XSEDE BOF: Science Clouds

Kate Keahey, David Lifka, Manish Parashar, Warren Smith, Carol Song, Shaowen Wang
Clouds Available to Science
FutureGrid Overview

• A distributed infrastructure to support computer and computational science experiments
  – Performance analysis, software testing and evaluation, interoperability

• A rich education and training platform
  – University courses, multi-day training sessions, informal learning and exploration

• Includes Cloud, Grid, and High-Performance Computing environments
  – Allows users to configure environments to meet their needs
  – Typically available interactively

• Provides tools to support rigorous experimentation
  – Documenting configurations, recording experiments

• Allocatable via XSEDE

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All sites are connected via a core router that is attached to a configurable network impairment device. Dedicated network links are shown in red.

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## IaaS Partitions

<table>
<thead>
<tr>
<th>Site</th>
<th># Cores*</th>
<th>TFLOPS*</th>
<th>Total RAM* (GB)</th>
<th>Secondary Storage* (TB)</th>
<th>Platforms</th>
</tr>
</thead>
<tbody>
<tr>
<td>IU</td>
<td>1308</td>
<td>11</td>
<td>2048+</td>
<td>335</td>
<td>Eucalyptus, OpenStack</td>
</tr>
<tr>
<td>TACC</td>
<td>768</td>
<td>8</td>
<td>1152</td>
<td>30</td>
<td>Nimbus, OpenStack</td>
</tr>
<tr>
<td>UC</td>
<td>672</td>
<td>7</td>
<td>1344</td>
<td>120</td>
<td>Nimbus</td>
</tr>
<tr>
<td>SDSC</td>
<td>672</td>
<td>7</td>
<td>2688</td>
<td>72</td>
<td>Nimbus, OpenStack</td>
</tr>
<tr>
<td>UF</td>
<td>256</td>
<td>3</td>
<td>768</td>
<td></td>
<td>Nimbus</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>3676</strong></td>
<td><strong>42</strong></td>
<td><strong>9344</strong></td>
<td><strong>557</strong></td>
<td></td>
</tr>
</tbody>
</table>

*All partitions on cluster

- Partitions mostly independent (Nimbus ones share authentication credentials)
- Accessed via implementation-specific interfaces and Amazon interfaces
- IU system includes large memory/disk nodes

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Virtual Machine Images and Appliances

- Provide a set of generic Linux images
- Provide appliance images for specific tasks
  - Virtual cluster
  - Condor
  - MPI
  - Hadoop
- Users create and share their own images

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On-Demand Research Computing
  – Infrastructure as a Service –
  – Software as a Service –
  – Cloud Storage Solutions –

www.cac.cornell.edu/redcloud
Commercial Clouds AWS (Kate)

• **Instances**
  – From $0.02 per hour to Top500 membership
  – Xen hypervisor

• **Storage**
  – Transient: 160 GB-48 TB on VM
  – Persistent: Elastic Block Storage (EBS) 1BG-1TB

• **Networking**
  – Internal: up to 10 Gb Ethernet for Cluster Compute
  – AWS Direct Connect (for large volume users)
  – Sneakernet

• **Pricing**
  – Reserved instances (up to 71% savings), 1-3 year commitment
  – Spot instances
Other Major Commercial Offerings (Kate)

• Google Compute Cloud (since 06/12)
  – Target high performance market, emphasizes consistent performance
  – Uses KVM
  – Pricing by the minute

• Windows Azure (since 2010)
  – Started out as a platform offering
  – Uses Windows Azure Hypervisor (can do Linux)

• Rackspace
  – Based on OpenStack (since 2012)
  – Uses Xen hypervisor

• See more at scienceclouds.org…
Science Cloud Solutions: from Private and Community Clouds to Commercial Clouds from Proof-of-Concept to Solution
Image Management
Contextualization

• Mainstream ctx tools: Chef, Puppet
• Providing abstractions, scalability, repeatability and control
  – StarCluster, Nimbus Context Broker, cloudinit.d

How can I create virtual clusters automatically?

How can I automate multi-dependency deployments?

How can I automate upgrades?

How can I monitor the changes to the environment consistently?

