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

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Research Proposal

- This project aims to upload a virtual machine that runs a protein-ligand molecular interaction simulation program called DOCK to a commercial cloud platform. This platform allows tasks to be performed on a large scale cheaply and efficiently. Three areas will be investigated: 1) the elasticity of the virtual clusters, 2) the fault tolerance of the system, and 3) the use of several virtual clusters on the commercial clouds to form a single system. By utilizing a commercial cloud(s) the system performance will be increased and will allow millions of protein-ligand interaction simulations to be run in a massively parallel manner.
- I will focus on the research of subtopic: Fault Tolerance.

Research Progress

- 6/26: Anthony, Katy, and I arrived in NAIST
- 6/27-29
  - Familiarized ourselves with the new living and working environment
  - Explored and experienced Nara and Osaka
- 6/30
  - Skype Meeting with Dr. Jason Haga, discussed project current and long-term goal
  - Applied for a FutureGrid account for project management
  - Completed FutureGrid project application, waiting for Dr. Haga and Ichikawa Sensei's FutureGrid account approval for submission
  - Met with Ichikawa Sensei to set up all related software and website accounts, and went through the steps to create a Virtual Machine on the NAIST Cluster

Research Progress

- 7/1
  - Practiced creating VMs on the NAIST Cluster, installing operating system onto VMs, and accessing VM created from our personal computers
  - Read more on Hadoop regarding installation, setup, and running on VMs
  - Discussed with fellow lab students and transferred/installed part of Hadoop onto testing VM
  - Successfully connected and transferred files between the VM and our personal computers

Research Expectations

- Obtain FutureGrid accounts from Dr. Haga and Ichikawa Sensei and submit project application for FutureGrid
- Produce numerous VMs for testing
- Transfer, install, and test Hadoop on a VM
- Transfer, install, and test DOCK on a VM

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