Atomic Clusters

Parallel algorithms for Global Geometry Optimisation

Einar de Gruyl — Patrick Hibbs — Donghwi Kim — Marco van Veen — Simon Van Hulle

TUDelft

Contents

TU Delft

Atomic Clusters

What are they?

- Between molecule and bulk
- Surface to volume ratio
- Unique properties

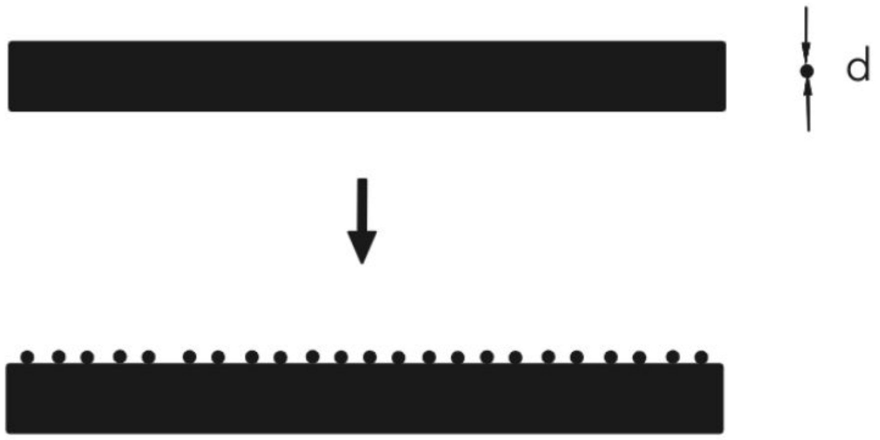
Retrieved from [Doye & Wales (1998)]

- Exact geometry very important

Atomic Clusters

Applications

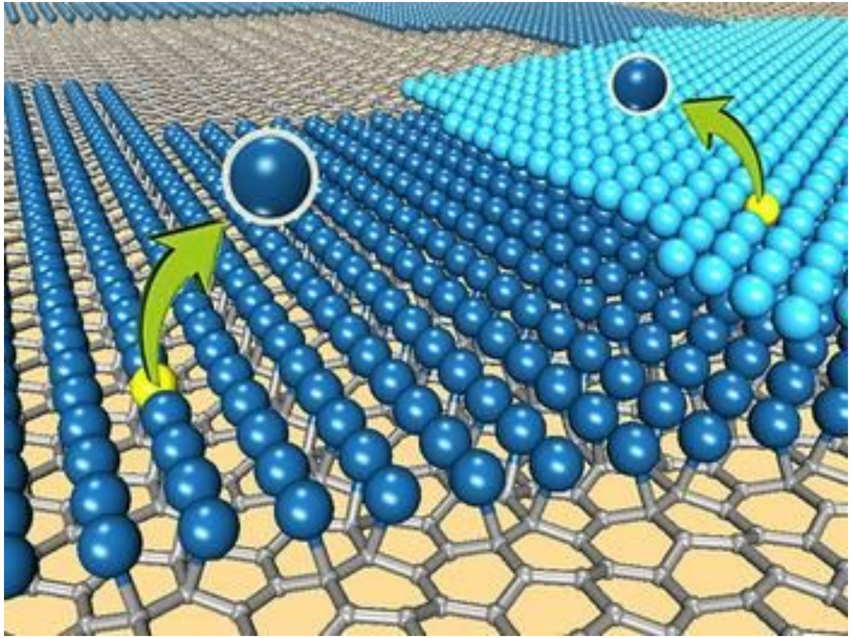
- Batteries and Supercapacitors



Atomic Clusters

Applications

- Batteries and Supercapacitors
- Catalysis

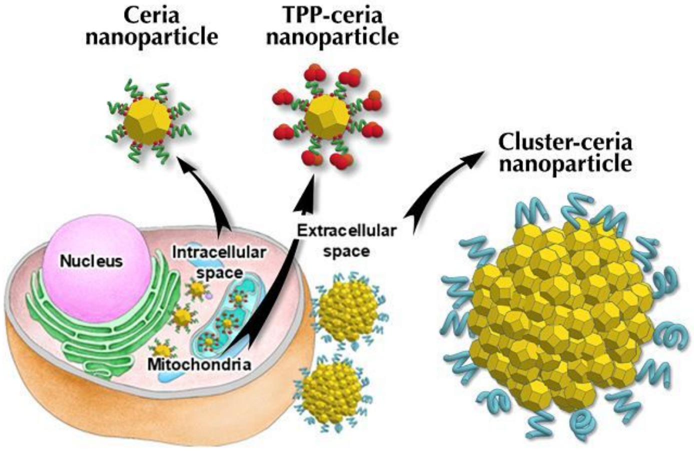


Retrieved from Choi et al. (2019)

Atomic Clusters

Applications

- Batteries and Supercapacitors
- Catalysis
- Medical applications (Parkinson's Disease)

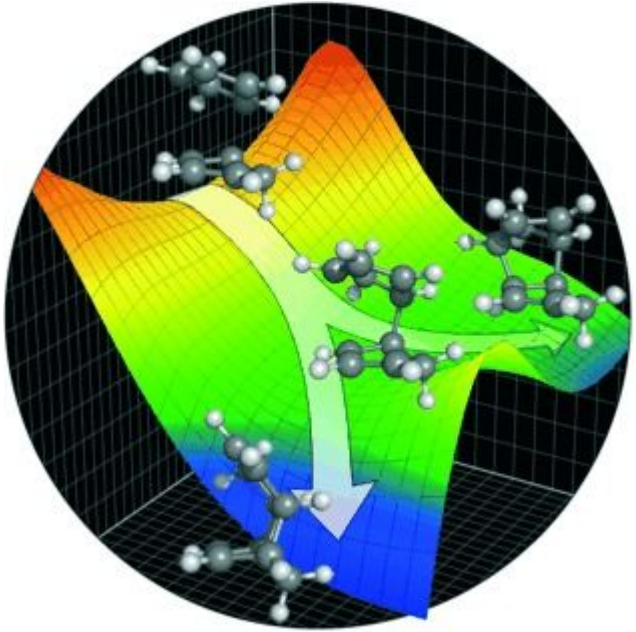


Retrieved from Kwon et al. (2018)

