“…computation may someday be organized as a public utility…”

John McCarthy, Professor at Stanford, 1961

Lecture A.2:
Large-Scale Processing on the Cloud

CS205: Computing Foundations for Computational Science
Dr. David Sondak
Spring Term 2021

HARVARD
School of Engineering
and Applied Sciences

INSTITUTE FOR APPLIED
COMPUTATIONAL SCIENCE
AT HARVARD UNIVERSITY

Lectures developed by Dr. Ignacio M. Illorente

Before We Start

Where We Are

Computing Foundations for Computational and Data Science

How to use modern computing platforms in solving scientific problems

Intro: Large-Scale Computational and Data Science

A. Parallel Processing Fundamentals

- A.1. Parallel Processing Architectures
- A.2. Large-scale Processing on the Cloud
- A.3. Practical Aspects of Cloud Computing
- A.4. Application Parallelism
- A.5. Designing Parallel Programs

B. Parallel Computing

C. Parallel Data Processing

Wrap-Up: Advanced Topics

CS205: Contents

APPLICATION SOFTWARE

APPLICATION PARALLELISM

PARALLEL PROGRAM DESIGN

PROGRAMMING MODEL

Optimization

OpenACC

OpenMP

MPI

Spark

Map-Reduce

PLATFORM

B. BIG COMPUTE

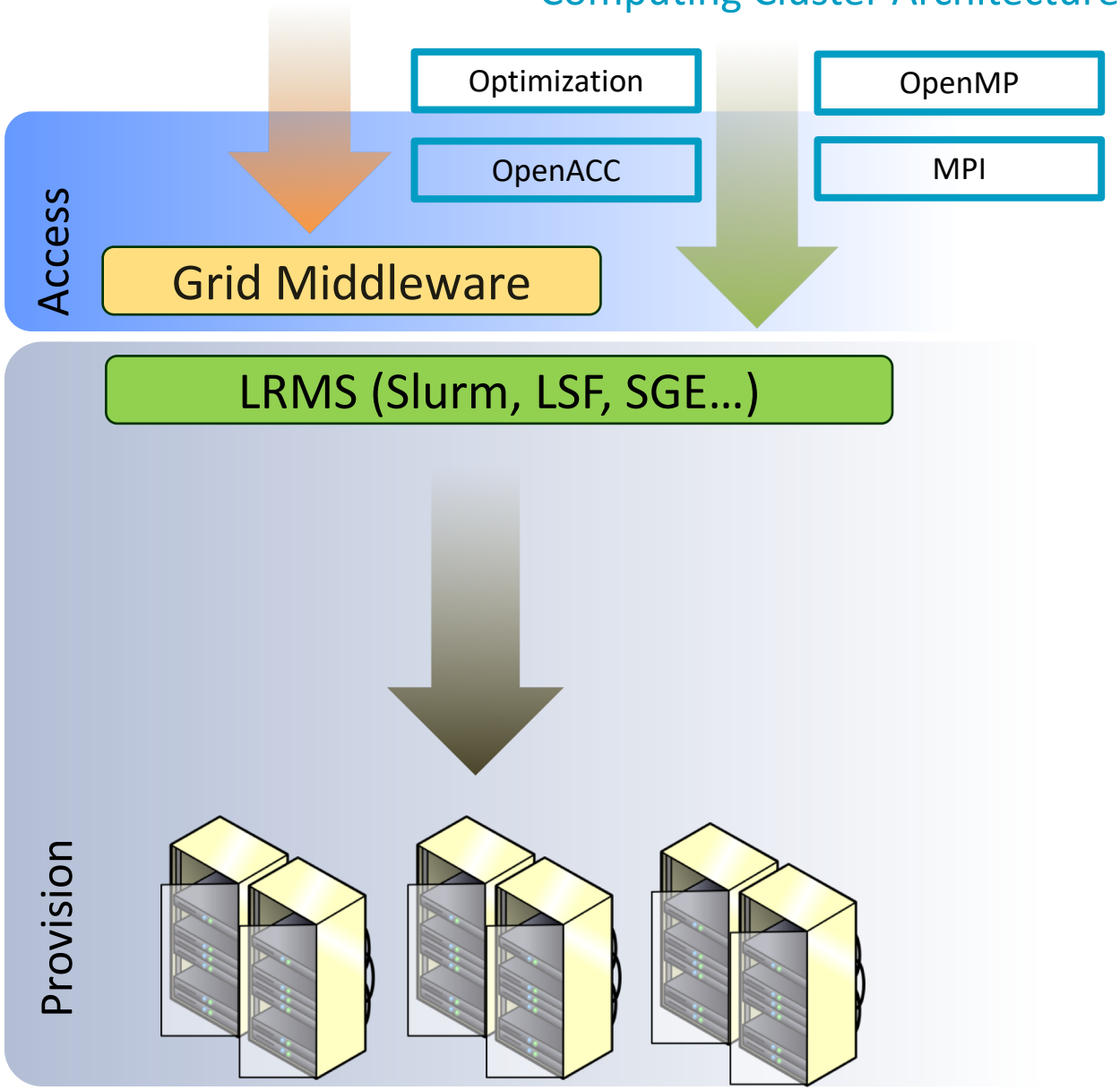
C. BIG DATA

CLOUD COMPUTING

PARALLEL ARCHITECTURES

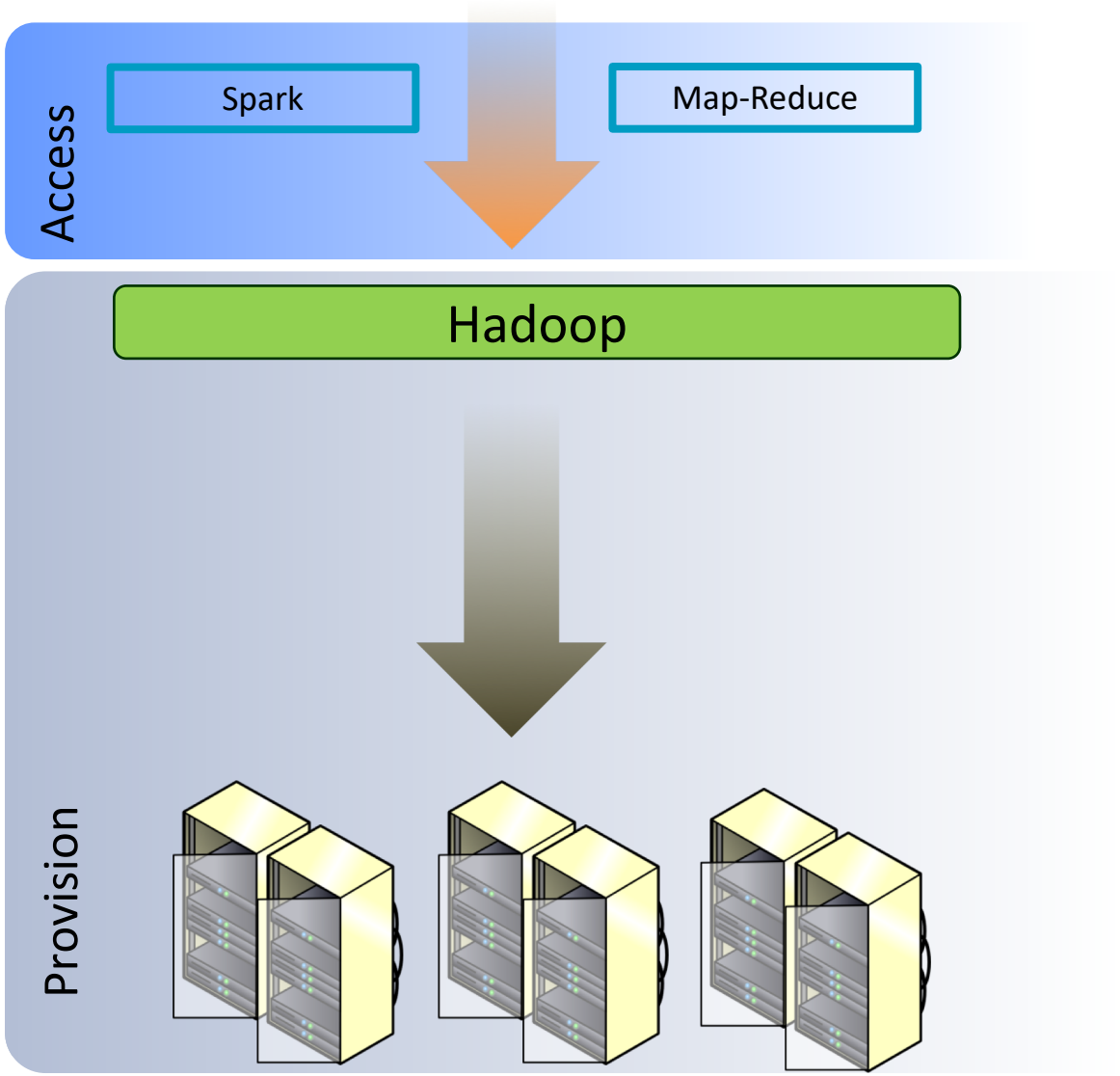
Context

Computing Cluster Architecture



Context

Computing Cluster Architecture



BIG DATA

Context

The Cloud as an Infrastructure Tool

Service/Provisioning Decoupling

Access

- Common interfaces

Service

Slurm / Hadoop

- Custom environments
- Dynamic elasticity

Virtual Worker Nodes

Provision

- Consolidation of WNs
- Simplified management
- Physical – Virtual WNs
