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 8 Progress

- Completed the yarn-pseudo distributed operation job and it worked successfully
- Set up the Hadoop cluster using Tokyo VM as the master and Fanship VM as the slave
- Edited the configuration files core-site.xml and yarn-site.xml – specified the ip addresses for the hosts
- Ran into problems while setting up the hadoop cluster: one of them was related to firewall being up (although we thought that we permanently disabled firewalls on our VMs)
- Another problem was that when turning on the services for Namenode and Datanode, only Tokyo showed up as being connected → solution: hadoop required all machines to have a list of the hostnames of all machines in the cluster inside the hostfile
- In order to facilitate the use of Hadoop with ViNe (for future usage), we decided to edit the configuration file hdfs-site.xml so that there's no need to keep the /etc/hosts file consistent on all nodes (easier because ViNe assigns an IP address for each node dynamically)
- Successful Run through of a sample yarn job on the hadoop cluster

Final Results:

- Installation of Java version 8 on the VMs in order to install Hadoop
- Successfully installed Hadoop on Barco Front End 1 VM
- Successfully tested Hadoop in standalone mode
- Successfully tested Hadoop in pseudo-distributed mode
- Successfully tested Hadoop in fully-distributed mode
- Performed cloning of Barco Front End 1 VM to make Tokyo VM and Fanship VM
- Creation of cluster made up of Tokyo VM (master) and Fanship VM (slave)
- Ran multiple sample commands in each mode to verify that Hadoop was working properly

Exploring the Culture

SHIMOJO SENSEI'S LAB TRIP

- **Amanohashidate**
  - Ate Japanese Seafood Donburi
  - Went on a sightseeing ship
  - Got to be at the beach for a little
  - Went to the top of Kasamatsu park after (literally) riding the ropeway
  - Went to winery to do wine tasting
  - Stayed at an onsen hotel in Kinosaki (situated in city full of onsens!)
  - Experienced the onsen experience! Put on yukatas, ate traditional Japanese dinners and went to onsens!
  - Fireworks!
- **Izushi**
  - Had traditional Japanese breakfast
  - Went to an onsen one more time
  - Experienced making soba noodles from scratch (super interesting and fun), then got to eat our own soba!
  - Walked around Izushi and did sake tasting

Exploring the Culture

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Shimojo Sensei's Lab at Kasamatsu Park!
Thank you for inviting us, Shimojo Sensei!

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