Cloud Computing Technology in Scientific Research

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Outline

• What is Cloud Computing

• A case-study of Scientific Research of the Cloud

• Conclusion
A Golden Era in Computing

- Powerful multi-core processors
- General purpose graphic processors
- Superior software methodologies
- Virtualization leveraging the powerful hardware
- Explosion of domain applications
- Proliferation of devices
- Wider bandwidth for communication

Proliferation of devices
Explosion of domain applications
Wider bandwidth for communication
Global Data, Global Science

- Sloan Digital Sky Survey (SDSS) year 2000
  - about 200 GB every night
  - amassed more than 140 TB
- LHC (Large Hadron Collider)
  - 15 PB/year, Total data: Several hundred PB total
  - Analysed by thousands of physical scientists worldwide
- Walmart
  - handles 1 million customer transactions every hour
  - estimated to contain more than 2.5 PB data
- FaceBook
  - handles 40 billion photos from its user base
Challenges

• Alignment with the needs of the business / user / non-computer specialists / community and society

• Need to address the scalability issue: large scale data, high performance computing, automation, response time, rapid prototyping, and rapid time to production

• Need to effectively address
  ✓ ever shortening cycle of obsolescence
  ✓ heterogeneity
  ✓ rapid changes in requirements

• Transform data from diverse sources into intelligence and deliver intelligence to right people/user/systems

• What about providing all this in a cost-effective manner?
Answer: The Cloud Computing?

- Typical requirements and models:
  - Platform (PaaS),
  - Software (SaaS),
  - Infrastructure (IaaS),
  - Services-based application programming interface (API)
- A cloud computing environment can provide one or more of these requirements for a cost
- Pay as you go model of business
- When using a public cloud the model is similar to renting a property than owning one.
- An organization could also maintain a private cloud and/or use both.
What is the cloud computing

• **Cloud Computing** is a general term used to describe a new class of network based computing that takes place over the Internet,
  ✓ basically a step on from Utility Computing
  ✓ a collection/group of integrated and networked hardware, software and Internet infrastructure (called a platform).
  ✓ Using the Internet for communication and transport provides hardware, software and networking services to clients

• These platforms hide the complexity and details of the underlying infrastructure from users and applications by providing very simple graphical interface or API (Applications Programming Interface).
What is the cloud computing

• In addition, the platform provides on demand services, that are always on, anywhere, anytime and any place.

• Pay for use and as needed, elastic
  ✓ scale up and down in capacity and functionalities

• The hardware and software services are available to
  ✓ general public, enterprises, corporations and businesses markets
## Cloud Deployment Model

**NIST Deployment Models**

<table>
<thead>
<tr>
<th>Cloud Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Public Cloud</td>
<td>Cloud infrastructure made available to the general public.</td>
</tr>
<tr>
<td>Private Cloud</td>
<td>Cloud infrastructure operated solely for an organization.</td>
</tr>
<tr>
<td>Hybrid Cloud</td>
<td>Cloud infrastructure composed of two or more clouds that interoperate or federate through technology</td>
</tr>
<tr>
<td>Community Cloud</td>
<td>Cloud infrastructure shared by several organizations and supporting a specific community</td>
</tr>
<tr>
<td>Virtual Private Cloud</td>
<td>Cloud services that simulate the private cloud experience in public cloud infrastructure</td>
</tr>
</tbody>
</table>

... and one other
Typical Cloud Platform

Windows Azure

Amazon EC2

Google App Engine
Outline

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• Conclusion
CAS is a leading academic institution and comprehensive research and development center in natural science, technological science and high-tech innovation in China.

It was founded in Beijing on 1st November 1949 on the basis of the former Academia Sinica (Central Academy of Sciences) and Peiping Academy of Sciences.
The total number of graduates in the whole academy has now reached 44,978, including 45.5% PhD candidates.
Scientific Data Deluge in CAS

- Large scientific facilities produce huge data
  - +20 being operation
  - +20 under construction
- Long-Term field observation stations
  - +100 stations including Ecology, Environment, Space, etc.
- Long-Term Research data need to be archived and curation and sharing
  - 100+ institutes
Computer Network Information Center (CNIC)

- is a supporting institute of CAS for the Construction, Operation and Services of Cyberinfrastructure

- China Science and Technology Network Center
- Supercomputing Center
- Scientific Data Center
- ARP Operation Support Center
- Internet-based Science Communication Center
- China Internet Network Information Center

[Graph showing percentages: 154, 20% and 606, 80%]
Data Centers Distribution of CNIC

- **Scientific Data**
  - ~1PB
  - Above 60 institutions
  - Multiple Disciplines

- **Storage Capacity**
  - ~22PB (50PB)
  - 1 major center
  - 1 archive center
  - 12 middle-size center

- **Computing Capacity**
  - ~5000 (10000) CPU cores
  - Dedicated design for DIC
New challenge and requirement in Modern scientific research

Cloud Computing can help?