Global Optimisation

- Only local energy minima can be stable
- The lower the better
- Need for efficient algorithm

$$E = 4\epsilon \sum_{i<j} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

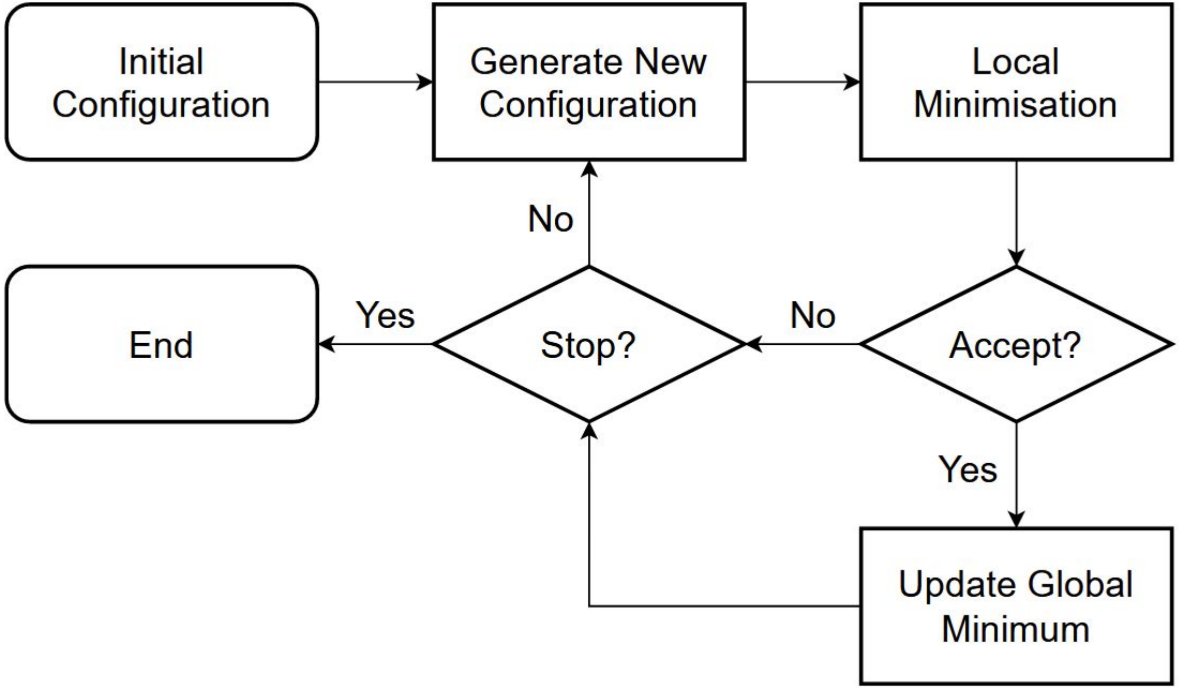


Retrieved from Ess et al. (2008)

