The background of the slide is a blue-tinted underwater photograph. It shows several fish swimming in the water, including a large, spotted fish on the left and a manta ray in the lower right. A stream of bubbles rises from the bottom right towards the center of the frame.

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

Subtopic: Multi-Cloud

**Nara Institute of Science and
Technology (NAIST)**

Nara, Japan

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08/06/2014**

The background of the slide is a blue-tinted underwater photograph. It features several large fish, including what appear to be groupers or snappers, and a large school of smaller fish. Bubbles are visible on the right side, suggesting an underwater environment. The text is overlaid on this background.

Week 6 Progress

- FutureGrid
 - The networking problem with using FutureGrid has been resolved.
 - VMs can now successfully be launched and accessed.
 - All VMs on FutureGrid have also been installed with ViNe and have full connectivity, through ViNe, with the VMs on NAIST and AIST clusters.

The background of the slide is a blue-tinted underwater photograph. It features several large fish, including what appears to be a grouper in the upper center and a large snapper or sea bream in the lower left. There are also smaller fish, possibly manta rays or stingrays, and a lot of bubbles rising from the bottom right, suggesting a diver's presence. The overall scene is serene and aquatic.

Week 6 Progress

- AIST
 - A new VM has been launched on AIST. Networking is set up but ViNe has not yet been installed.
- Multi-Cloud Environment
 - The current Multi-Cloud environment with full connectivity via ViNe includes one VM on AIST, one VM on NAIIST, and two VMs on FutureGrid.

The background of the slide is a blue-tinted underwater photograph. It features several fish of different species, including what appears to be a large grouper in the upper center, a large fish with a prominent white stripe (possibly a snapper or sea bream) in the lower left, and several rays or manta fish in the lower right. Bubbles are visible on the right side, suggesting a diver's presence. The overall scene is a vibrant, deep-sea environment.

Week 6 Progress

- DOCK
 - DOCK is now being run on the Multi-Cloud Environment.
 - mpirun command is being used to send DOCK jobs to the the VMs connected via ViNe
 - Fully Functional
 - Parameters are being changed to test performance of DOCK in a Multi-Cloud environment.

Road Blocks -> Approach -> Outcomes

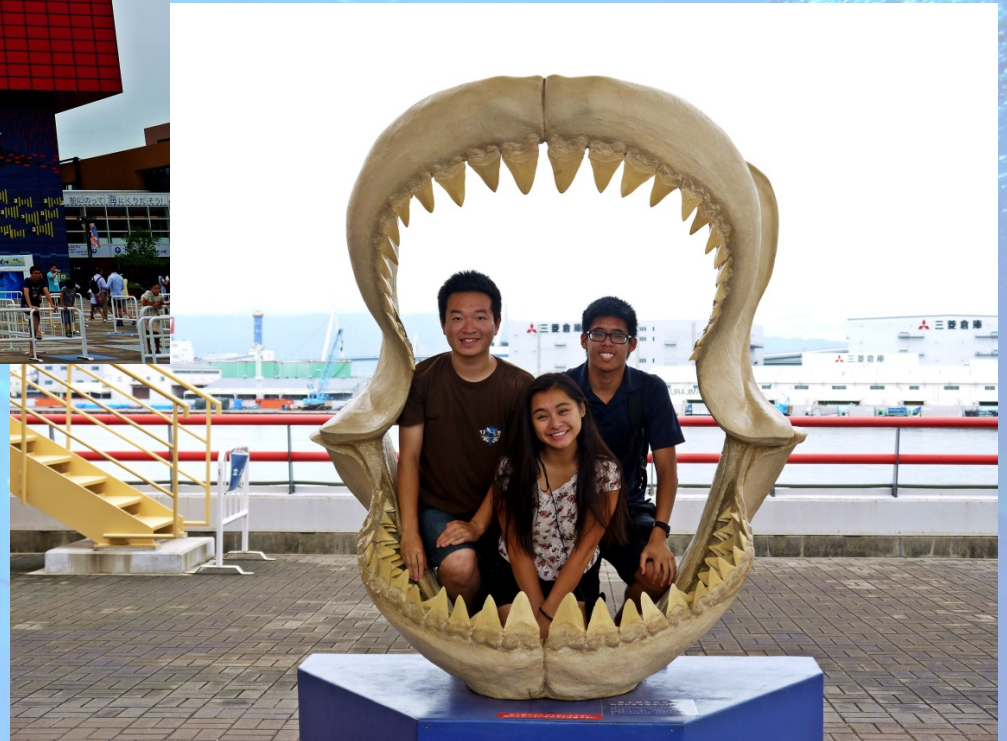
- Command mpirun misunderstanding
 - The initial understanding of the mpirun command was that input files would be sent from the source VM to all other VMs where processing and running of the DOCK simulation would occur.
 - However, upon testing it became apparent that mpirun solely sends the command to all machines listed in the machinefile, it does not send the input
 - Hadoop, a job distribution and scheduling program, should be able to solve this issue.
 - For now, all input files are able to be transferred via scp command and the full connectivity available through ViNe.