- HPC (scientific computing)
- BigData (scientific data)
Case 1: High-Performance Cloud Computing

- Scientific computing often requires the availability of a massive number of computers for performing large scale experiments. Traditionally, these needs have been addressed by using high-performance computing solutions and installed facilities such as clusters and super computers, which are difficult to setup, maintain, and operate.

- Cloud computing provides scientists with a completely new model of utilizing the computing infrastructure. Compute resources, storage resources, as well as applications, can be dynamically provisioned (and integrated within the existing infrastructure) on a pay per use basis. These resources can be released when they are no more needed.
Case 1: High-Performance Cloud Computing

Move the computing work to cloud

An example of SaaS:

CAS Data Cloud Computing Service

We provide some simple scientific computing service. People can submit Application Wares jobs through a website, then our scheduler assign adequate resources for this job.
Case 1: **High-Performance Cloud Computing**

*Move the computing work to cloud*

**Application Wares**

**Gauss Computation**

**Group:**
You are the group manager

**Description:**
The application is now serving for Prof. Hao Wen’s Research Group from Institution of Engineering, CAS. Gaussian 09 is the latest in the Gaussian series of programs. It provides capabilities for electronic structure modeling. Gaussian 09 is licensed for a wide variety of applications. All versions of Gaussian 09 contain every scientific/modeling feature, and none impose limitations on calculations other than your computing resources and patience.

**Operation:**
- Submit Single Job
- Submit Batch Jobs
- Submit Zip Jobs

People can submit batch of jobs at one time.

When huge amounts of jobs come, our computing resource get an effective utilization.
Case 1: High-Performance Cloud Computing

Move the computing work to cloud

Management and statistics of submitted jobs are extended functions.

<table>
<thead>
<tr>
<th>JobID</th>
<th>Command</th>
<th>Arguments</th>
</tr>
</thead>
<tbody>
<tr>
<td>234501</td>
<td>/panfs/MPIBlade_Users/libzdcn/lib/beast1.7.1</td>
<td>BEAST_Cayratia_small.xml</td>
</tr>
<tr>
<td>234498</td>
<td>/panfs/MPIBlade_Users/libzdcn/lib/beast1.7.1</td>
<td>BEAST_Cayratia_7.25.xml</td>
</tr>
<tr>
<td>231143</td>
<td>/panfs/MPIBlade_Users/libzdcn/lib/beast1.7.1</td>
<td>combine_new8.xml</td>
</tr>
<tr>
<td>231142</td>
<td>/panfs/MPIBlade_Users/libzdcn/lib/beast1.7.1</td>
<td>combine_new7.xml</td>
</tr>
</tbody>
</table>
Case 2: Public Cloud of CAS Based on OpenStack

OpenSource help us to establish our own cloud

“OpenStack is a global collaboration of developers and cloud computing technologists producing the ubiquitous open source cloud computing platform for public and private clouds. The project aims to deliver solutions for all types of clouds by being simple to implement, massively scalable, and feature rich. The technology consists of a series of interrelated projects delivering various components for a cloud infrastructure solution.”
Platform Architecture of Public Cloud in CAS

- Horizon Dashboard
- Unified Authentication of SDC
- keystone
- nova-api
- nova-volume
- VM
- Shared Storage
the Status of Public Cloud in CAS

- 9 nodes (one controller + 7 compute node + one storage node)
  - 32G RAM, 16cores, 4T DISK
  - OS: ubuntu 11.10
  - Hypervisor: KVM
- Openstack Release: ESSEX
- Network: FlatDHCP, multi-host
- 7 months
- Use Puppet to deploy and manage
- Maximum VMS: 300+
the Future Plan of Public Cloud in CAS

- **Openstack HA**
  - HA MySQL
    - DRBD Master/Slave
    - Multi Master
  - HA RabbitMQ
    - DRBD Master/Slave (Deprecated)
    - RabbitMQ Active/Active (Mirrored Queues)
  - HA Glance/Keystone
    - Glance API
    - Glance Registry
    - Keystone
  - Nova
    - Front-end API Servers - HW/SW load balancer
    - Other services

