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

Nara Institute of Science and Technology (NAIST), Japan
Katy Pham, 07/15/14
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 1st 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 1st 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
Exploring the Culture
Acknowledgements

I would like to thank:

- The graduate students, professors & assistant professors for being so friendly, welcoming and helpful
- Dr. Haga for his constant guidance and for providing us with this incredible opportunity
- Ichikawa-Sensei for always answering our questions and teaching us more about Japan
- The amazing PRIME Staff (Dr. Gabriele Wienhausen – Principal Investigator, Mrs. Teri Simas, Mr. Jim Galvin) for continuous support and guidance
- Dr. Abbie Celniker for her generous donations that are allowing for me to participate in this program
- JASSO for the scholarship
- NAIST for providing the accommodations
- Karen Rodriguez and Kevin Lam for training us during Spring Quarter
- Previous PRIME students for their excellent advice