Global Optimisation

Basin Hopping

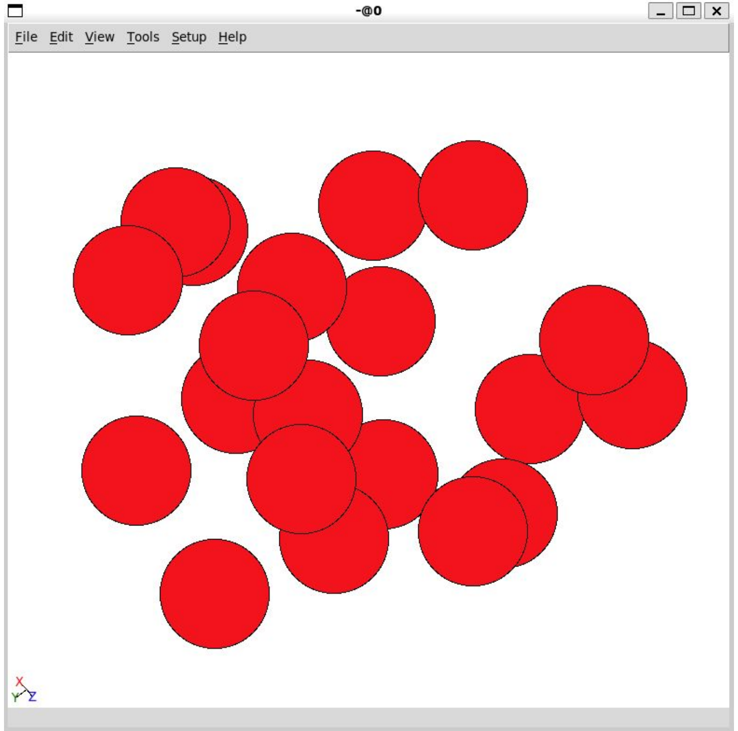
Wales and Doye, 1997



Basin Hopping

Initial Configuration

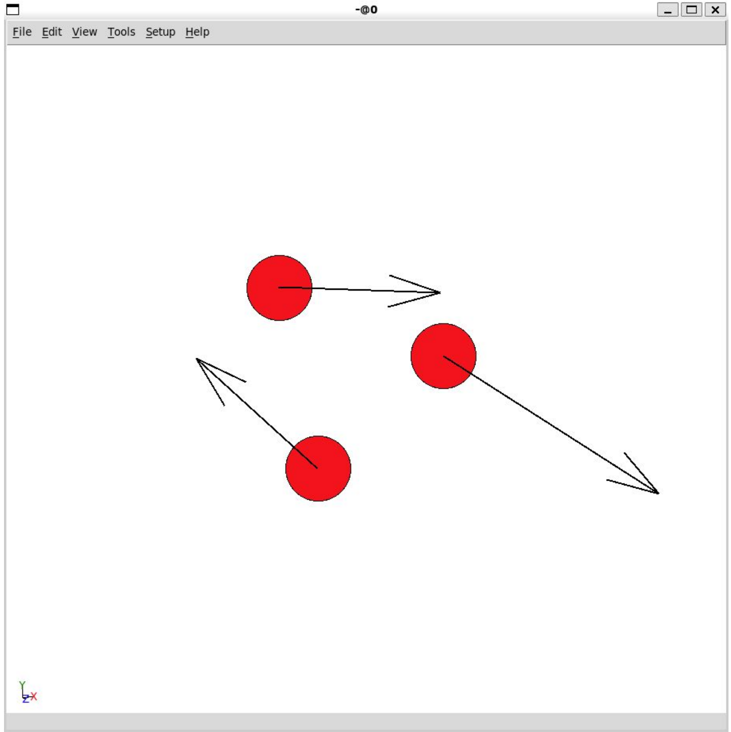
- Uniform distribution in a sphere with a radius of 1Å, or 0.1 nanometre.



Basin Hopping

Generating new configurations

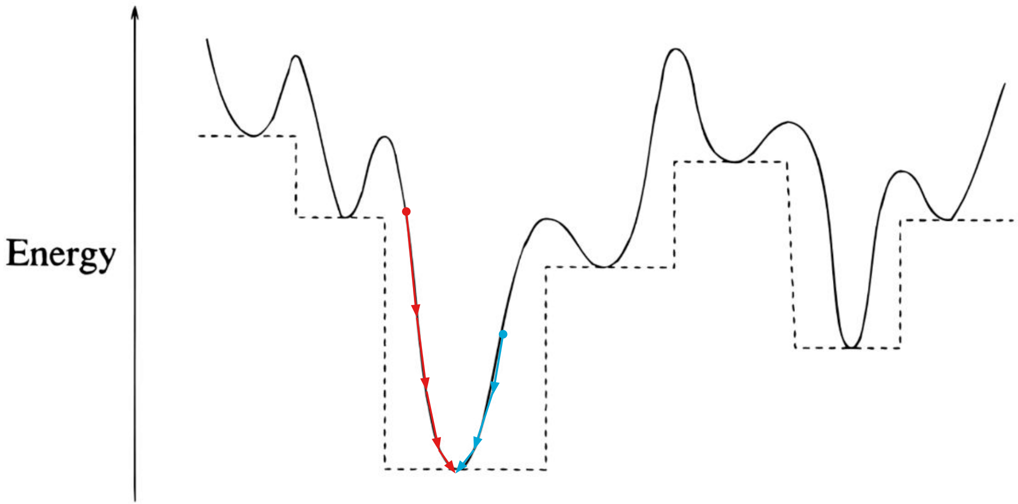
- Random displacement of all atoms by a dynamic step size.
- Step size is adjusted every few loops in order for the algorithm to find unique cluster configurations.



Local minimisation

$$\tilde{E}\left(\mathbf{A}\right) = \min\left\{E\left(\mathbf{A}\right)\right\}$$

- Gradient descent on potential energy surface



Retrieved from Wales & Doye (1997)

Acceptance Criteria

Metropolis acceptance criteria

$$P(\mathbf{A}) = \begin{cases} \exp(-\Delta\tilde{E}/T) & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases}$$

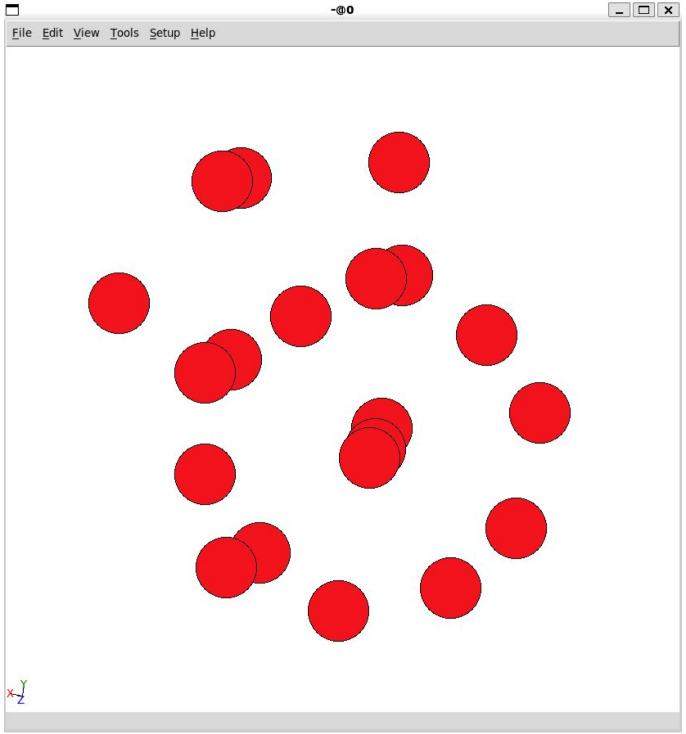
- T is the boltzmann constant ≈ 8.617 x 10^{-5} eV K^{-1}
- All configurations with a lower potential energy will be selected.
- Some configurations with a higher potential energy will be selected.
- Adjust step size to achieve a specific acceptance ratio.