- **HPC in Openstack**
  - Dedicated configuration and optimization for VMS

- **Schedule algorithm**
  - Different types of application scenario
  - Customized requirements

- **Monitor Components**
Case 3: A Migratory Birds’ Spatial Distribution Prediction System Based on *Hadoop*

Lots of algorithms used by scientific computing can be divided to adapted to the MapReduce model. MapReduce can describes problems suitable for clouds. MapReduce covers many high throughput computing applications including "parameter searches". Many data analysis applications including information retrieval fit the MapReduce paradigm.
Case 3: A Migratory Birds’ Spatial Distribution Prediction System Based on Hadoop

The Bird-SDPS uses birds’ GPS tracking data and remote sensing data as input to build multiple distribution models, which are implemented by different programming languages. And the system provides online access and visualization functions. In order to store large dataset of remote sensing data, we design a hybrid storage structure based on Hbase.
Case 3: A Migratory Birds’ Spatial Distribution Prediction System Based on Hadoop

- we have to confront a much larger dataset (larger than 100 GB). The dataset is so large that it cannot be stored and accessed through relational database.
- Therefore, we employed HBase, which is a typical NoSQL database based on Hadoop framework, to store and process these text data.
Case 4: Collaboration with Microsoft (Windows Azure)

Windows Azure

- Enterprise-level on-demand capacity builder
- Fabric of cycles and storage available on-request for a cost
- You have to use Azure API to work with the infrastructure offered by Microsoft
- Significant features: web role, worker role, blob storage, table and drive-storage
Case 4: Collaboration with Microsoft (Windows Azure)

We got a certain amount of Windows Azure Resources and we are trying to use them properly. More in-depth cooperation will be carried out.

Windows Azure Collaboration Timeline

2012

• February 15 Effective Date of Microsoft Online Subscription Agreement
• February 22 Our account is ready for activation in the system
• April 02 Deploy our first Windows Azure testing service
• July 10 Our experimental mapreduce job running on Azure Hadoop
• October 22 We made a plan of further collaboration with MicroSoft
Case 4: Collaboration with Microsoft (Windows Azure)

The use of Azure

Open Azure to our graduate student to help them establish experiments environment. Also, we can get high-performance Windows/Linux hosts from Azure to establish distributed Matlab environment to run some algorithms.
Case 4: Collaboration with Microsoft (Windows Azure)

Hadoop Azure is an exciting product

Reduce to deduce!

Your Cluster: test2cnic.cloudapp.net

Hadoop Azure make people can generate their own Hadoop cluster on cloud. All you need to do is submitting mapreduce job on the website. It will make everything easy and safe.
Case 4: Collaboration with Microsoft (Windows Azure)

Plans of Windows Azure academic collaboration

we will issue a statement about an academic collaboration. You can fill in a simple proposal paper and send it to us. We will collect the proposal and do some associated review work with Microsoft, we can provide Window Azure resources to users who can offer their stated requirement.
Case 5: Geospatial Data Cloud
Welcome to the Age of Data-intensive GIScience!
Data-intensive GIS = principles and applications of geoinformatics for handling very large data sets
Challenges for data-intensive GIScience

Which data is out there?
How to organize big spatial data?
How to get the data I need?

How to model big data?
How to access and use big data?
GIS technology for big data
Geospatial Data Cloud

• The management, processing and utilization of these mass data is a big and difficult challenge for scientists

  • Distributed: The RS data was stored in different data centers around the world
  • Spatial-temporal: Scientists want to search their focused data quickly by spatial and temporal characteristics
  • Massive data entities, Petabytes or more: A great challenge to view, store, move, share these massive data for scientists

To solve these problems, the recent cloud computing and cloud storage technology can meet these requirements
Geospatial Data Cloud--Objectives

• Based on CASDC, Constructing a highly scalable Geospatial Data Cloud for the Geographical research, Remote Sensing application and related research

• To meet the requirements of:
Geospatial Data Cloud-- **Key technologies**

- Aggregating open data resources
  - Crawling metadata and cache data entities from the Internet
  - Reorganizing raw data and push them to the cloud database

- Providing an user-friendly search engine
  - Users can find their favorite data records easily and quickly
    - Online open data entity, download directly
    - Offline open data entity, submitting application form. Crawling tools fetch and cache data from Internet, then provide for downloading
    - Commercial data entity, providing quick link to the data provider
Geospatial Data Cloud-- Key technologies

- Integrating typical analytical models and GIS tools:
  - Encapsulating models as services in the cloud computing environment
  - Providing online calculation for scientists: NDVI, EVI, Land Surface temperature, projection, clip, resample, format conversion et al.

