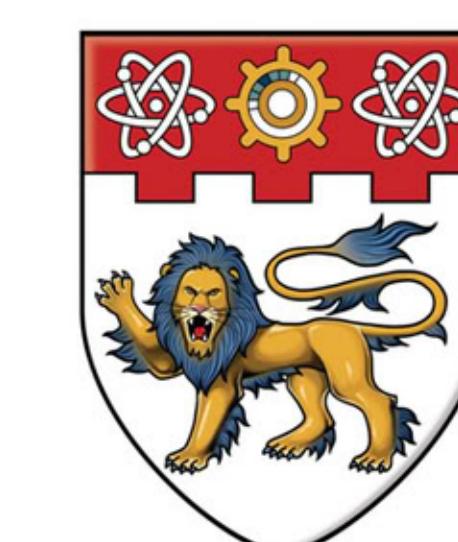


OPENCL ACCELERATED MOLECULAR DOCKING WITH HISTORICAL GENETIC ALGORITHM

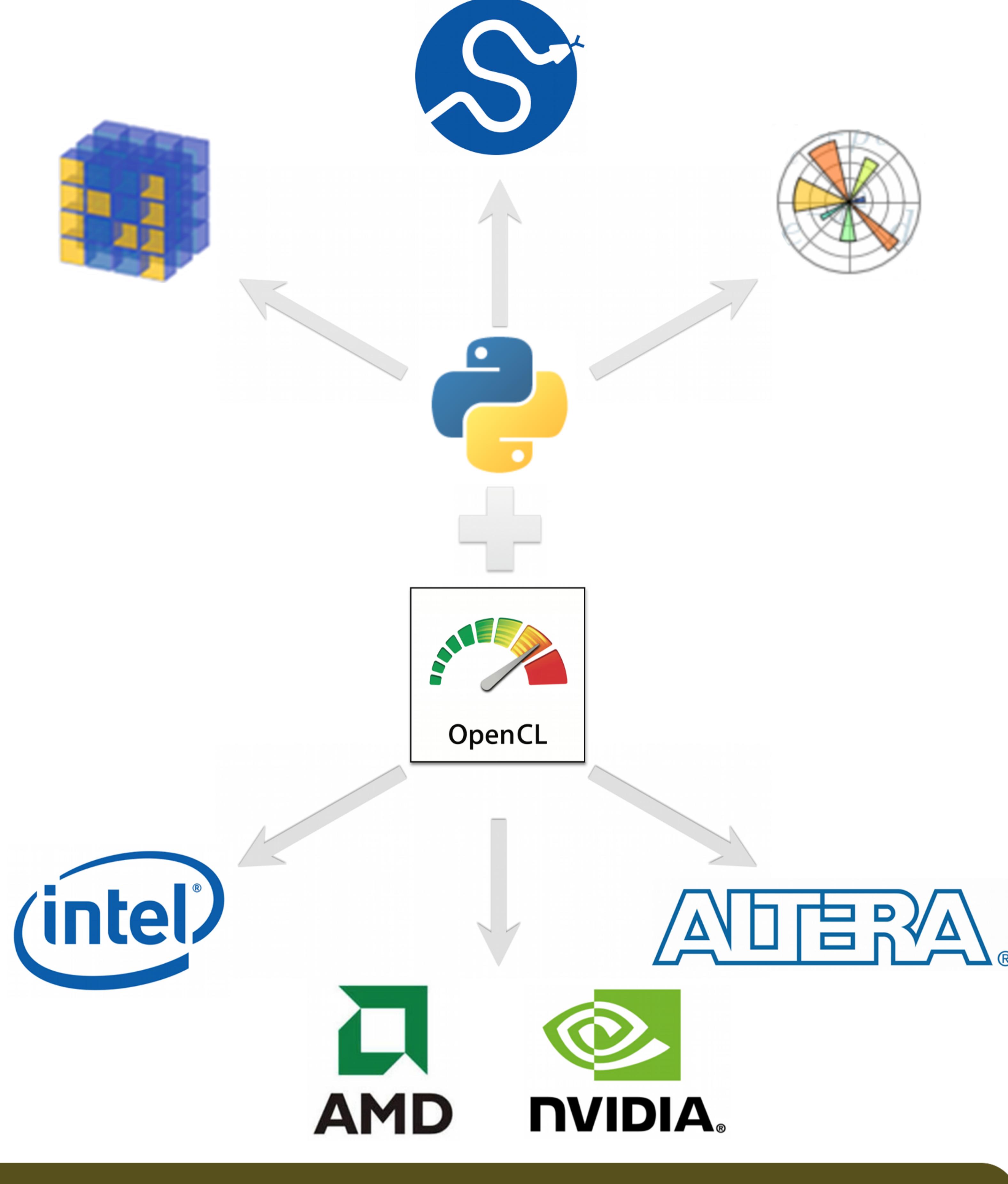
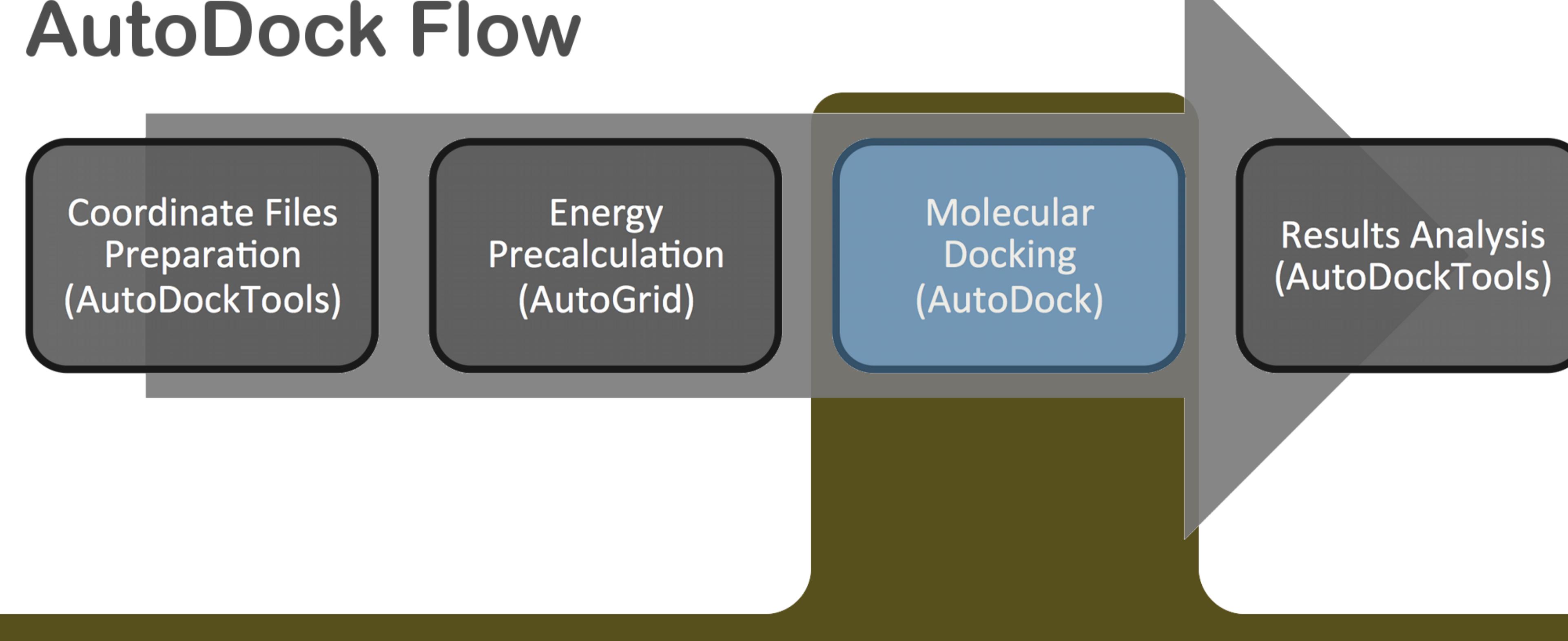


