

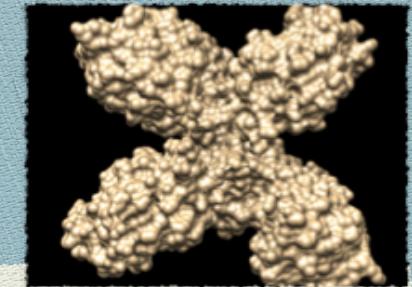
Deployment of Virtual Clusters on a Commercial Cloud Platform for Molecular Docking & Fault Tolerance

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Expectations from Previous Week

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

Research Progress



- Utilized private key to connect to VM Barco on Cyberduck, and now able to transfer Dock preparation files between Barco and personal computers
- Prepared a protein receptor DUSP4, and generated molecular spheres with Chimera
- Generated molecular box and docking grid for receptor DUSP4, and performed rigid docking between DUSP4 and 0_top ligands (obtained from Karen)
- Obtained the full list of protein ligands from Karen

Research Progress

- Requested Anthony to clone VM Barco, removed and reinstalled dock6 onto the VM for practice
- Prepared and performed Rigid Docking for protein receptor SSH2 and protein ligand slice 0_top.mol2
- Cut out 5 protein ligands (test.mol2) from 0_top.mol2 for Rigid Docking and Amber Scoring with SSH2 due to extremely long processing time of 0_top.mol2
- Preparing SSH2 and test.mol2 for Amber Scoring
- Reading and learning Python 3.4



Overall Plan of Action

- After successfully transferring large amount of preparation files onto VM Barco via Cyberduck, I was able to test the functionality of Dock. Now I am running a full cycle of Dock from beginning to end, and I plan to understand the format and information provided by all the output files in order to continue screen for protein receptor SSH2. I also plan to work with Katy to learn Python and figure out how big of a slice of protein ligands we need for the most efficient Docking.

Research Expectations

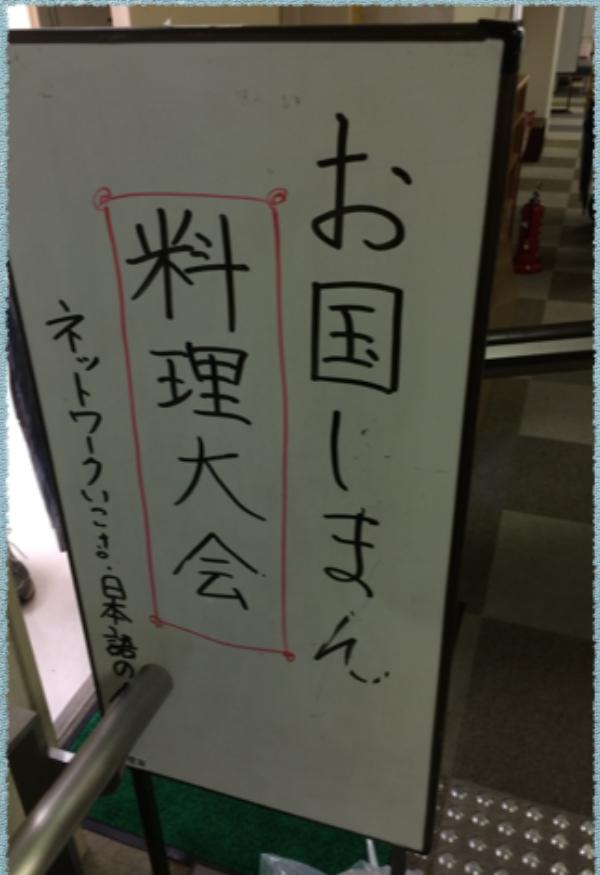
- Finish Amber Scoring and complete one cycle of running Dock
- Read and learn more about Python 3.4 with the goal to appropriately split protein ligand slices
- Test VM function and Dock completion when disconnected with terminal
- Understand the format and output of Rigid Docking and Amber Scoring
- Make a plan to continue screen for protein receptor SSH2 with the ligand list



Above = *Sanjūsangen-dō* in Kyoto

Right = *Fushimi Inari Shrine*





International Cooking Party in Ikoma, Nara



#UCSDPRIME2014

Kinkaku-ji (Temple of the Golden Pavilion), Kyoto, Japan

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