- Dynamic capacity partitioning
- Faster upgrades

Context

Cloud as a Provisioning Tool

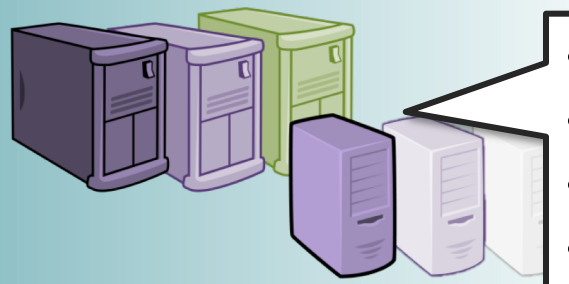
Access

IaaS Interface

- Simple Provisioning Interface
- Raw/Appliance VMs

Service

Pilot Jobs, SSH…

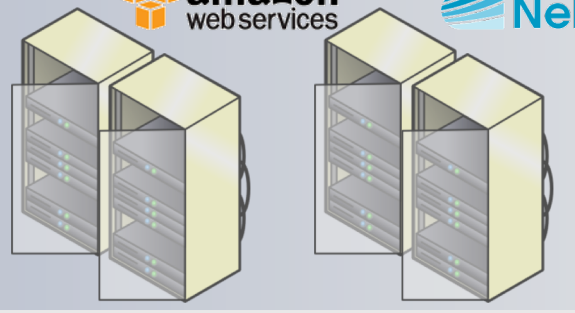


- Dynamic scalable computing
- Custom access to capacity
- Not only batch workloads
- Not only scientific workloads

Provision

amazon web services

Open Nebula



- Improve utilization
- Reduced service management
- Cost efficiency

Roadmap

Large-scale Data Processing on the Cloud

Virtualization

What is Cloud Computing?

Types of Cloud Services

Cloud Services for Parallel Processing

Breakout Room

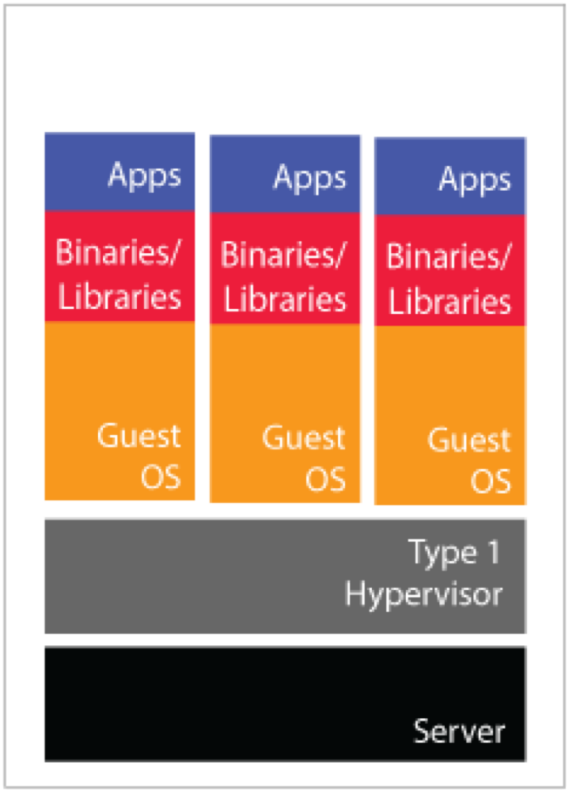
10 mins

Figure out who got up the earliest? They will be the ”spokesperson.”

