Deployment of Virtual Clusters in a Multi-Cloud Environment for Molecular Docking

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October 17, 2014

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Background

- Multi-cloud computing is both cost efficient and offers a high degree of versatility and flexibility.
  - No hardware cost (pay for time used)
  - Essentially limitless resources
  - Can easily scale and alter computational environment
  - Adds a degree of fault tolerance (If one cloud has high traffic or goes down for maintenance others still run)

Objective

- The goal is….
  - Develop a multi-cloud environment to run virtual screenings
    - Virtual screenings of molecular dockings performed via DOCK program
- Anticipating that the multi-cloud environment will…
  - Simplify process to scale the number of screenings
  - Maintain same performance level as grid computing

Run DOCK Test

Project Approach

Phase 1

- Launch VMs on Different Clouds

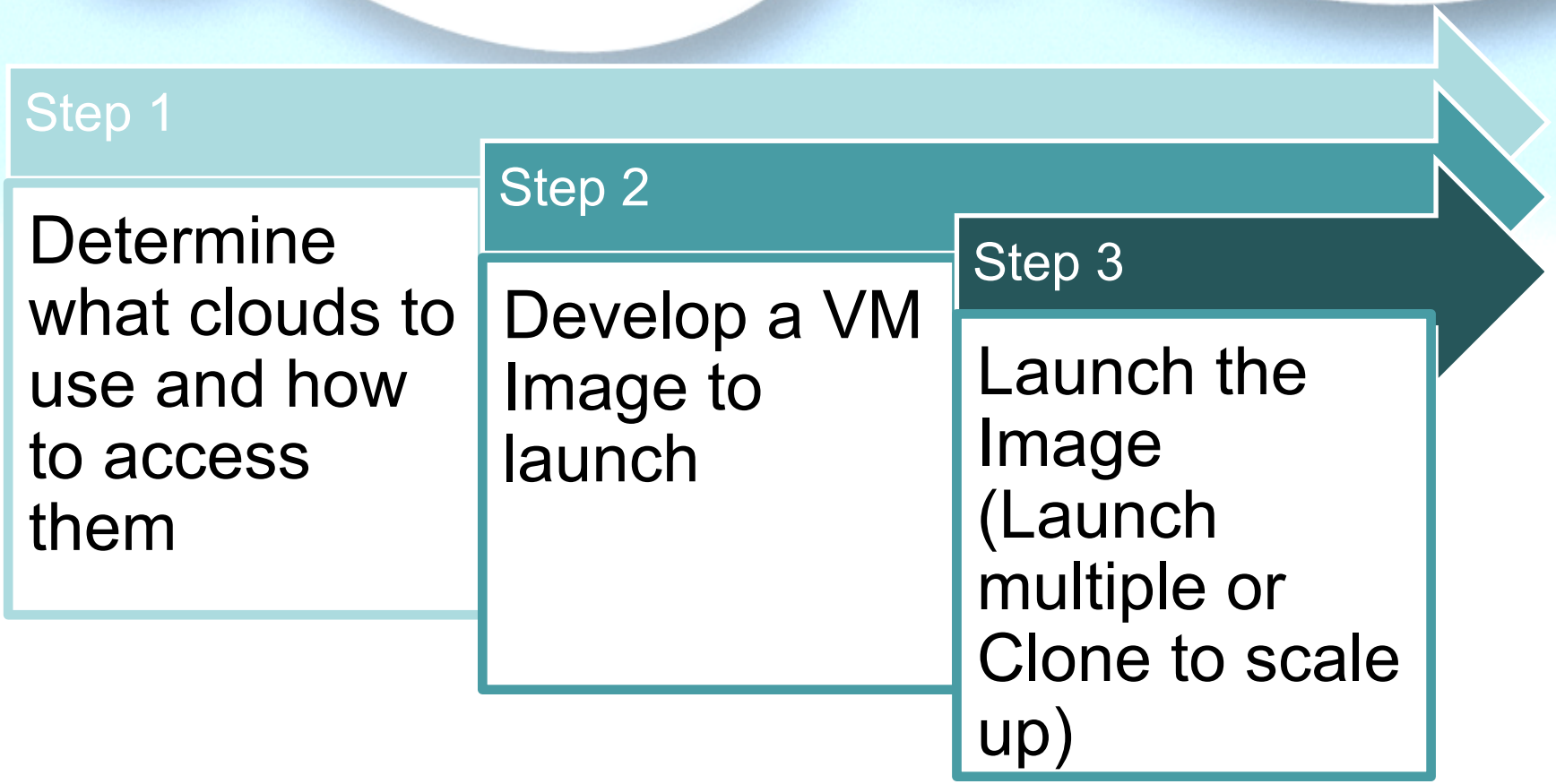
Phase 2

- Establish Connectivity Across Clouds

Phase 3