How can I securely create a trust layer?
Multi-Cloud, Availability and Scalability

• Creates and manages “domains”, groups of resources in the cloud
• Scalability and availability
  – regulate domain properties based on system and application metrics
• Multi-cloud
  – Mitigate risks by working with multiple providers
• Extensible monitoring
  – VM-based, provider-based, and domain data
  – OpenTSDB, traffic sentinel, AWS CloudWatch, etc.
• Policy agnostic
  – From pre-defined policies to python programs
Integrating On-Demand Resources

Phantom → Workflow → Process Dispatcher → Torque Scheduler → Condor Scheduler
Science Cloud Applications
Ocean Observatory Initiative

- Towards Observatory Science
- Sensor-driven processing
  - An “always-on” service
  - Real-time event-based data stream processing capabilities
  - Highly volatile need for data distribution and processing
- Nimbus team building platform services for integrated, reactive support for on-demand science
  - High-availability
  - Auto-scaling
- From regional Nimbus clouds to commercial clouds
Building a Plant Observatory

Spectral Indices*
NDVI • SAVI • EVI • NDWI

Multi-Temporal Hyperspectral Cubes and Spectral Index Images

Diseases

application images courtesy of Yuki Hamada, ANL

Joint project with Pete Beckman, Nicola Ferrier, Yuki Hamada, Rao Kotamarthi, Rajesh Sankaran and others (ANL)
The iPlant Collaborative

- Challenge: to build a lasting, community driven Cyberinfrastructure for the Grand Challenges of Plant Science

Building a platform that can support diverse and constantly evolving needs.

- Storage
- Computation
- Hosting
- Web Services
- Scalability
iPlant Cloud Investments

• Atmosphere (pre-configured virtual machines)
  – Private science cloud @ University of Arizona
  – Eucalyptus -> OpenStack
  – Custom UI & API

• Discovery Environment (web-based access to tools and data)
  – Several services running in the cloud
  – DevOps in the cloud

• Foundation API (programmatic access to iPlant)
  – Running on multiple clouds (FutureGrid, HP, Rackspace)
  – Leveraging PaaS and SaaS (HP, Iron.io)
  – DevOps in the cloud
  – Supports execution to arbitrary IaaS providers.
Apache Airavata
Science Gateway Framework

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Courtesy of Suresh Marru, Indiana University
SWATShare – Online SWAT Simulation and Model Sharing

http://water-hub.org

- An XSEDE science gateway
- Available to broad SWAT user community
- Being integrated with Hydroshare project funded by NSF SI2 award
- Used by researchers and classes
  - Simulation of daily streamflow for water resources management in Wabash River Basin
  - Simulation of monthly flows for drought prediction and crop management
  - Simulation of daily, monthly and annual streamflows for nutrient loading
- Technical implementation
- Using different resources based on job nature:
  - Simulation
  - Calibration
  - Sensitivity experiment
- Challenges relevant to cloud computing
  - On-demand scalability
  - Adaptability
    - E.g., migrate from one resource to next
Discussion:
How can clouds complement the existing XSEDE resources?
XSEDE Cloud Investigation

• Investigation Team
  – Ian Foster, Steve Tuecke, ANL/University of Chicago
  – David Lifka, Susan Mehringer, Paul Redfern, Cornell University CAC
  – Craig Stewart, Indiana University
  – Manish Parashar, Rutgers University

• Cloud Survey Motivation
  – The goal of XSEDE is to enhance research productivity
  – XSEDE must embrace cloud
  – XSEDE must have a clear understanding of how researchers using the cloud today and why
  – Based on this information XSEDE plans to integrate cloud services into its portfolio to support use cases that are not well served by its current resource offerings

• Survey Status ([www.xsede.org/cloudsurvey](http://www.xsede.org/cloudsurvey) - closed end of March; report by July 1)
  – 80 cloud projects from around globe, broad participation (21 disciplines + HASS), extensive technical data (19 categories), user perspectives, e.g., cloud benefits/challenges
  – Focused exclusively on use of cloud for research and education
User Identified Benefits

1. Pay as You Go
2. Lower Costs
3. Compute Elasticity
4. Data Elasticity
5. Software as a Service
6. Education as a Service
7. Broader Use
8. Scientific Workflows
9. Rapid Prototyping
10. Data Analysis
User Identified Challenges

1. Learning Curve
2. Virtual Machine
3. Bandwidth
4. Memory Limits
5. Databases
6. Interoperability
7. Security
8. Data Movement
9. Storage
10. Cost/Funding