TUDelft

Basin Hopping

Result after 200 iterations

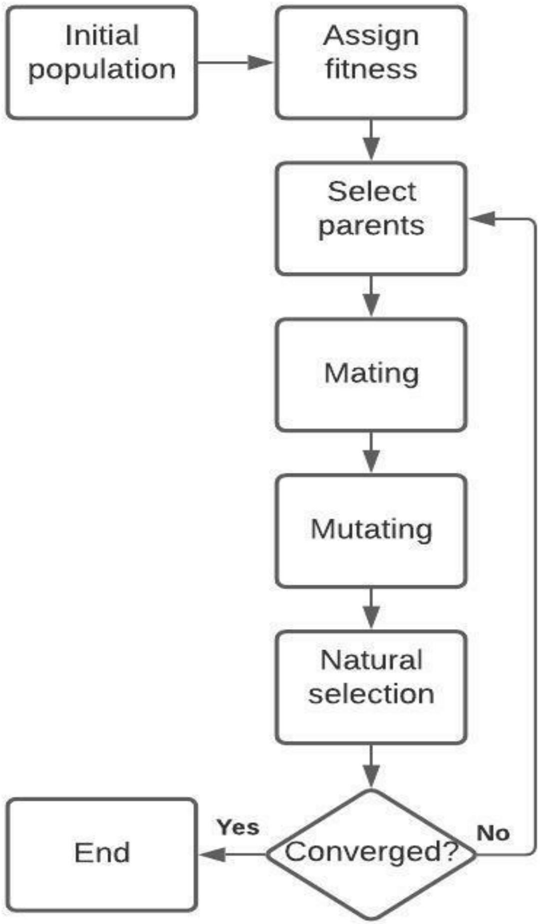
- N = 20
- E = -76.137 eV



Global Optimisation

Genetic Algorithm

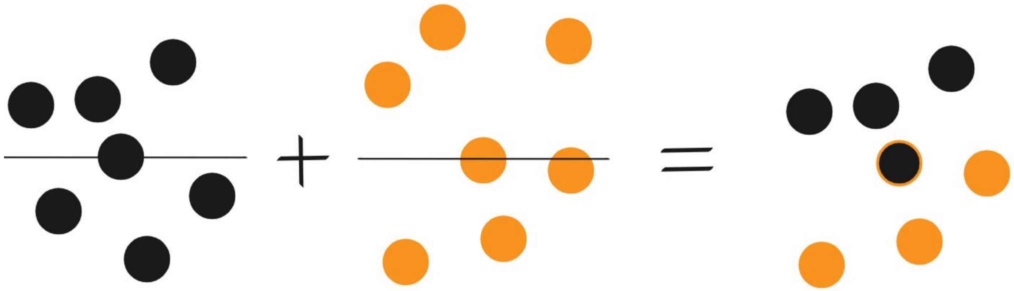
- Inspired by the process of biological evolution
- Maintains a population of clusters
- Evolves over time using natural selection



TU Delft

Genetic Algorithm
Mating

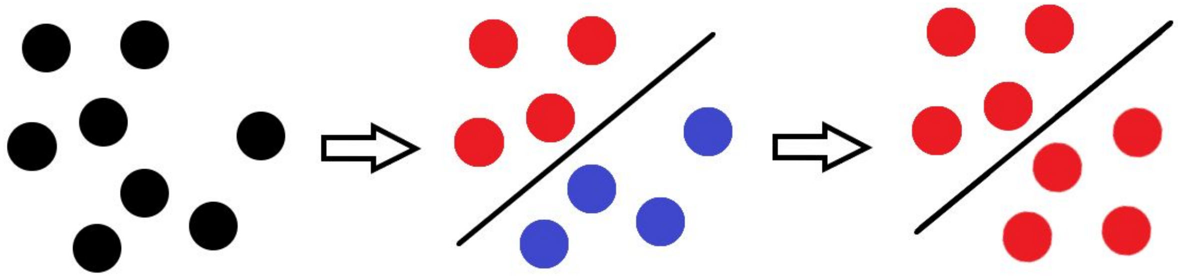
- Choose parents based on fitness
- Combine parent clusters



Genetic Algorithm

Mutating

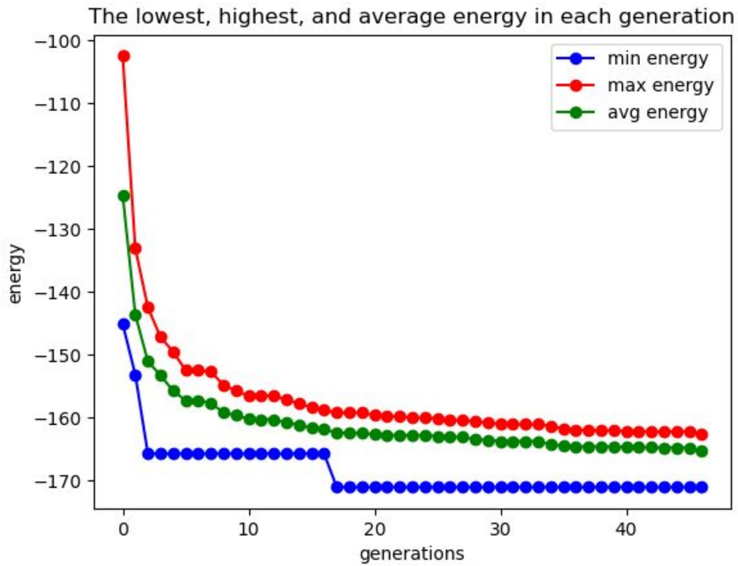
- Displacement
- Rotation
- Replacement
- Mirror-and-shift