- Who has ever used virtualization?
- Have you ever used a cloud?
- What are the benefits of the cloud?

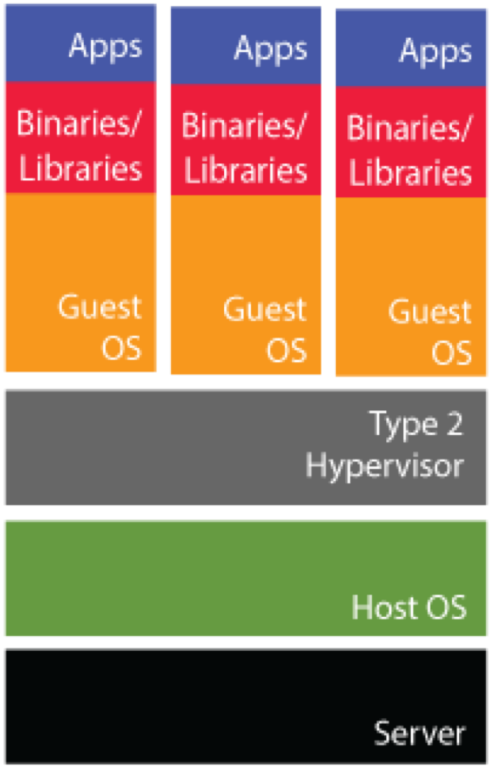
Virtualization

The Key Enabler of Cloud Computing



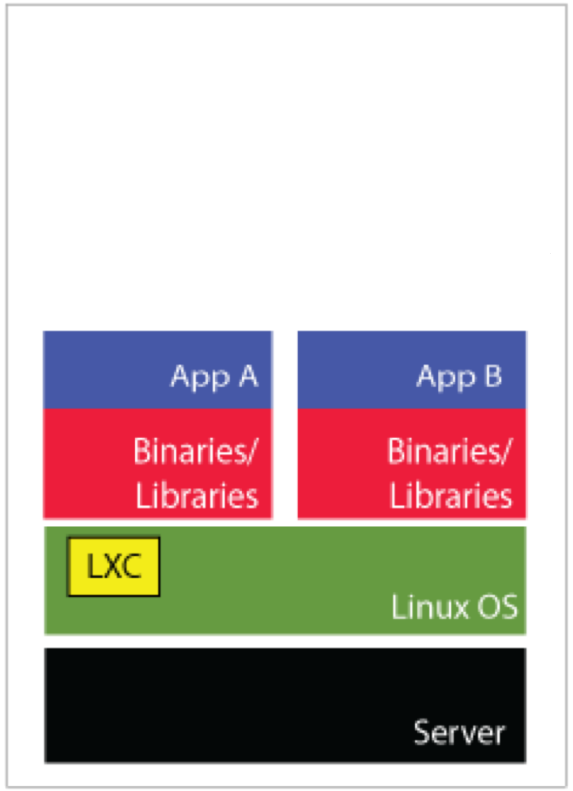
Type 1 Hypervisors

VMware, Xen Project, Hyper-V



Type 2 Hypervisors

KVM, VirtualBox



OS Containers

LXC, OpenVz

Which one offers the best performance?

Virtualization

Pros and Cons

End User Benefits

- Run multiple OS on the same machine
- Test/development
- Hardware/OS independent
- Replicate environments => Scientific method!

Operator Benefits

- Backup and recovery
- Live migration and consolidation
- Automation => “Software defined hardware”
- Cost savings

Drawbacks

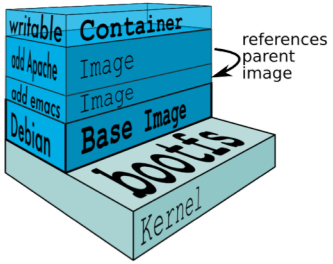
- Less efficiency => HPC!

Virtualization

Application Containers

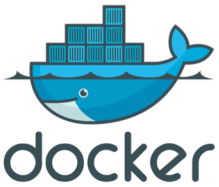
Encapsulation of Application Execution Environments

- Built on top of OS containers
- Provide lightweight, portable, self-sufficient execution environments from any application.
- Same container that a developer builds and tests on a laptop can run at scale, in production, on VMs, bare metal, public clouds...