The background of the slide is a blue-tinted underwater photograph. It features several fish, including a large, spotted fish in the upper center and a large, spotted fish in the lower left. There are also many small, silvery fish and a large plume of white bubbles on the right side. The overall scene is bright and clear.

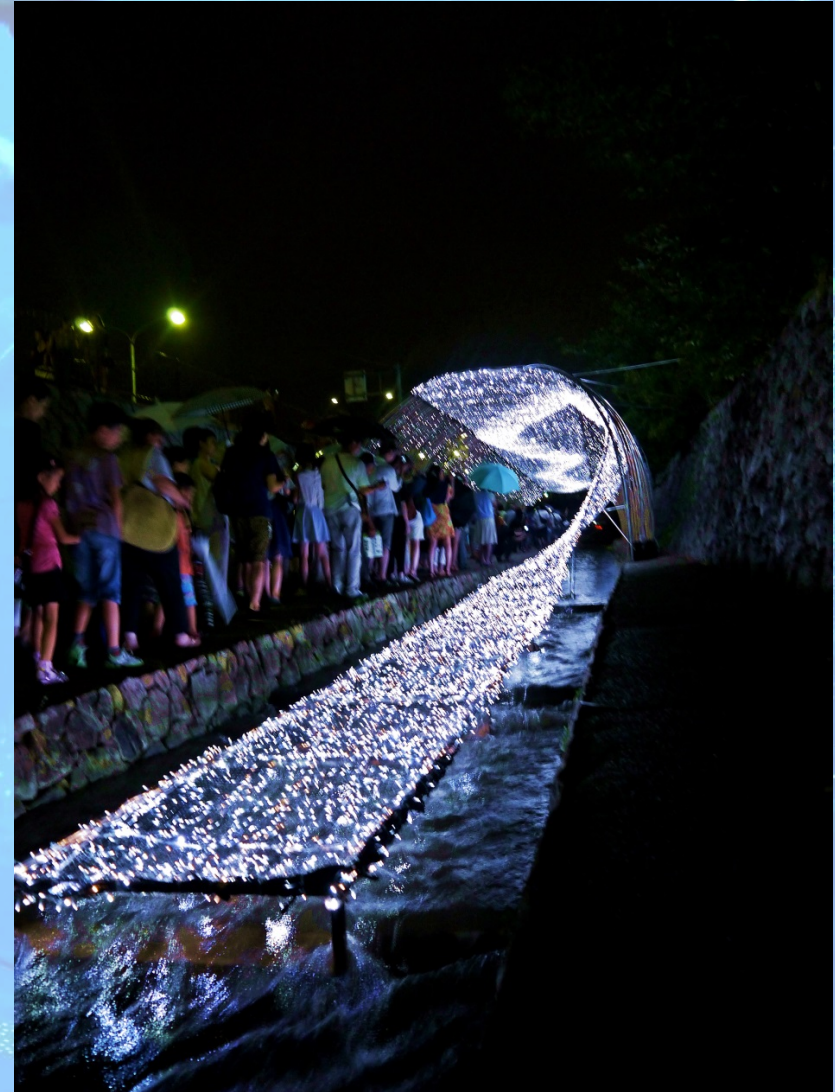
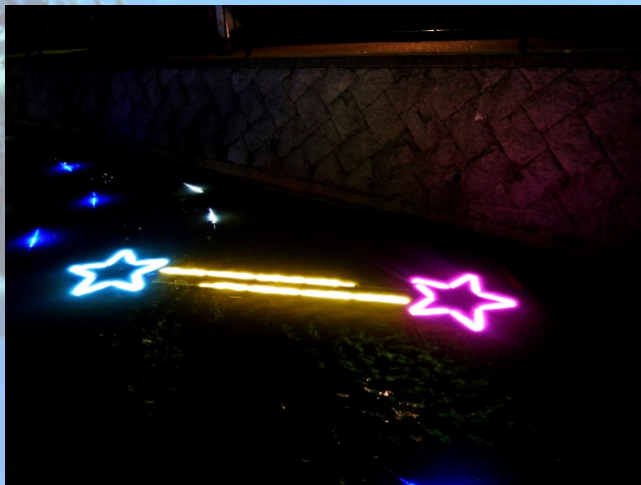
Week 7 Plans

- **Multi-Cloud**
 - Connect the new VM on AIST with ViNe and add another VM with ViNe on NAIST to make a total of six VMs, two on AIST, two on NAIST, and two on FutureGrid
 - All will be connected via ViNe
- **DOCK**
 - Continue running tests by altering variables and checking completion rate to determine performance of DOCK in Multi-Cloud Environment.

Cultural Exploration



Cultural Exploration



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