Genetic Algorithm

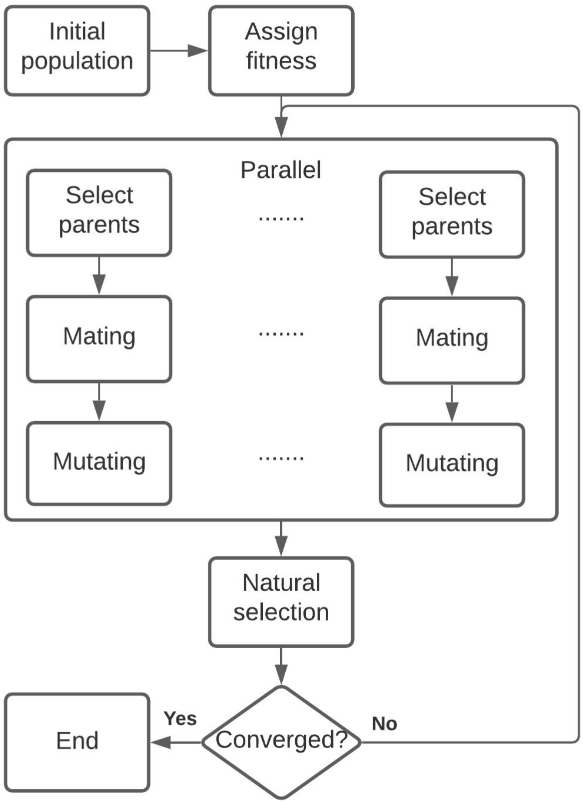
Natural selection

- Fittest members are chosen
- Different energy values required for variety
- Repeat the entire process

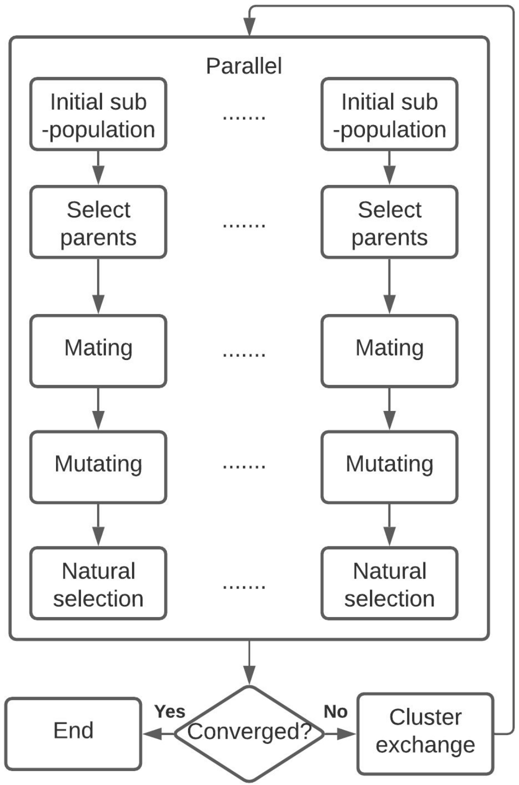


Genetic Algorithm
Parallel

Distributed Genetic Algorithm



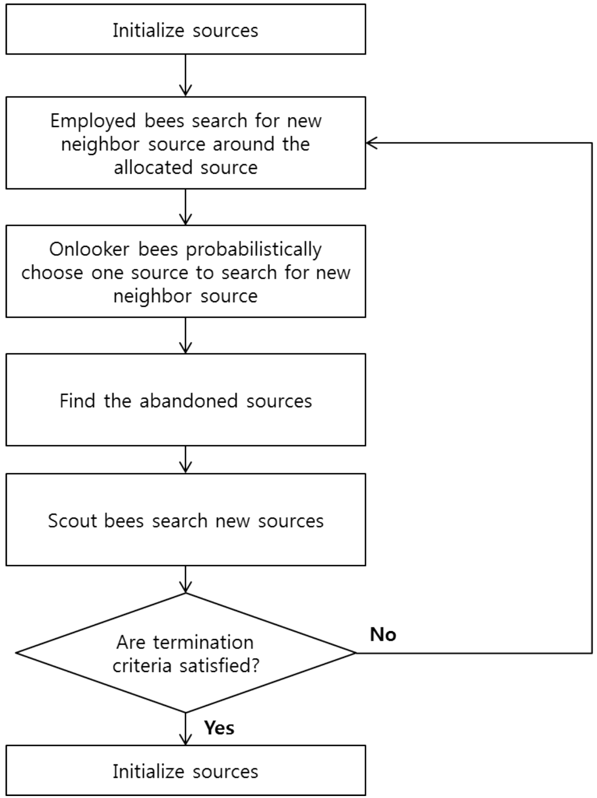
Sub-population Genetic Algorithm



Global Optimisation

Artificial Bee Colonies Algorithm

- Recently proposed by [Karaboga & Basturk (2007)]
- Imitates intelligent hunting behavior of honey bee swarm
- Bee swarm consists of three bees: employed bee, onlooker bee and scout bee

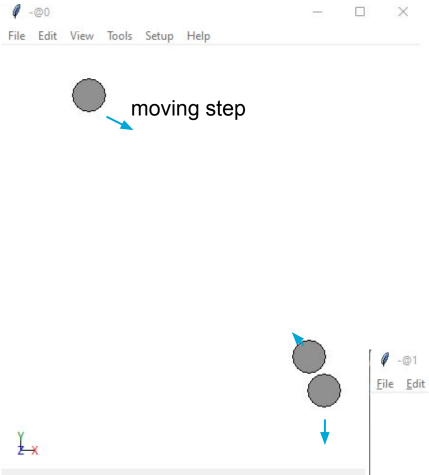


TU Delft

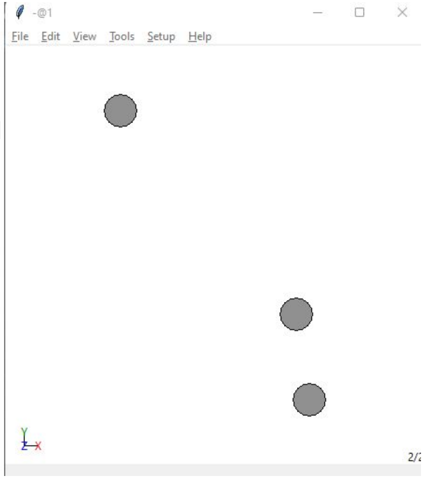
Artificial Bee Colonies Algorithm

Employed bee

- Generates the new structure for each clusters in population:
  - trigonometric mutation operator
  - modified Monte-Carlo method
- Existing cluster is replaced when new cluster has better energy
  - greedy method