- Providing private cloud storage for scientists
  - Free, secured, and permanent cloud storage
  - Users can manage their private data
  - Permanent store model results
  - Share data between users
Geospatial Data Cloud-- Key technologies

- Efficient mass data management strategy
  - All earth observation data stored in the parallel cloud databases
    - System Architecture: postgresql + postgis + pgpool
    - The data table is divided properly, and dispersed on database nodes
  - Establish attribute indexes and geospatial indexes enables fast retrieval become possible
Geospatial Data Cloud-- **Key technologies**

- Web crawling technique for geospatial data
  - Developing web crawling tools to fetch data from Internet
  - Rearranging the raw metadata, push to the cloud database for search service
  - Automatically fetch metadata & data entities from NASA and USGS web sites
Geospatial Data Cloud-- Key technologies

- Online geospatial model calculation
  - Analysis models and GIS tools were wrap as web services
  - Providing online parameter pages for users to submit tasks
  - Users can use private data and platform data for model calculation
  - All user tasks were dispatched by task scheduler asynchronously
Geospatial Data Cloud-- **Key technologies**

- Data localized task scheduling
  - Big Data File System
    - A smart distributed file system for big data computation
    - High scalable, dynamically expanding storage space
    - Smart Data Replication
      - Automatically balance data distribution when a computer node breaks down
Data localized task scheduling (cont.)

- **File Allocation Strategy**

  🌐 A file has at least 2 copies, the file stored as data chunks, the first copy distributed in a node, and other copies distributed in other nodes.

  🌐 With this strategy, high read speed up to 800MB/s, VS single disk only up to 60MB/s.
Geospatial Data Cloud-- Key technologies

- Data localized task scheduling (cont.)
  - Task Scheduling Strategy
    - Goal: Minimized the data transmission through network
    - Data localized task scheduler:
      - First, find the node location of data chunks of all model input files
      - Then dispatch the computation task to the corresponding node
Geospatial Data Cloud-- Online data resources

- Original Data from Internet: 76 datasets
  - Several data resources. Including LANDSAT, MODIS, MODIS_L1B, EO-1, DEM, NCAR, AVHRR......
  - The amount of data reached 220 TB, the number of metadata reached to 6 million

- Processed data products: 40 datasets
  - Including Land Surface Temperature, NDVI, EVI of 5 days, 10 days, 15 days and 30 days ...

- All these open data are providing online services for free

- All data covered China and the surrounding region
Geospatial Data Cloud-- Online data resources

- Data Products produced by CNIC
  - The maximum value of Land Surface Temperature, NDVI, EVI in 5 days, 10 days, 15 days and 30 days, from 2000 – 2010
  - Calculated from original modis hdf files
Geospatial Data Cloud- System Introduction

- Homepage(www.gscloud.cn)
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Conclusion

• The use of the cloud provides a number of opportunities
  ✓ It enables services to be used without any understanding of their infrastructure.
  ✓ Cloud computing works using economies of scale:
  ✓ Data and services are stored remotely but accessible from “anywhere”.
Conclusion

- In parallel there has been backlash against cloud computing:
  - Use of cloud computing means dependence on others and that could possibly limit flexibility and innovation:
    - The others are likely become the bigger Internet companies like Google and IBM, who may monopolise the market.
    - Some argue that this use of supercomputers is a return to the time of mainframe computing that the PC was a reaction against.
  - Security could prove to be a big issue:
    - It is still unclear how safe out-sourced data is and when using these services ownership of data is not always clear.
  - There are also issues relating to policy and access:
    - If your data is stored abroad whose policy do you adhere to?
    - What happens if the remote server goes down?
    - How will you then access files?
    - There have been cases of users being locked out of accounts and losing access to data.
Conclusion

• should be able to run a variety of scientific applications on the cloud

• Microsoft and CNIC will issue a **statement about an academic collaboration**

  ✔ You can fill in a simple proposal paper and send it to us. We will collect the proposal and do some associated review work with Microsoft, we can provide Window Azure resources to users who can offer their stated requirement
The End
Thanks!
Please contract me:
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