

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

Subtopic: Multi-Cloud

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Overview

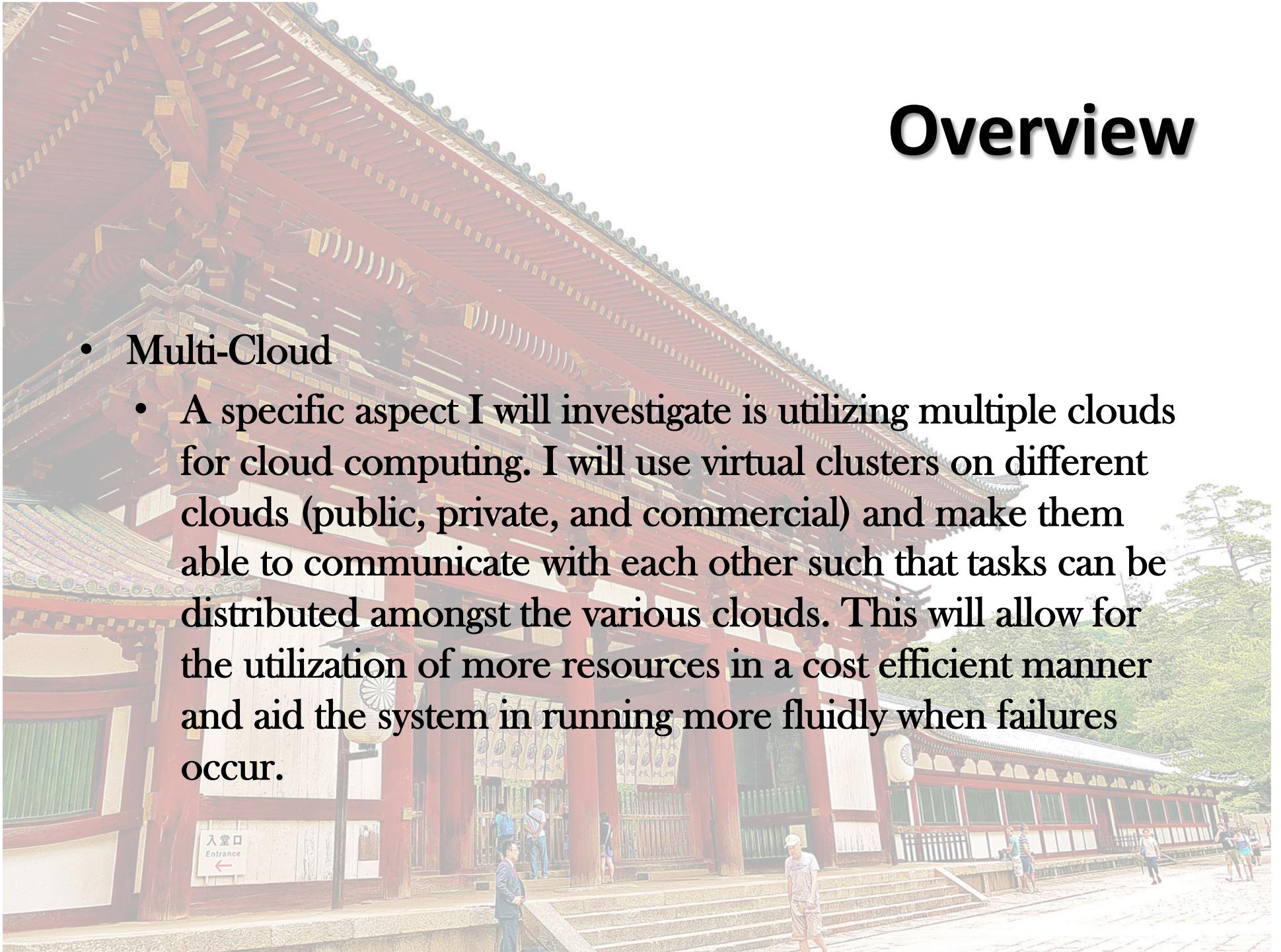
- Background
 - A popular form of computational research used is Grid Computing. However, when doing simulations on a large scale, this becomes costly and unfeasible due to hardware costs. This project takes a newer approach to computational research aiming to utilize a method known as Cloud Computing which will be a more cost efficient method than standard Grid Computing

Overview

- Objective
 - The goal of this research is to upload and clone virtual machines that are capable of running a molecular docking simulation program called DOCK on a cloud system.
 - DOCK is a program that simulates protein-ligand interactions
 - By the end of the research, a system that can run millions of protein-ligand simulations simultaneously will be developed and usable for drug development

Overview

- Multi-Cloud
 - A specific aspect I will investigate is utilizing multiple clouds for cloud computing. I will use virtual clusters on different clouds (public, private, and commercial) and make them able to communicate with each other such that tasks can be distributed amongst the various clouds. This will allow for the utilization of more resources in a cost efficient manner and aid the system in running more fluidly when failures occur.