Existing cluster



new cluster

Artificial Bee Colonies Algorithm

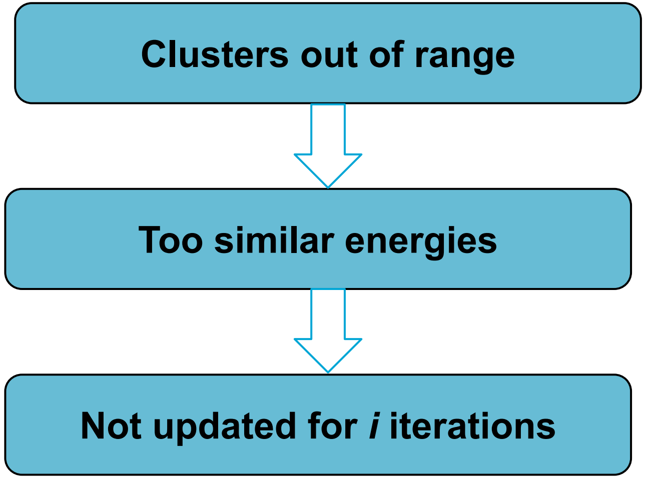
Onlooker bee

- Selects one good cluster
- Searches neighbour of chosen cluster by using Monte-Carlo method
- Decides whether to accept or not by using greedy method

Artificial Bee Colonies Algorithm

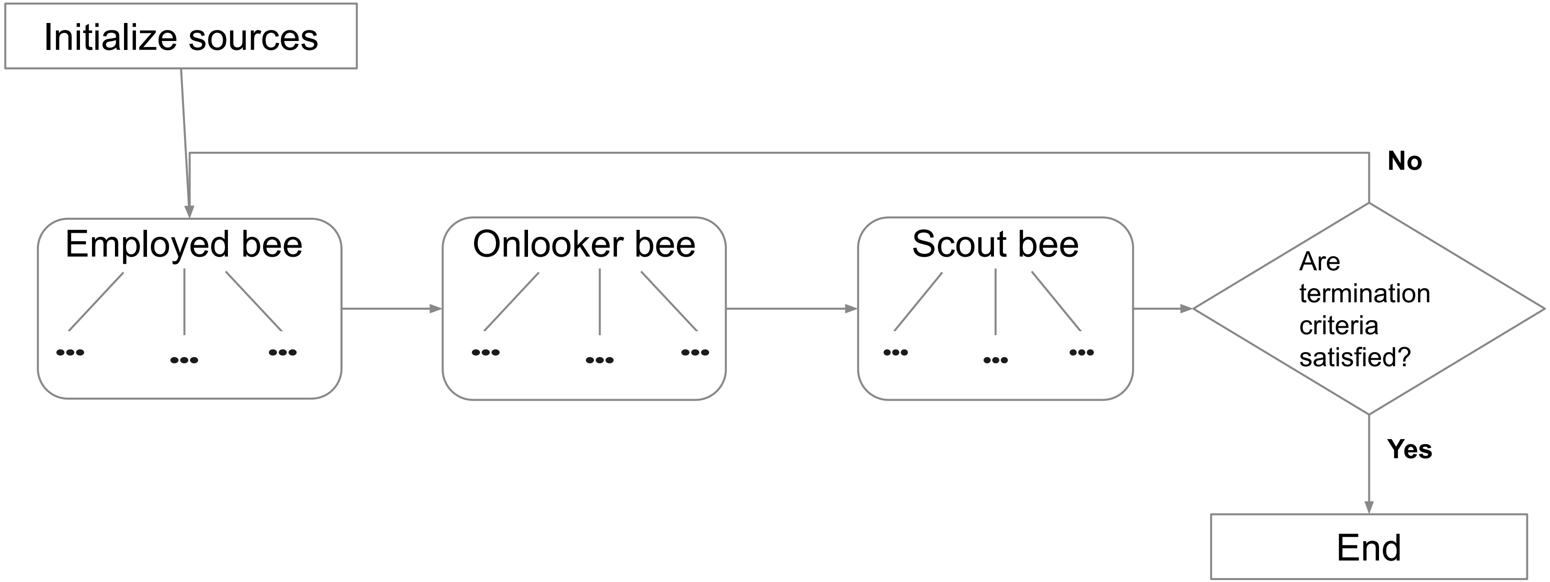
Scout bee

- Removes clusters that are not “worth it”