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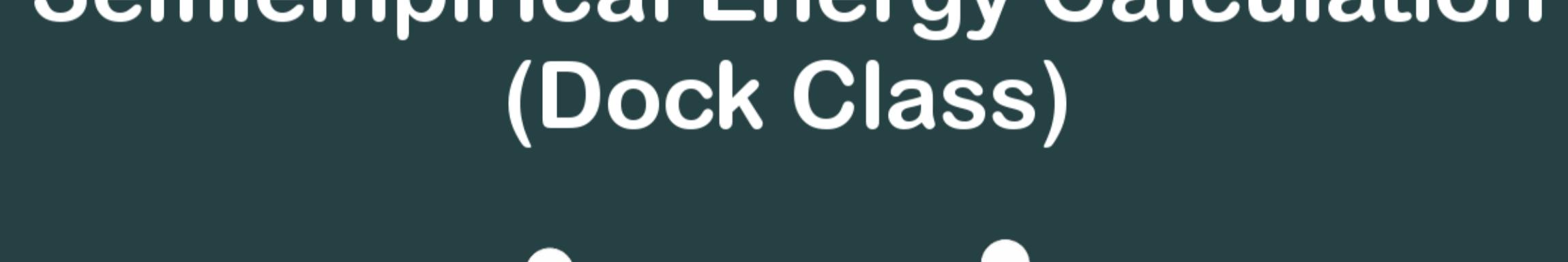
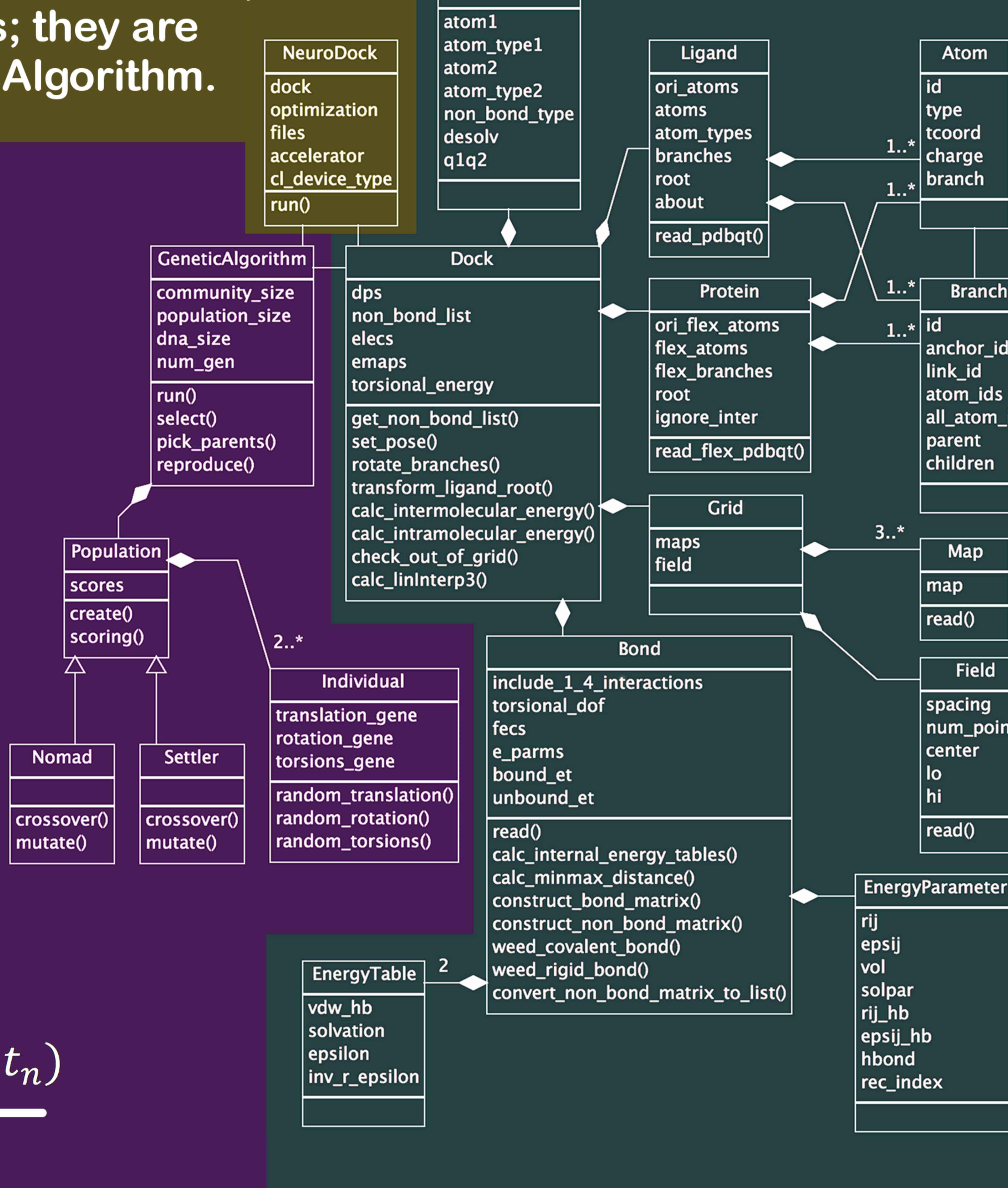
1. BACKGROUND