- Run DOCK Tests and Analyze Results

Phase 1: Launch VMs on Different Clouds



Step 1: Cloud Selection

- Factor
  - Low Cost or Free
- Clouds Selected
  - NAIST Private Cluster Environment
  - AIST Private Cluster Environment
  - FutureGrid Alamo Cloud Computing Resource
    - Proposal Submitted to attain access to FutureGrid resources.

Step 2: Developing VM Image

- Used a KVM Virtual Image designed by UCSD PRIME 2013 Interns
  - This Virtual Image was set up to optimize DOCK program performance with regards to consistency in results.
  - Some modification were necessary to match specific requirements of cloud (network configuration)

Step 3: Launch the Image

- Each Cluster uses a different Cloud Middleware System so image launch method varied from cloud to cloud
  - NAIST: Libvirt (KVM)
  - AIST: OpenNebula
  - FutureGrid Alamo: Nimbus

Project Approach

Phase 1

- Launch VMs on Different Clouds

Phase 2

- Establish Connectivity Across Clouds

Phase 3

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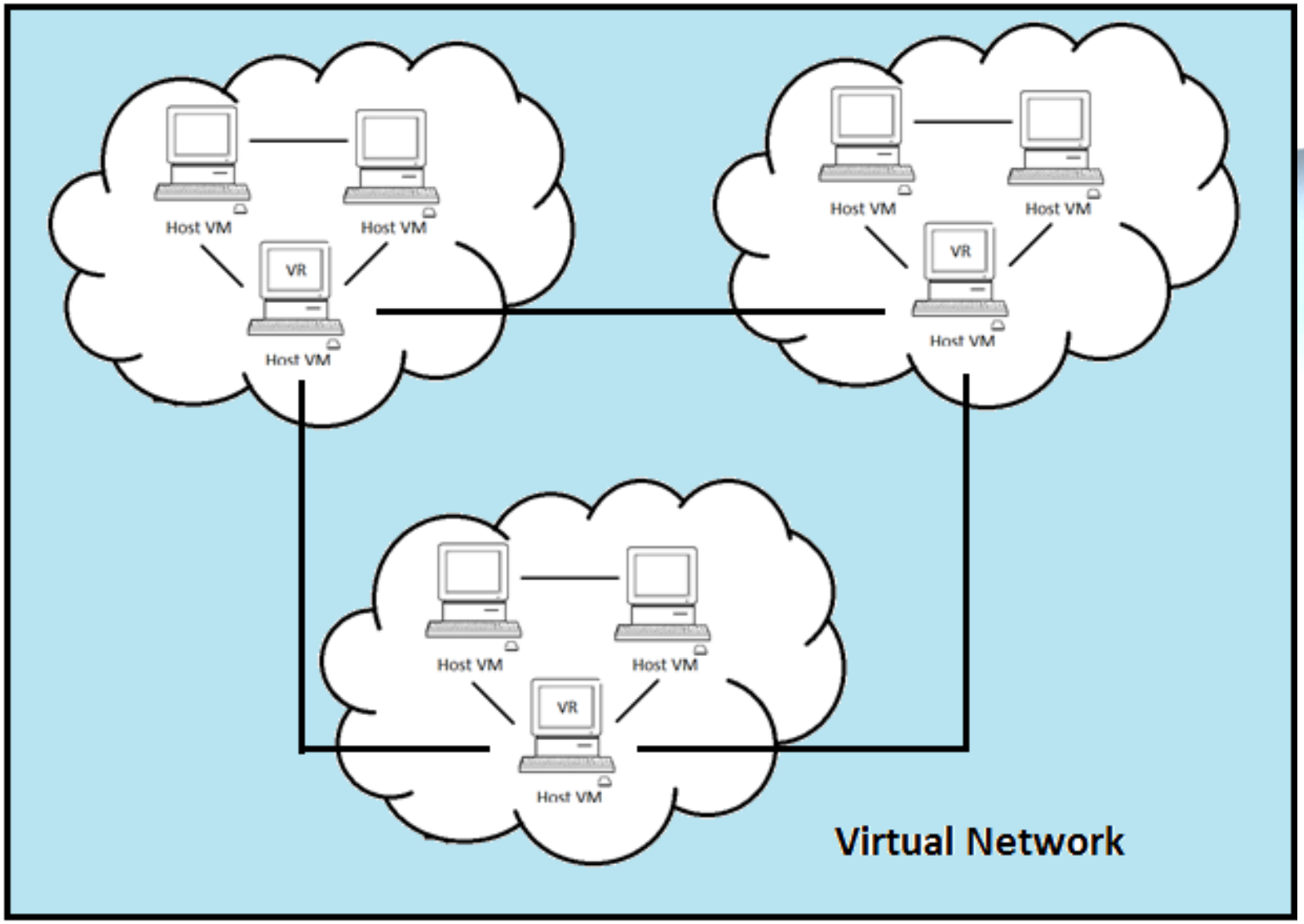
Phase 2: Establish Connectivity

