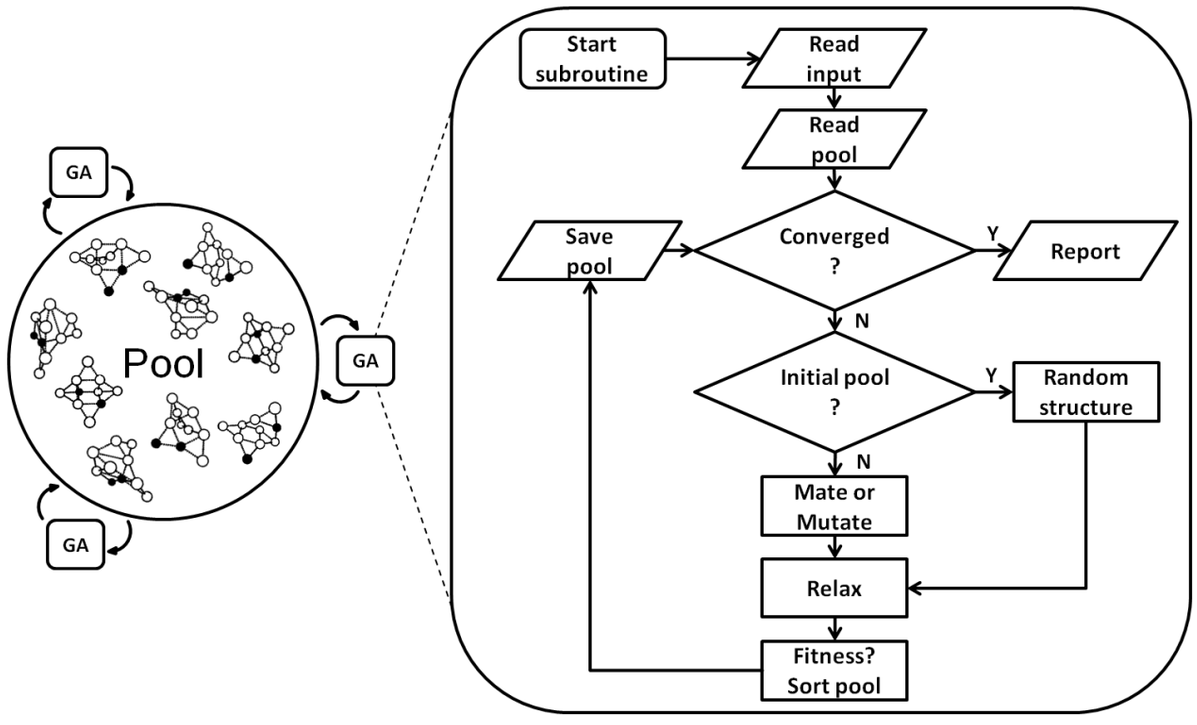
- Direct MPI parallisation is not possible. We would not be able run DFT codes in parallel alongside the GA.

Database Method

- Pool GA methodology insures efficiency within a parallel scheme.