Molecular docking tools are developed to help scientists to discover new drug efficiently. The objective of this work is to implement molecular docking tool using Python programming language that is well known to natural scientists so they can work on their own representation of semiempirical energy function. Also, for computer scientists so they can easily implement new optimization algorithm for the conformational search.



2. IMPLEMENTATION

The implementation (called nppNeuroDock) consists of three major classes; they are **NeuroDock**, **Dock**, and **GeneticAlgorithm**.

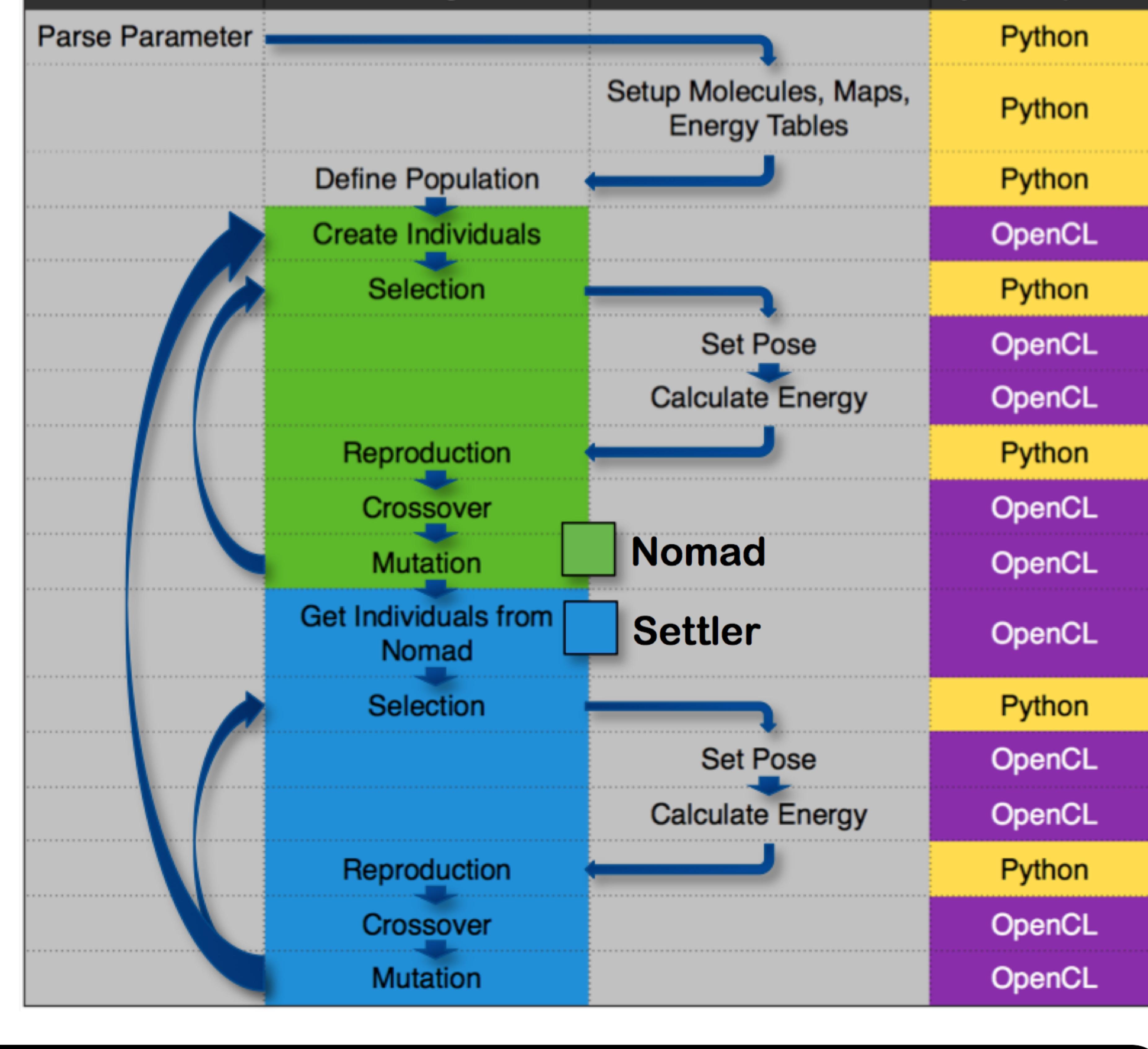
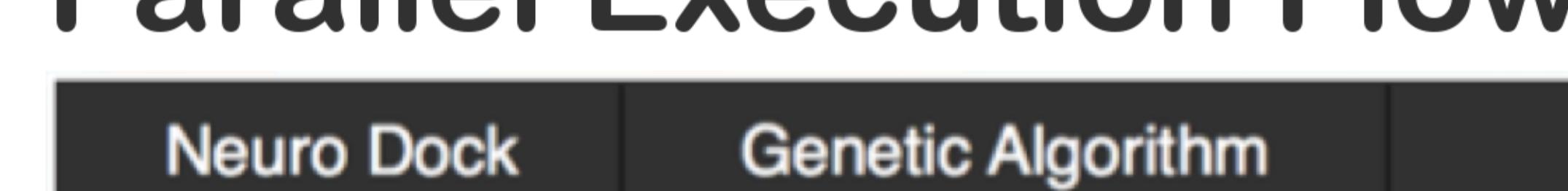
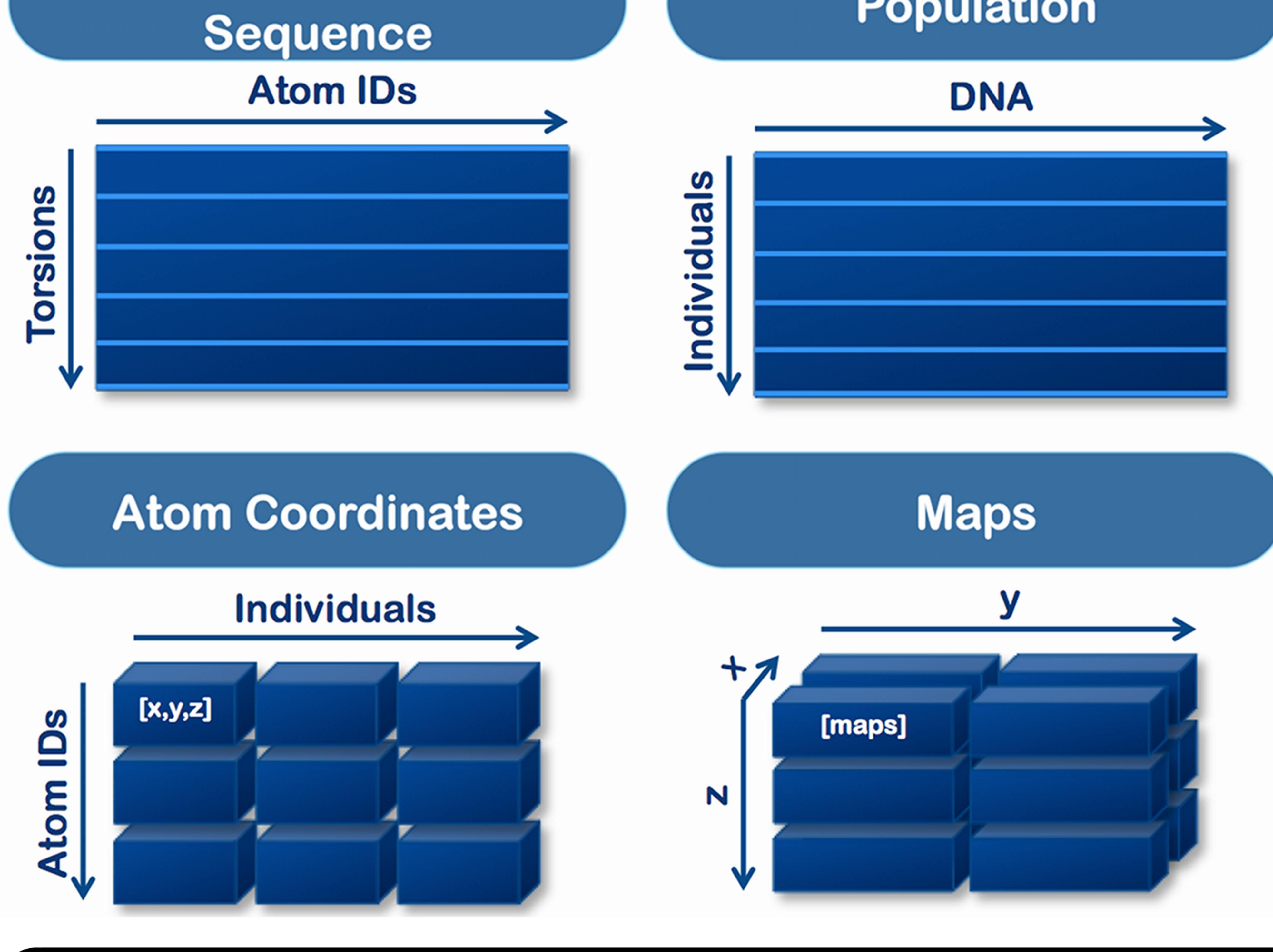