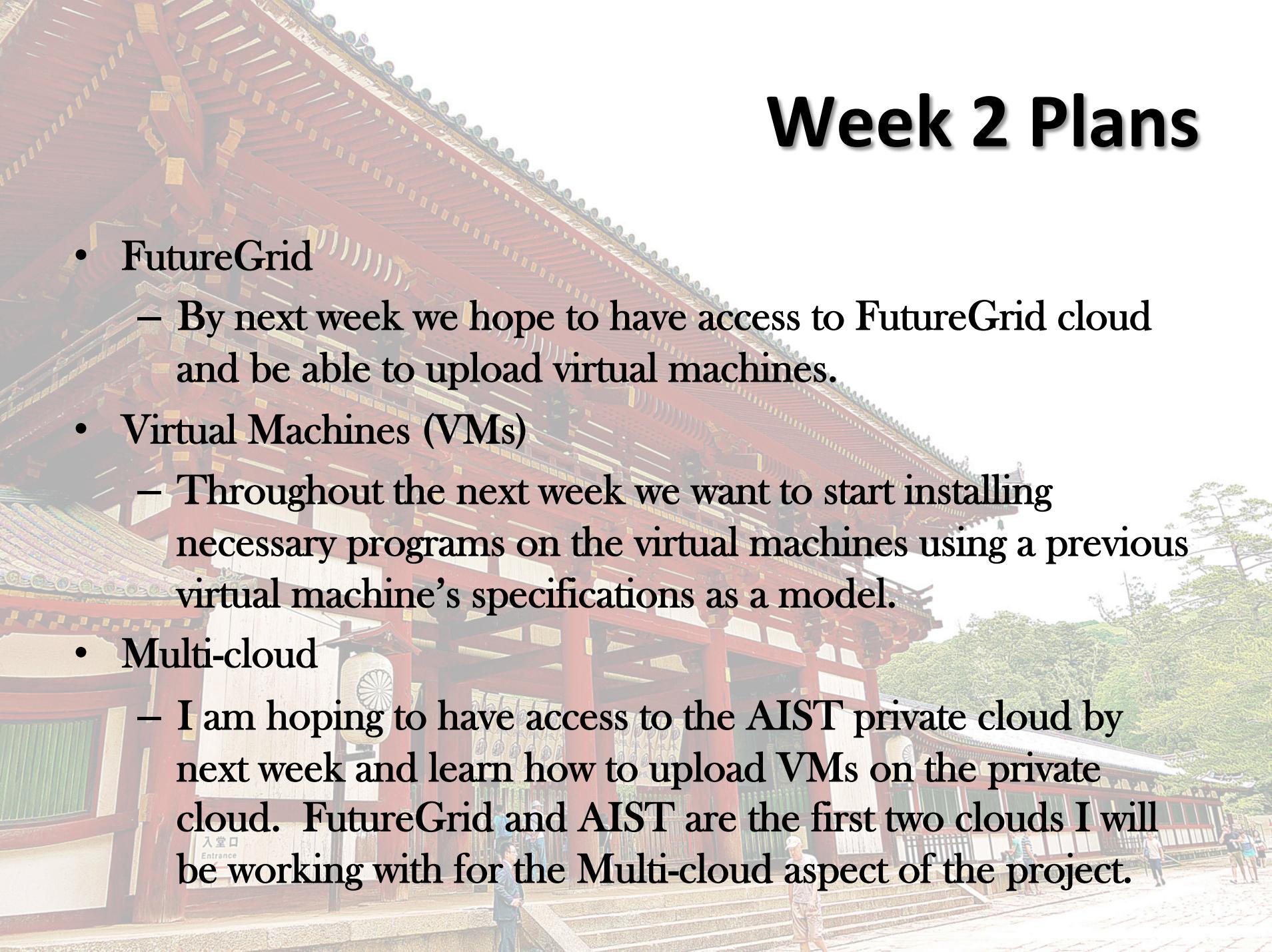
Week 1 Progress

- FutureGrid
 - FutureGrid is a free cloud service that we will put virtual clusters on. To gain access to this cloud, a project proposal must be submitted and approved by FutureGrid. We have written the proposal and it will be submitted within the next few days after accounts have been approved.
- Virtual Machines (VMs)
 - Virtual Machines have been made on a local server. We will be using this local server to do initial testing before moving VMs to the clouds.



Week 1 Progress

- Multi-Cloud
 - For my multi-cloud work, I have been researching how to upload virtual machines on FutureGrid, the primary cloud we will be using.
 - Permission was asked to grant me access to AISt private cloud.
 - I have begun researching ViNe, a networking software that will help with making virtual clusters on different clouds communicate with each other.



Week 2 Plans

- FutureGrid
 - By next week we hope to have access to FutureGrid cloud and be able to upload virtual machines.
- Virtual Machines (VMs)
 - Throughout the next week we want to start installing necessary programs on the virtual machines using a previous virtual machine's specifications as a model.
- Multi-cloud
 - I am hoping to have access to the AIST private cloud by next week and learn how to upload VMs on the private cloud. FutureGrid and AIST are the first two clouds I will be working with for the Multi-cloud aspect of the project.