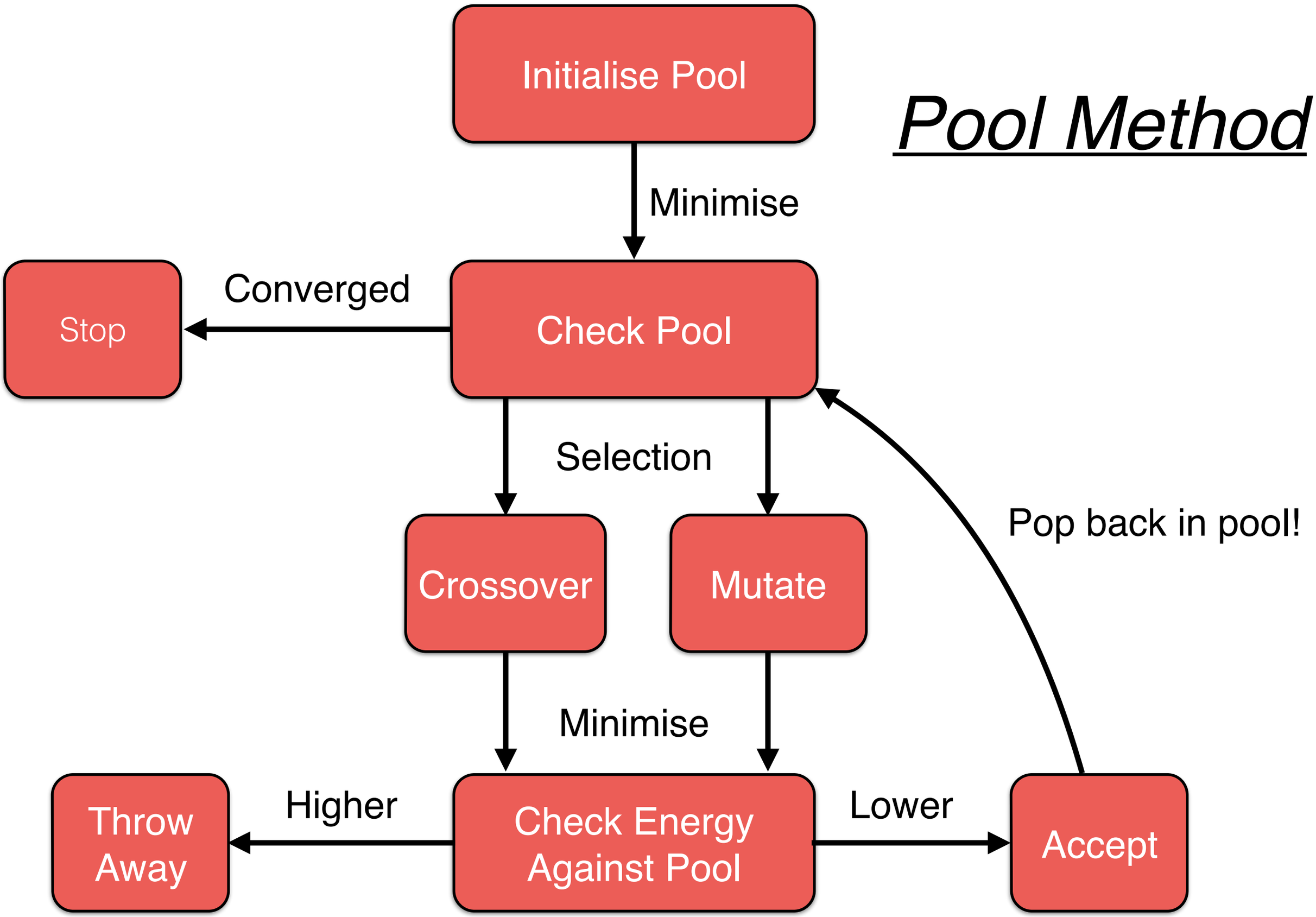
- The pool is updated whenever a lower energy structure is found.

- The pool of structures is kept within a text file. This allows multiple instances of the code access to the structures.