Benefits

- Reproducibility and mobility of compute
- Ability to re-use and manage similar applications
- Content and hardware agnostic
- Easy to automate and integrate with other tools

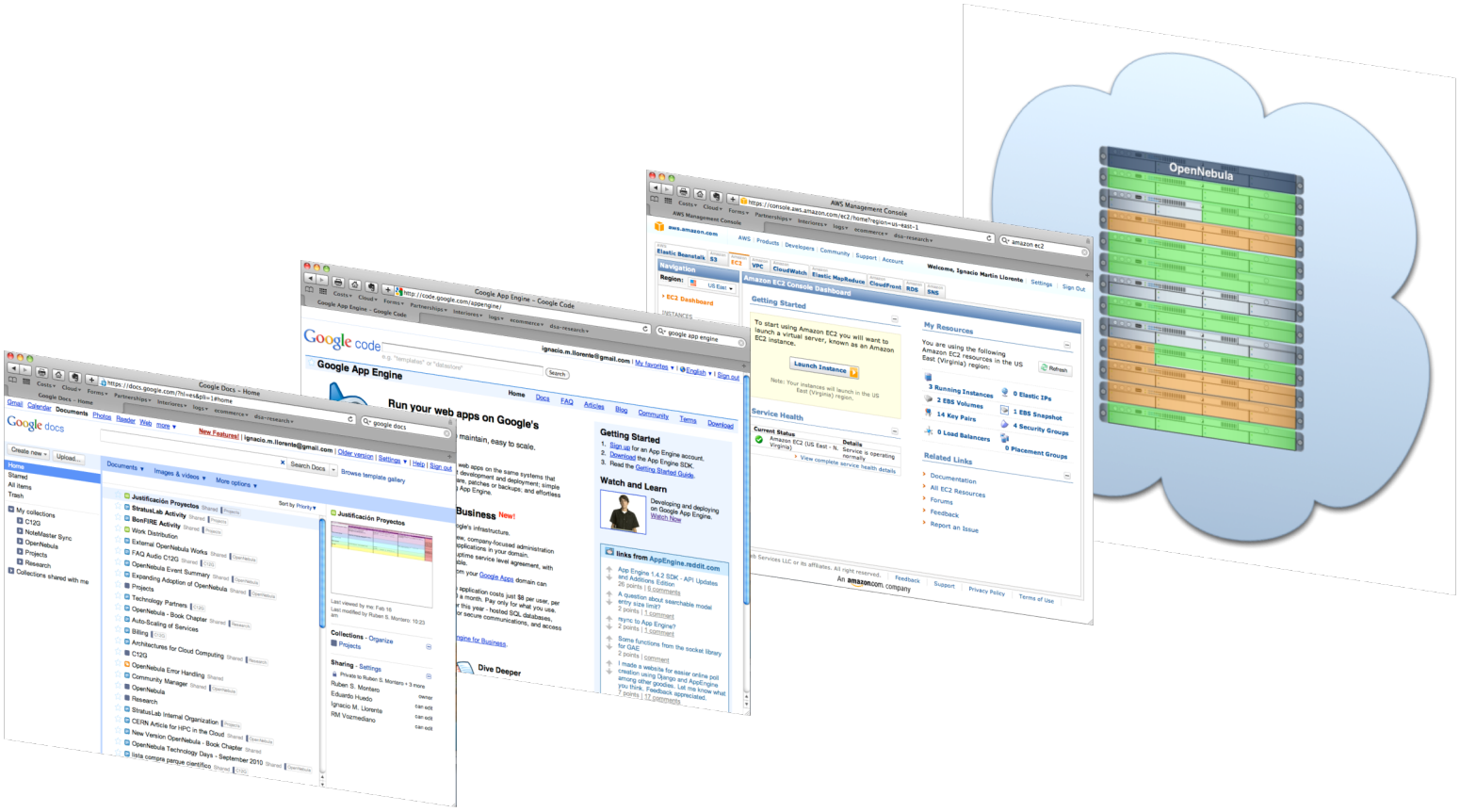


What is Cloud Computing?

An New Provision Model

Definition as a New IT Model

- Provision of resources (applications, development platforms and infrastructure) as a service, on-demand, with elastic capacity, through the internet.



What is Cloud Computing?