Artificial Bee Colonies Algorithm

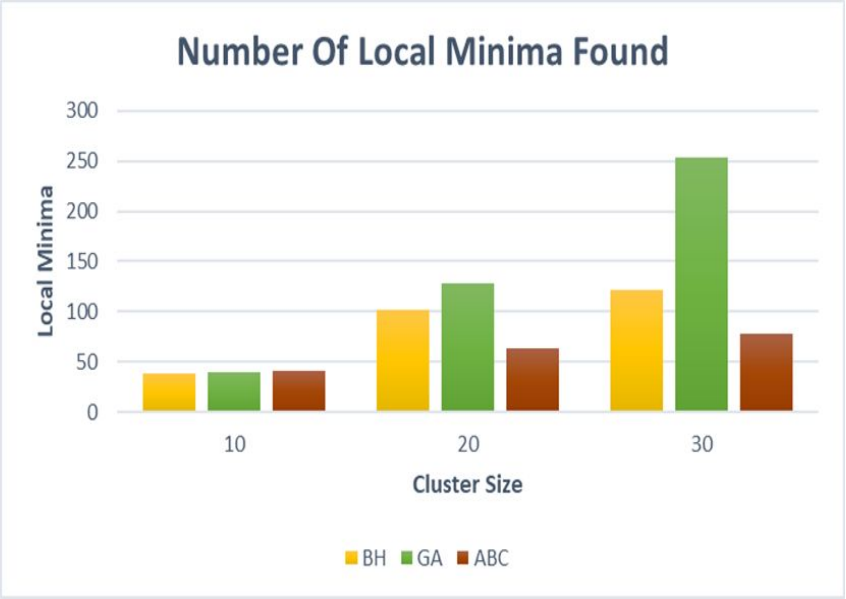
Parallel



TU Delft

Comparison of algorithms

Different cluster sizes

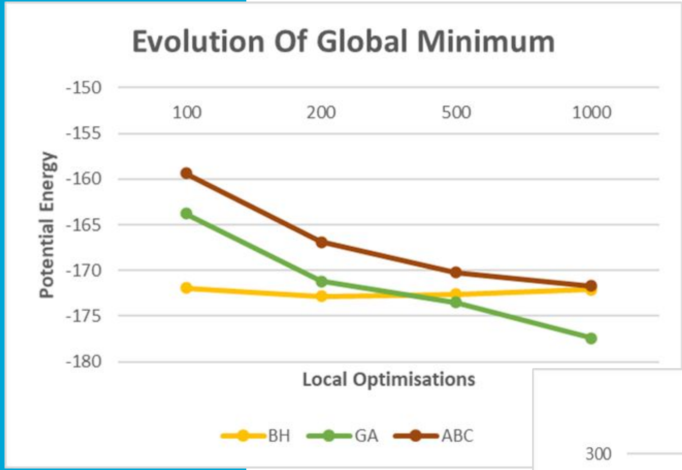


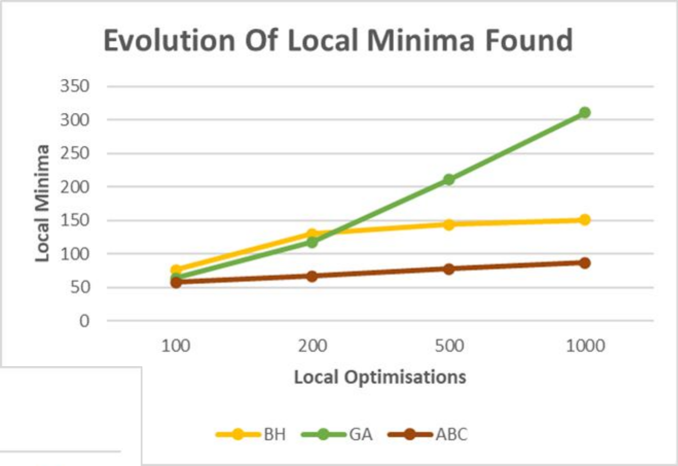
Note: All the data has been averaged over 5 separate runs. For the global minimum, the best result was chosen.

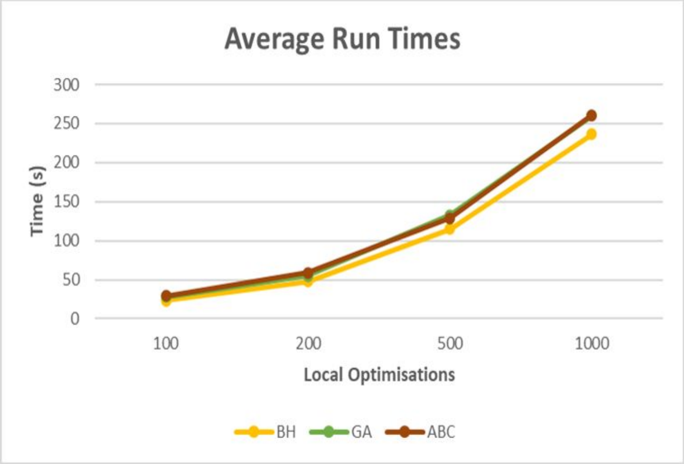
TUDelft

Comparison of algorithms

Evolution of algorithms







Note: All the data h … global minimum, the best result was chosen.

Comparison of algorithms

Best use cases

- Basin Hopping
  - Good solution required within short period of time
- Genetic Algorithm
  - Best overall when plenty of resources are available
- Artificial Bee Colony
  - Alternative for Genetic Algorithm when other local minima not of interest

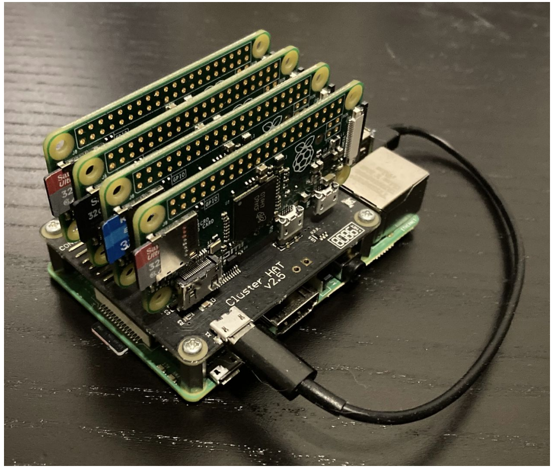
Conclusion

- Basin Hopping
- Genetic Algorithms
- Artificial Bee Colonies

- Little extra:
    - Raspberry Pi Cluster Demo

Raspberry Pi Cluster

- Raspberry Pi 3 (2 CPU)
- 4x Raspberry Pi Zero (1 CPU)
- Total 6 CPU cores
- Slurm workload manager



Questions?