Shayeghi, PCCP, 2014, Accepted

Pool Method

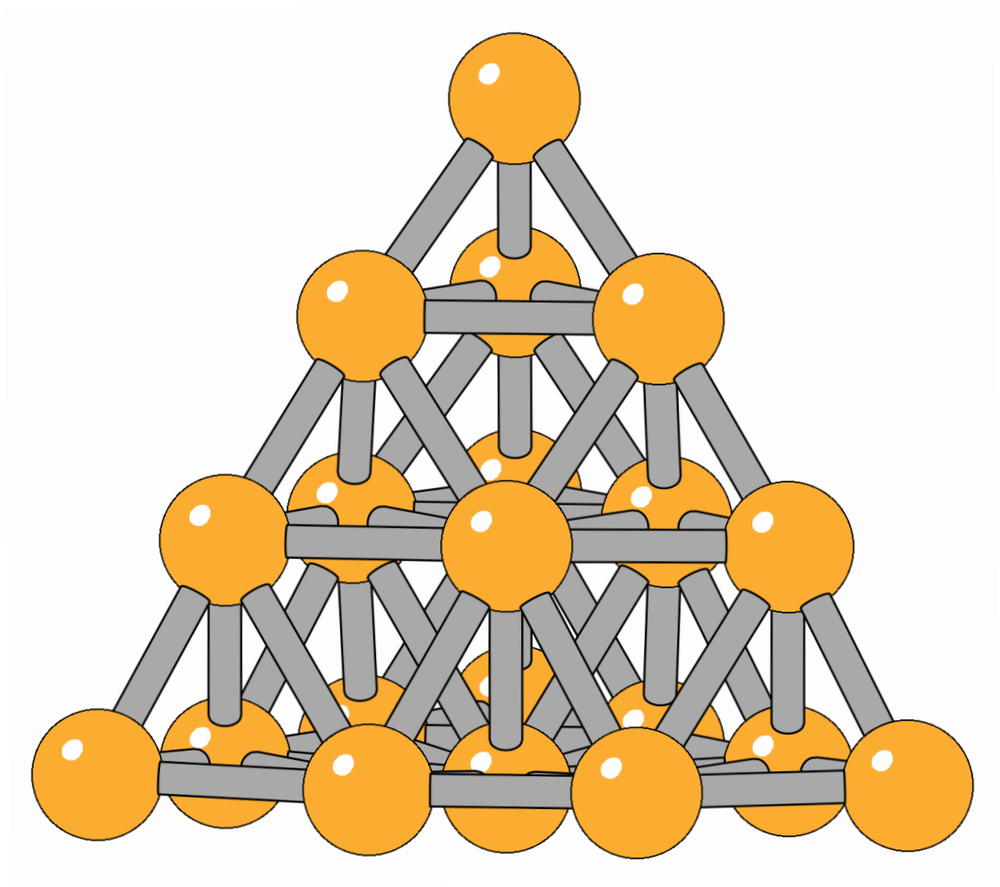

Initialise Pool
Minimise
Converged
Stop
Check Pool
Selection
Crossover
Mutate
Pop back in pool!
Minimise
Higher
Throw Away
Check Energy Against Pool
Lower
Accept

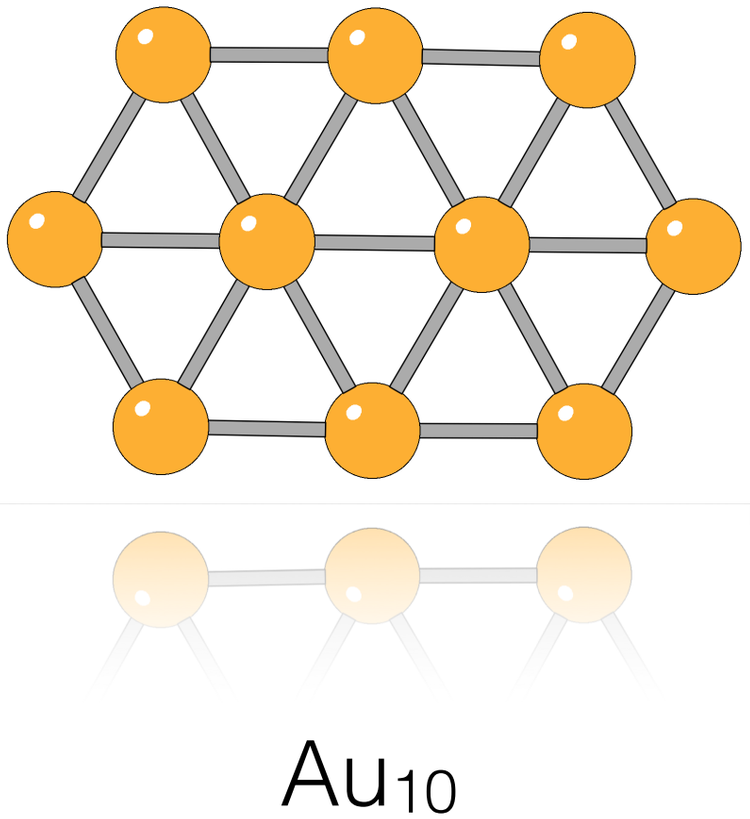
Au_{20}

- The pool/database methodology has been benchmarked and applied to Au_{20}.