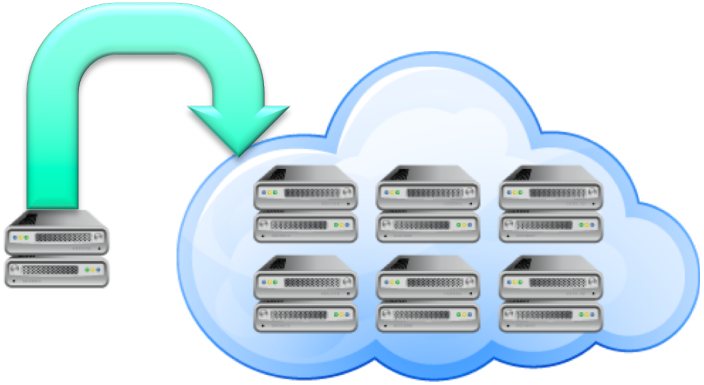
Elasticity on the Cloud

Vertical Scaling (Scale-Up)

Allocate additional resources to VMs, requires a reboot, no need for distributed app logic, single-point of OS failure

Horizontal Scaling (Scale-Out)

Application needs logic to work in distributed fashion (e.g. HA-Proxy and Apache Hadoop)



What is Cloud Computing?

A New Model, but an Old Idea

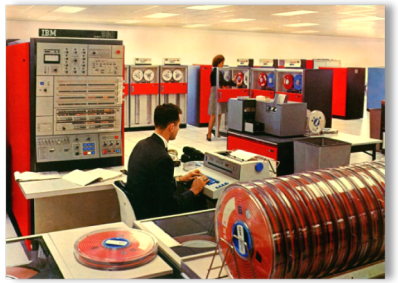
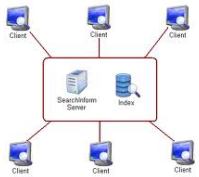
1961, John McCarthy "…*computation may someday be organized as a public utility…*"

https://www.youtube.com/watch?v=gwsDEgiN6_M

In 1974 Arthur C Clarke Predicts the Remote Worker and Future of the Internet and Computers

What is Cloud Computing?

The Third Era of Computing

	Technology	Management	Costs
Mainframe 	Centralized computing and storage based on high performance special-purpose systems, accessed through terminals	Optimized for maximum performance due to their high cost	Very high cost, both for hardware and software
Client/Server 	Distributed computing and storage based on commodity workstations and personal computers	Optimized for maximum agility due to their lower cost	Lower, incremental cost for hardware, and perpetual license-based model for software
Cloud 	Centralized computing and storage based on commodity systems, accessed through devices	Optimized for maximum performance and agility	Pay per use

What is Cloud Computing?

The Future of Resource Provisioning

"The horse is here to stay but the automobile is only a novelty, a fad"

President of Morgan Saving Bank to Ford Motor Co. Lawyers, 1903

What is Cloud Computing?

Different Perspectives

Use Model

- Focus on the result and not its implementation

Access Model

- Ubiquitous access from any device

Cost Model

- From Capital expenditures (CAPEX) to operating expenses (OPEX)

Infrastructure Model

- Virtualized, elastic, on-demand, multi-tenant IT capacity

What is Cloud Computing?

