

# 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

- Clarification of the type of slicing we want to have – we want to pre-slice the slices before Hadoop; thus, we can use Python language to write the code
- Attempted to run the Hadoop tutorial – still running problems that will be looked upon more this week
- Started learning Python language, went through more than 12 tutorials ! Almost reaching the end of the course
- Continued reading on the relationship between the parsing files and the input Hadoop files
- Practiced checking if Dock6 was installed properly by creating new outputs and comparing them with the developer's scores

# Coming up: Next Week's Goals

- Successful run of Hadoop tutorials on the front end 1 of Barco
- Completion of tutorials for Python language
- Completion of the 1<sup>st</sup> 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

- On Saturday:
  - Took the subway to Kyoto
  - Explored
    - Kinkakuji Temple (known for its Golden Pavillion)
    - Sanjusangendo Temple (known for its 1031 statues)
    - Fushimi Inari Shrine (and an unplanned hike!)
  - Near Fushimi Inari Shrine – Food Discoveries
    - Tofu milk ice cream for the 1<sup>st</sup> time ever! Delicious
    - Cold Ramen noodles at a smaller restaurant – amazing!
- On Sunday:
  - Took the subway to Ikoma
  - Participated the International Cooking Party hosted by the senseis of Japanese class!
  - Got to mingle with international students from all over the world and cook as well as try out new specialties from other countries!
  - Walked to revolving sushi bar in Nara

# Exploring the Culture

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# Exploring the Culture

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