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

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Expectations from Previous Week

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

Research Progress

- Used output files of Rigid Docking and prepared SSH2 protein receptor for Amber Scoring
- Learned vim command for running commands in background
  - nohup command &
  - cat nohup.out
  - nohup command & 2>&1 </dev/null

Research Progress

- Ran Amber Scoring overnight with “nohup” command in Virtual Machine Barco with SSH disconnected from personal computer
- Completed Amber Scoring and ranked 5 sample ligands from 0_top.mol2
- Planing the process to continue screen ligands for SSH2 protein receptor
- Reading and learning Python 3.4

Overall Plan of Action

- Due to the long processing time of Rigid Docking and Amber Scoring, I have learned "nohup" commands from Ichikawa-Sensei, and with this support, I have now completed the entire process of Dock. The focus of this upcoming week is to learn Python and start coding for the splitting of ligand slices. At the same time, finish planning and start screening the rest of the ligands for SSH2 protein receptor.

Research Expectations

- Continue to learn Python and start coding for splitting of ligand slices
- Start screening all ligands for SSH2 protein receptor using DOCK

Gion Matsuri 2014, Kyoto

Below = Minoh Park Illumination, Osaka

Right = Kobe Port Tower, Kobe

#UCSDPRIME2014

Mount Wakakusa (on top of the third summit), Nara

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