Different Perspectives

Security
- Backup and HA provided by the provider

Ubiquity
- Access from everywhere and any device

Coherency
- No need for information synchronization

Pay per Use
- No licenses, only pay for the time you need it

Updates
- Software always patched and updated

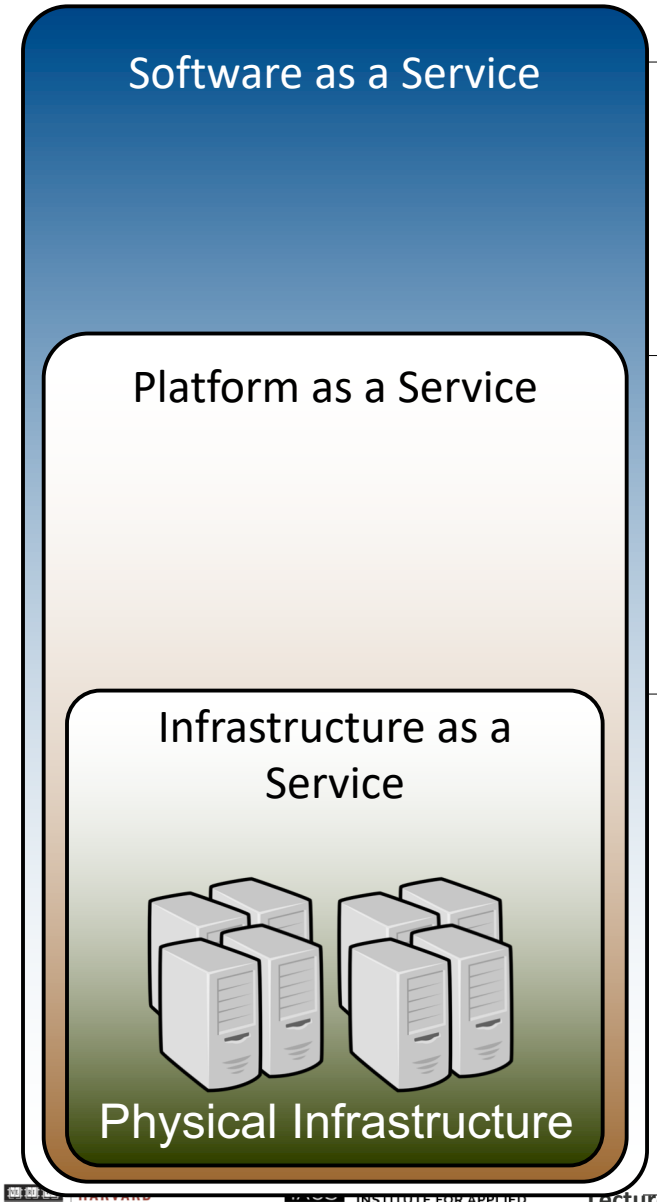
Lite Clients
- Does not require powerful client devices

