

Deployment of Virtual Clusters on a Commercial Cloud Platform for Molecular Docking & Fault Tolerance

*Derek Song
NAIST, Nara, Japan
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Expectations from Previous Week

- ◆ Obtain FutureGrid accounts from Dr. Haga and Ichikawa Sensei and submit project application for FutureGrid (Completed)
- ◆ Produce numerous VMs for testing (Not yet needed, since we just recently gained access to Karen and Kevin's Virtual Machine - Barco)
- ◆ Transfer, install, and test Hadoop on a VM (Completed by Katy)
- ◆ Transfer, install, and test DOCK on a VM (Completed)

Research Progress

- ◆ Reviewed and submitted Project Application for FutureGrid
- ◆ Utilized Cyberduck to transfer dock6 source file to Virtual Machine test-1
- ◆ Troubleshooted and Installed Dock 6.2 onto VM test-1
- ◆ Met with Dr. Haga and Ichikawa Sensei to report project progress, set goals, and learned how to create Kernel-based Virtual Machine
- ◆ Anthony and Ichikawa Sensei unlocked Karen and Kevin's Virtual Machine created last due to its preferable environment and parameters for Dock 6.2

Research Progress

- ◆ Ran a test suite and made sure Dock was processing correctly, and Dock yielded the exact same Grid scores compared to the Developer's
- ◆ Obtained protein ligands slices and protein receptors list from Karen for running Dock
- ◆ Reading and familiarizing with the Dock tutorial: structure preparation, sphere generation, grid generation, docking, and amber score generation
- ◆ Preparing a protein receptor for running dock
- ◆ Trying to connect Cyberduck to Karen and Kevin's VM

Overall Plan of Action

- With the gaining of access to Karen and Kevin's Virtual Machine - Barco created last year, we are in the process of installing all critical softwares onto Barco including Hadoop and Vines. I am testing Dock on Barco to make sure it is working correctly, and I plan to run a small slice of ligands with a receptor to further learn the process of Dock and the function of its parameters. Katy is installing Hadoop, and Anthony is installing Vines. Once all related softwares are up and running, we plan to test run Dock on a larger scale.

Research Expectations

- ◆ Connect Cyberduck to Karen and Kevin's VM for transfers of prepared molecule files
- ◆ Prepare a protein receptor and protein ligands slice to run Dock
- ◆ Read and familiarize more on adjustments of Dock parameters
- ◆ Obtain the complete set of protein ligands needed for docking from Karen and Kevin
- ◆ Learn and understand Anthony and Katy's parts of the project especially on Hadoop



Below = Ikebana (Flower Arrangement) in Japanese Culture Class at NAIST

Left = Bamboo forest in Kyoto





Left = Akame 48 Waterfalls

Middle = Kyoto Monkey Park

Right = Kyoto Monkey Park



#UCSDPRIME2014

Akame 48 Waterfalls, Nabari City, Mie, Japan

Acknowledgments

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