

# Deployment of Virtual Cluster on a Commercial Cloud Platform for Molecular Docking and Elasticity of the Clusters

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# Overview

- Objective: upload a virtual machine that runs a protein-ligand interaction simulating program (Dock6) onto FutureGrid
- Purpose: having Dock6 onto the commercial cloud will allow tasks to be performed cheaply and efficiently
- 3 areas will be investigated:
  - Elasticity of the clusters (Katy)
  - Fault tolerance of the system (Derek)
  - Use of several virtual clusters on various commercial clouds to form a single system (Anthony)

## Week 3 Progress

- Learned python language – still practicing coding through tutorials
- Practiced writing if/then statement and how to work with functions, dictionaries, looping etc...
- Researched how people write codes and read about key concepts of writing a program (regular expression, how to put data into files, how to find key word, etc...)
- Continued reading on the relationship between the parsing files and the input Hadoop files

# Coming up: Next Week's Goals

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- Successful run of Hadoop tutorials on the front end 1 of Barco
- Edit of the attempt to write the file splitting tool in Python in order to pre-slice the slices based on number of molecules in each slice (we want around 1,000 molecules)

# Exploring the Culture

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- On Thursday:
  - Ichikawa-sensei allowed us to have a day off to experience the Gion Matsuri Festival in Kyoto
    - Left around 6am from NAIST and took the subway to Kyoto
    - Watched the float procession
    - Had lunch at the Nishiki Market – tried octopus head filled with quail egg!
    - Watched the portable shrine procession – Shinko-Sai procession
- On Saturday:
  - Took the subway to Osaka
  - Explored
    - Bampaku Kinen Koen Park (Expo 70' Commemorative Park) – had a picnic there!
    - Watched the Mino-O Waterfall Illumination
- On Sunday:
  - Took the subway to Nara
  - Hiked Mount Wakakusayama
- On Monday:
  - Day off due to Sea Day
  - Took the subway to Kobe
    - Visited the Disaster Reduction and Human Renovation Institution
    - Ate lunch (KOBE BEEF!!) in Motomachi area
    - Visited Chinatown, Kitano area and Merikken park

# Exploring the Culture

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# Exploring the Culture

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