- ViNe
  - Can be used to establish a virtual network supporting symmetric communication beyond boundaries like firewalls
  - Requires no change to physical network
  - Requires no change to machines operating system

How ViNe Works



Project Approach

Phase 1

- Launch VMs on Different Clouds

Phase 2

- Establish Connectivity Across Clouds

Phase 3

- Run DOCK Tests and Analyze Results

Phase 3: DOCK Tests and Results

- With full connectivity in Multi-Cloud Environment, DOCK jobs were run using mpi (message passing interface)
- The tests that were run were used to assess effectiveness and flexibility of a multi-cloud environment.

Our Environment

- Three VMs on NAIST
  - One is master, two run DOCK
- Three VMs on AIST
  - All three run DOCK
- Three VMs on FutureGrid
  - All three run DOCK

Results

- Processing times for DOCK tests in same order of magnitude for Grid Computing and Multi-Cloud Environment
  - Grid Computing DOCK Test
    - 82s per compound per processor
  - Multi-Cloud DOCK Test
    - 30s per compound per processor

Results

- Processing times longer with increased workloads
  - Anticipate that this will no longer be the case when using larger clouds with more resources
- Jobs evenly distributed across clouds and VMs when scaling environment
  - Jobs distributed on a per VM basis, not a per cloud basis

