

# 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 5 Progress

- Still dealing with the hadoop tutorial
- Figured out how to get a rid of the error about public SSH key; now it works
- Concerned about the warning regarding not being able to find the hadoop native library – talked to graduate students and they said not to worry about it for right now
- Struggling with datanode. We can access the browser that gives us information about namenode and datanode; however, when we click on datanode we get no information (=this means that there is a problem with datanode starting up or being connected)
- Checked the configuration files of Hadoop to look for errors there. Seemed correct
- Checked the logs for errors, found an error saying that all directories in `.dfs.datanode.data.dir` are invalid
- In the process of figuring out this error

# Coming up: Next Week's Goals

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- Today: can only go through until Step 4 of Hadoop tutorial (copying of the input files into the distributed filesystem), when we reach that step → we get errors related to datanode.  
Goal: figure out the problem with datanode and fix it
- Continue and finish the hadoop tutorial which consists of running the MapReduce job locally
- Proceed to do the YARN on a single node part of the tutorial which will allow us to check if we can run a MapReduce job on YARN in a pseudo-distributed mode

# Exploring the Culture

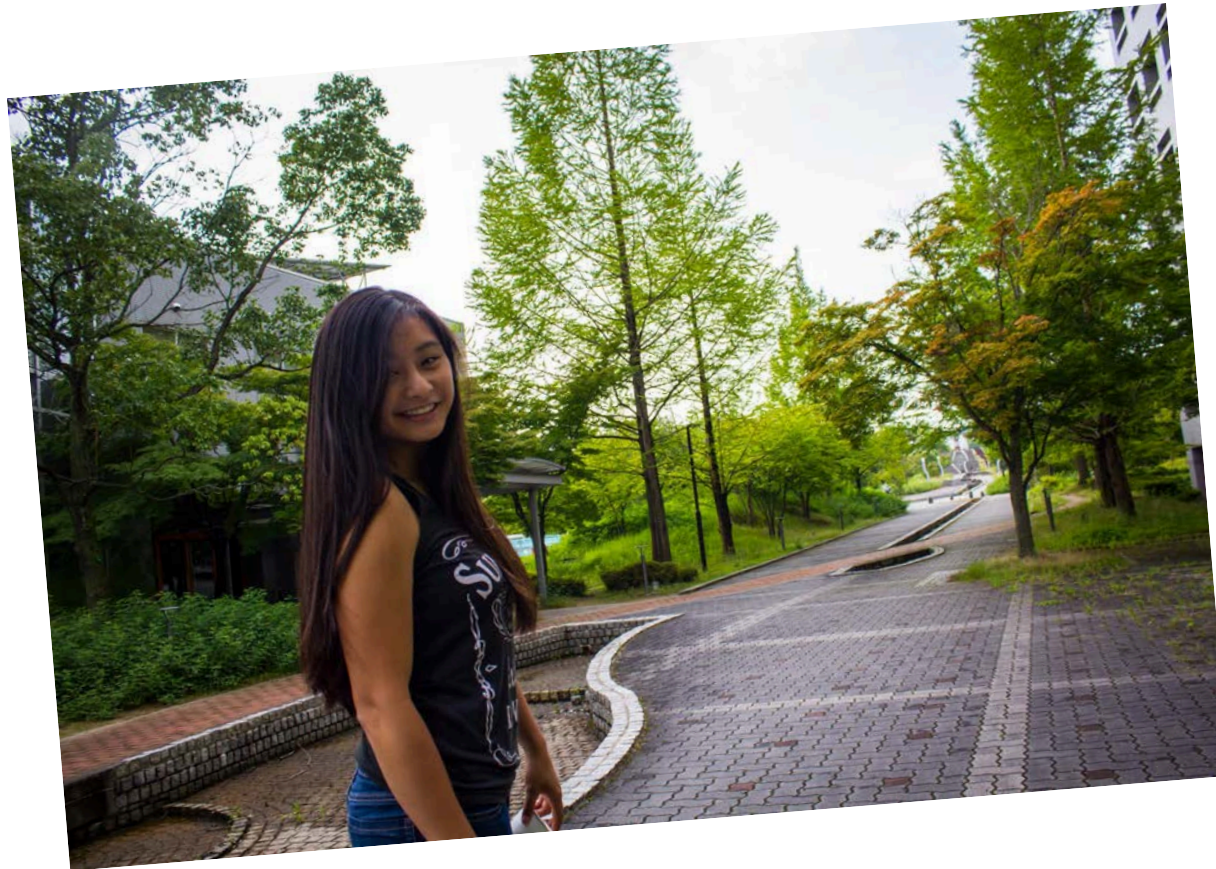
- On Wednesday:
  - Our lab hosted Takoyaki party
    - Made our own takoyaki !
- On Friday:
  - Went to Vietnamese cooking party
    - Made Vietnamese spring rolls and got the Japanese students to try to eat fermented duck eggs!



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# Exploring the Culture



Impromptu photoshoot courtesy of one of the Thai students at NAIST

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# Acknowledgements

- I would like to thank:
  - The graduate students, professors & assistant professors for being so friendly, welcoming and helpful
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