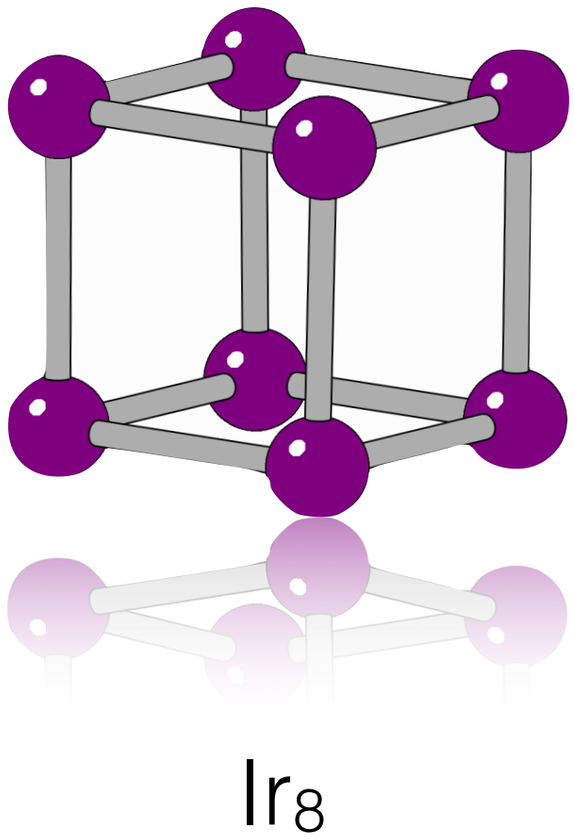
- The tetrahedral (T_d) structure of Au_{20} has been predicted by both theory and experiment.

- The pool-BCGA successfully finds this as the global minimum.

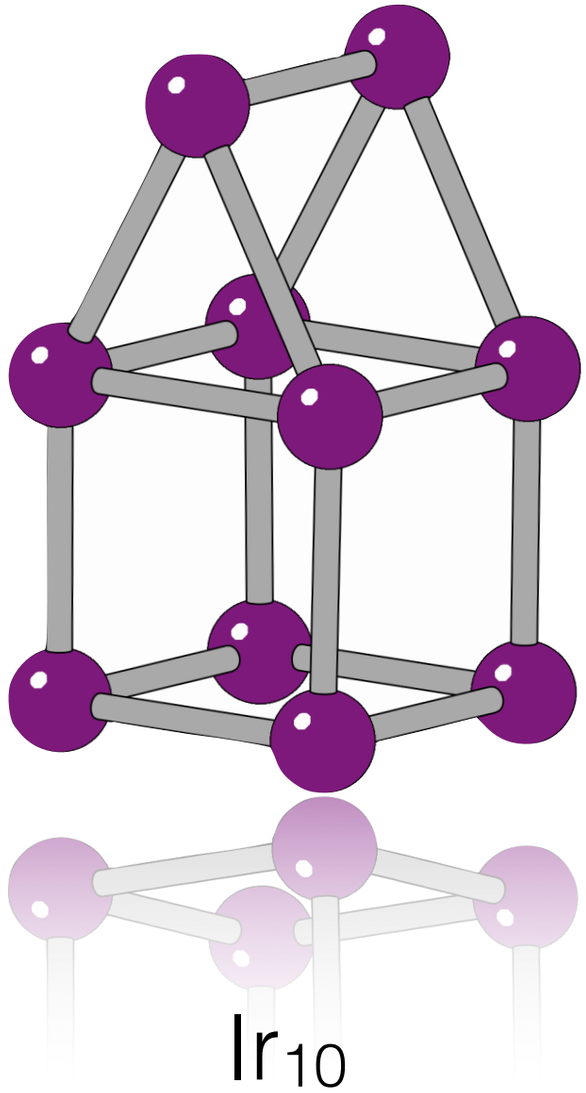




Au_{10}



Ir_8



Ir_{10}

Davis, J. Phy. Chem. A, 2014, **114**.

Conclusions & Future Work

- Continue to test the code on a variety of systems.
- More mutation schemes.
- Ligand and surface optimisation.
- Implementation of a an SQL database.

Acknowledgements

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- A. Shayeghi.
- Johnston Group.
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