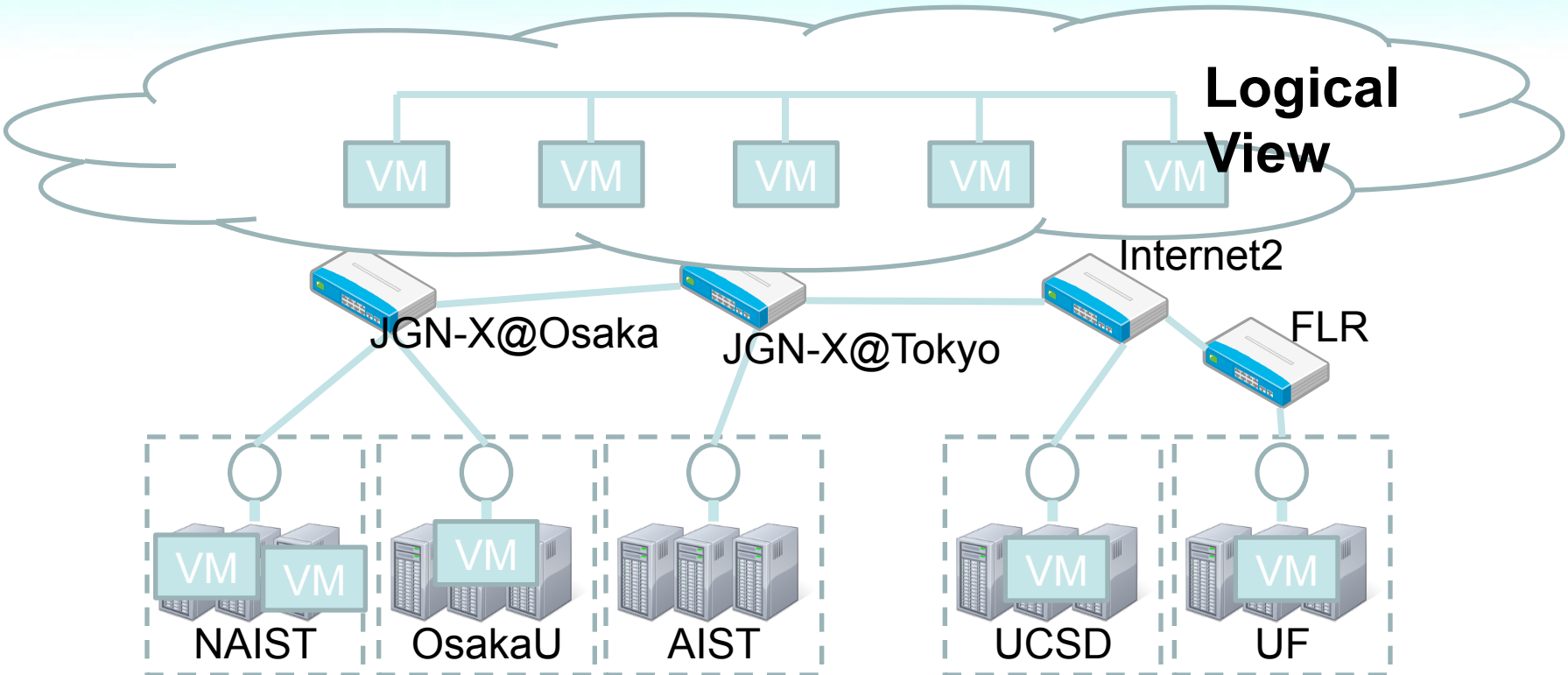
Our Demo Environment

- Two VMs on NAIST
  - One is master, one run DOCK
- One VM on Osaka U
- One VM on UF
- One VM on UCSD

*Connectivity through PRAGMA-ENT

PRAGMA-ENT

- Application using multisite resources
  - Pragma-ENT allows to provide a single L2 flat network for applications. This makes it easy for application users to use multisite resources simultaneously.



DOCK Demo Output

Conclusions and Future Work

- Scaling up of the number of virtual screenings and VMs on the environment was simple and quick
- Performance on the Multi-Cloud environment was equivalent to that on a grid computing environment

- Incorporate Hadoop for job distribution and fault tolerance
- Incorporate larger commercial clouds (Azure) for larger scale tests

Acknowledgements

- Previous PRIME students
  - Kevin Lam
  - Karen Rodriguez
- UCSD Pacific Rim Experiences for Undergraduates (PRIME)
  - Dr. Gabriele Wienhausen
  - Teri Simas
  - Jim Galvin
  - Madhvi Acharya
- Funding Sources
  - URS Ledell
  - PRIME Alumna Haley Hunter-Zinck
  - National Science Foundation

Rigid Test with Flexible Parameter Off

Molecules Processed per Host (100 total)			Test 1 (Small Workload)
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	10	10
AIST	13	11	14
FG	16	14	12

Molecules Processed per Host (100 total)			Test 2 (Large Workload)
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	14	13
AIST	10	12	12
FG	13	11	15

Rigid Test with Flexible Parameter Off

Average Processing Time per Molecule on each Host (sec) Test 1 (Small Workload)			Total Time: 1066 sec
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	96	140
AIST	79	90	70
FG	66	71	81

Average Processing Time per Molecule on each Host (sec) Test 2 (Large Workload)			Total Time: 3015 sec
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	197	222
AIST	280	237	233
FG	232	241	189

Rigid Comparison Test (100 Compounds)

Average Processing Time per Molecule on each Host (Multi-Cloud) (sec) Total Time: 24380			
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	1290	1561
AIST	3104	1184	1649
FG	1907	2603	1850

- Published Rate for Grid Computing DOCK Test
  - **82 seconds per compound per processor**
- Multi-Cloud DOCK Test
  - **30 seconds per compound per processor**

Unbalanced Rigid Test

Molecules Processed per Host (Balanced) (100 total)			Test 1
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	10	10
AIST	13	11	14
FG	16	14	12

Molecules Processed per Host (Unbalanced) (100 total)						
Cloud	**Host 1**	**Host 2**	**Host 3**	**Host 4**	**Host 5**	**Host 6**
NAIST	MASTER	8	9	-	-	-
AIST	9	8	7	-	-	-
FG	9	11	10	9	11	9

Unbalanced Rigid Test

Average Processing Time per Molecule on Each Host (Balanced) (sec) Total Time: 1066 sec			
Cloud	**Host 1**	**Host 2**	**Host 3**
NAIST	MASTER	96	140
AIST	79	90	70
FG	66	71	81

Average Processing Time per molecule on each Host (Unbalanced) (sec) Total Time: 766 sec						
Cloud	**Host 1**	**Host 2**	**Host 3**	**Host 4**	**Host 5**	**Host 6**
NAIST	MASTER	91	82	-	-	-
AIST	73	89	97	-	-	-
FG	78	60	65	80	64	85