$$V = W_{vdw} \sum_{i,j} \left(\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6} \right) + W_{hbond} \sum_{i,j} E(t) \left(\frac{C_{ij}}{r_{ij}^{12}} - \frac{D_{ij}}{r_{ij}^{10}} \right) + W_{elec} \sum_{i,j} \frac{q_i q_j}{\epsilon(r_{ij}) r_{ij}} + W_{sol} \sum_{i,j} (S_i V_j + S_j V_i) e^{-r_{ij}^2 / 2\sigma^2}$$

electrostatic **desolvation**

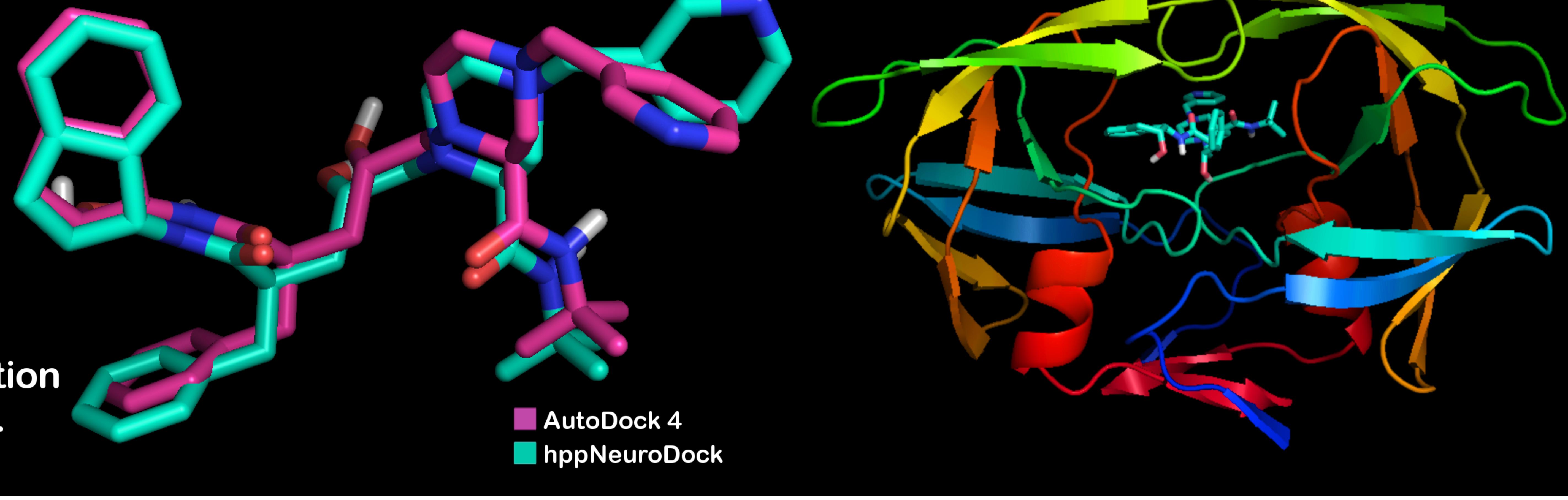
Parallel Data Structure

Branch Rotation



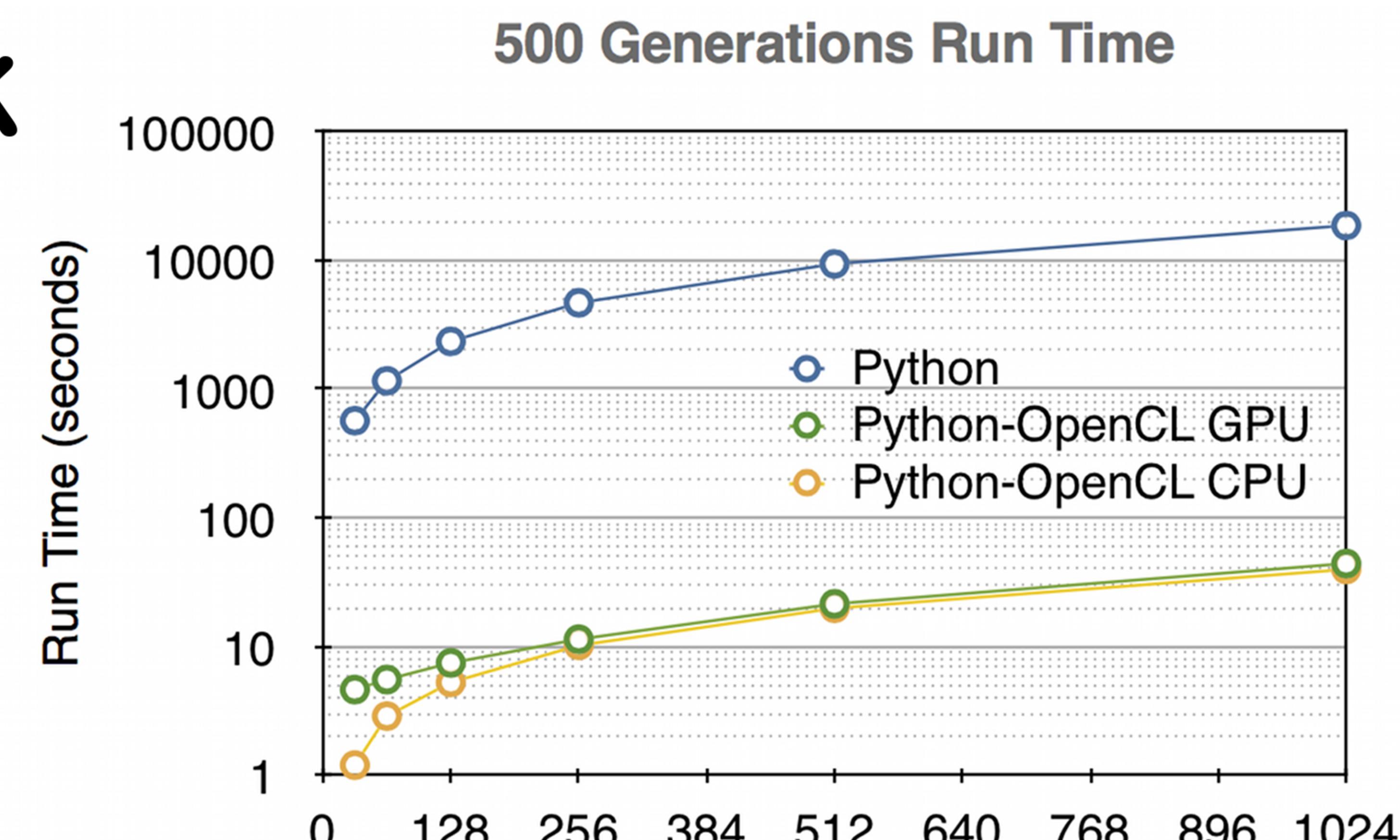
3. RESULT

Protein and ligand used to evaluate the implementation are HIV-1 and Indinavir respectively. It achieves lowest free energy of -14.27 kcal/mol as compared to AutoDock 4 with -15.66 kcal/mol. The ligand location and conformation RMSD of the two are 1.53 Å apart.



4. BENCHMARK

Runtime comparison of different implementations over different population size in 500 generations taken using NVIDIA GeForce GT 650M GPU and Intel Core i7 CPU.



5. CONCLUSION

The main contributions of this work are implementing AutoDock 4 semiempirical energy function in Python, implementing new algorithm for conformational search called historical genetic algorithm, and implementing heterogeneous parallel program by integrating Python and OpenCL to achieve runtime improvement up to 477 times compared to sequential program