Deployment of Virtual Clusters on a Commercial Cloud Platform for Molecular Docking <u>& Fault Tolerance</u>

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Expectations from Previous Week

- Go over the process of running Dock with Anthony (In Progress)

- Finish unpacking, unzipping, and organizing raw ligand slices on virtual machine (Completed)

- Read more on Hadoop (In Progress)

Research Progress

* Ran grid2.dockin with a compressed ligand file and failed = Dock cannot be run with compressed ligand files (.mol2 only)

* Finished organizing the raw ligand slices (Clean Drug-Like from ZINC Database

  * all zipped .gz files are stored in Virtual Machine

  * unzipped .mol2 files are stored in my personal computer

  * 186 slices total. Splitting of slices can be operated upon test

Research Progress

- Measured the size of raw ligand data, will also measure the size of output files

- Supported Anthony with Dock for his Multi-cloud environment

- Read more on Hadoop

Overall Plan of Action

- This will be the last week of our research internship. For future reference of virtual machine and commercial cloud storage, I plan to figure out the size of all output files carried out by docking. I will support Anthony to fully test the function of dock on the multi-cloud environment between clusters. Finally, I hope to work with Katy and configure Hadoop so we can operate dock through Hadoop.

Research Expectations

- Operate dock6 and estimate the size of all output files

- Support Anthony with dock6 in the Multi-Cloud environment

- Work with Katy to operate dock6 on Hadoop

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