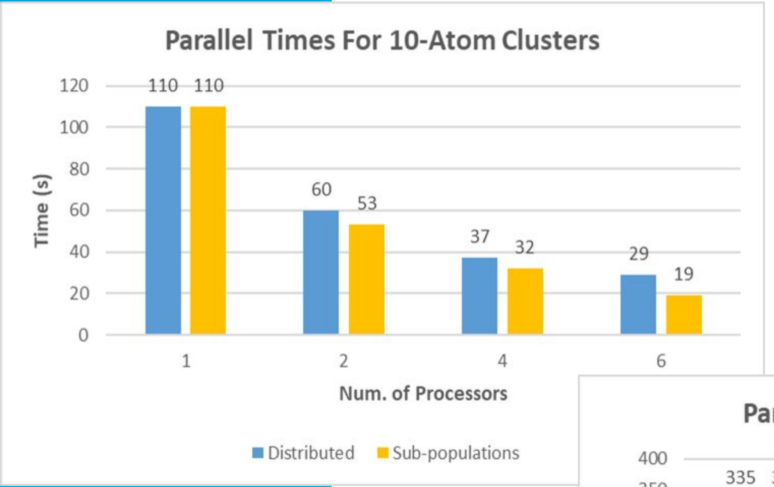
References

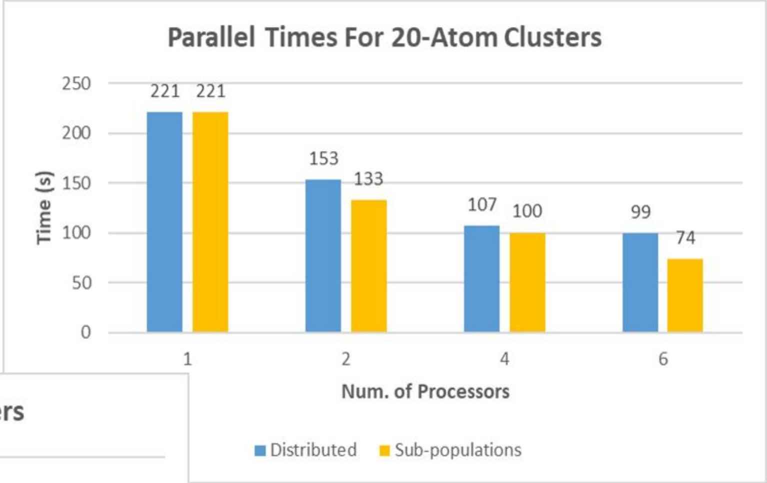
- Abakumov, A. M., Fedotov, S. S., Antipov, E. V., & Tarascon, J. M. (2020). Solid state chemistry for developing better metal-ion batteries. *Nature Communications.* 2020 11:1, 11, 1–14. https://doi.org/10.1038/s41467-020-18736-7
- Choi, J. I., Abdelhafiz, A., Buntin, P., Vitale, A., Robertson,A. W., Warner, J., Jang, S. S., & Alamgir, F. M. (2019). Contiguous and atomically thin pt film with suprabulk behavior through graphene imposed epitaxy. *Advanced Functional Materials*, 29. https://doi.org/10.1002/ADFM.201902274
- Doye, J. P. K., & Wales, D. J. (1998). Thermodynamics of Global Optimization. *Phys. Rev. Lett.*, 80, 1357–1360. https://doi.org/10.1103/PhysRevLett.80.1357
- Ess, D. H., Wheeler, S. E., Iafe, R. G., Xu, L., Çelebi-Ölçüm, N., & Houk, K. N. (2008). Bifurcations on Potential Energy Surfaces of Organic Reactions. *Angewandte Chemie International Edition*, 47, 7592–7601. https://doi.org/10.1002/ANIE.200800918
- Karaboga, D., & Basturk, B. (2007). A powerful and efficient algorithm for numerical function optimization: Artificial bee colony (abc) algorithm. *Journal of Global Optimization*, 39, 459–471. https://doi.org/10.1007/s10898-007-9149-xK
- Kwon, H. J., Kim, D., Seo, K., Kim, Y. G., Han, S. I., Kang, T., … Hyeon, T. (2018). Ceria Nanoparticle Systems for Selective Scavenging of Mitochondrial, Intracellular, and Extracellular Reactive Oxygen Species in Parkinson's Disease. *Angewandte Chemie*, 130, 9552–9556. https://doi.org/10.1002/ANGE.201805052
- Wales, D. J., & Doye, J. P. K. (1997). Global optimization by basin-hopping and the lowest energy structures of lennard-jones clusters containing up to 110 atoms. *Journal of Physical Chemistry A*, 101, 5111–5116. https://doi.org/10.1021/JP970984NW
- Wang, C., Li, J., Amatore, C., Chen, Y., Jiang,H., & Wang, X.-M. (2011). Gold nanoclusters and graphene nanocomposites for drug delivery and imaging of cancer cells. *Angewandte Chemie International Edition*, 50, 11644–11648. https://doi.org/10.1002/ANIE.201105573

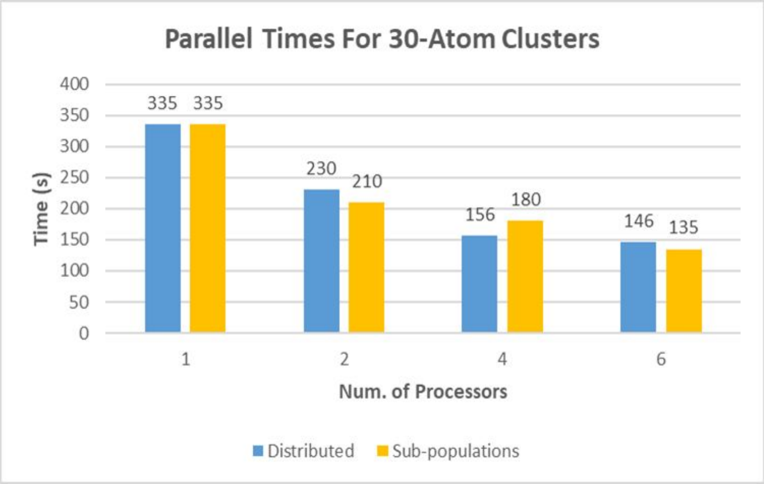
TU Delft

Extra Slide

GA Parallel Times







TU Delft