Collaborative Work
- Natural support for remote collaboration

Energy Saving
- Allows consolidation of resources

Types of Cloud Services

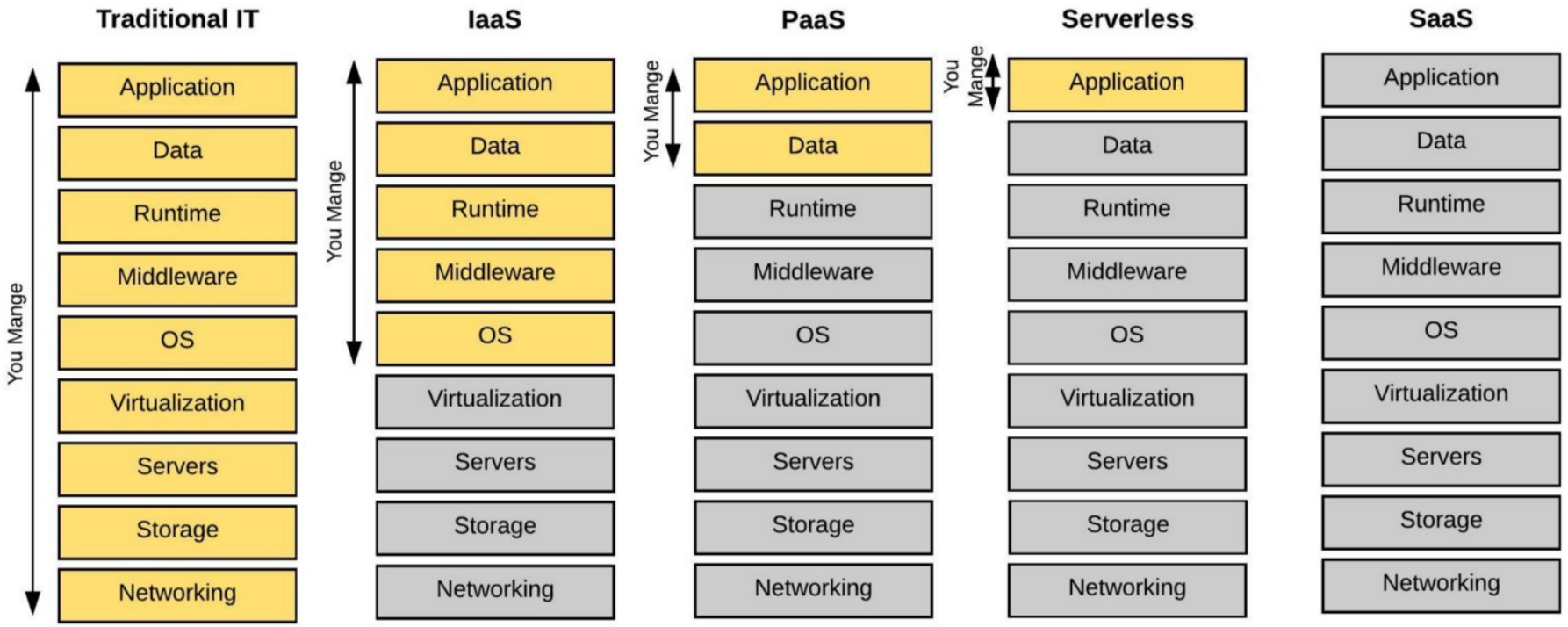
From Infrastructure to Application



What	Who
On-demand access to an application	Final user (not interested in sw/hw)
On-demand access to a platform to develop and test applications	Developer (not interested in hw)
IT resources	System administrators (complete management of the infrastructure)

Types of Cloud Services

From Infrastructure to Application



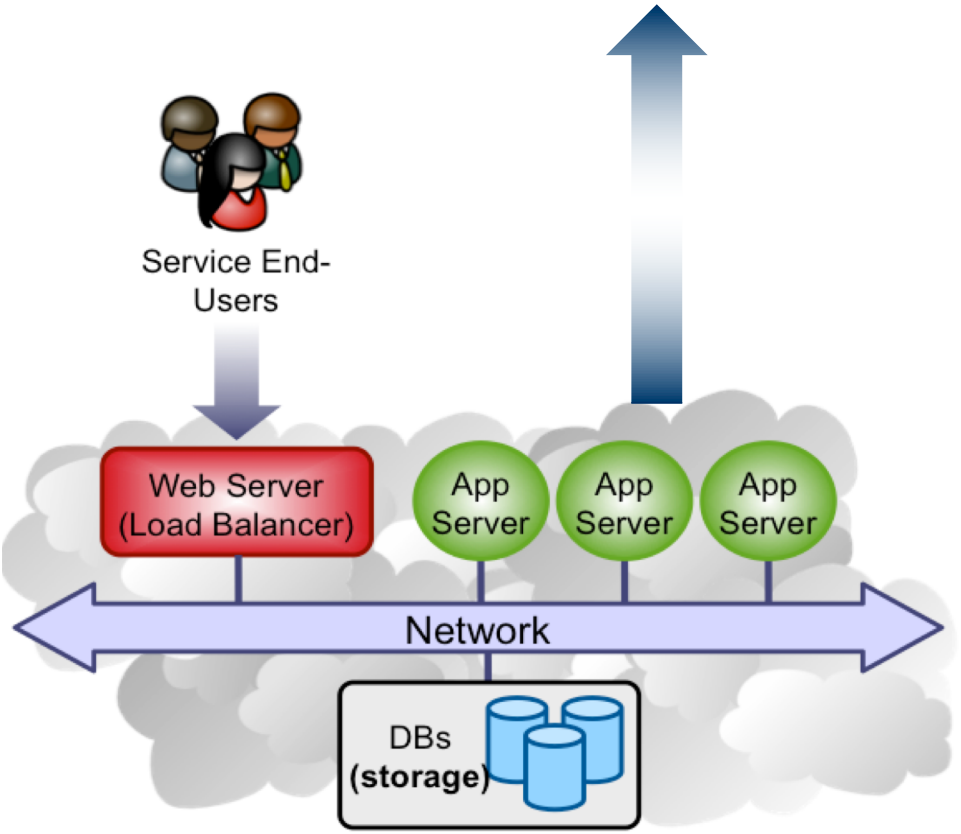
Types of Cloud Services

Infrastructure as a Service

On-demand Access to IT Resources

- Simple REST interface
- Pay per use
- Elastic capacity

$0.006 (1 vCPU 0.5 GiB) - $24.48 (64 vCPU 48 GiB) / Hour



Types of Cloud Services

Infrastructure as a Service

amazon web services™

On-Demand

With On-Demand instances, you pay for compute capacity by the hour with no long-term commitments or upfront payments. You can increase or decrease your compute capacity depending on the demands of your application and only pay the specified hourly rate for the instances you use.

On-Demand instances are recommended for:

- Users that prefer the low cost and flexibility of Amazon EC2 without any up-front payment or long-term commitment
- Applications with short-term, spiky, or unpredictable workloads that cannot be interrupted
- Applications being developed or tested on Amazon EC2 for the first time

See On-Demand Pricing

Spot Instances

Amazon EC2 Spot instances allow you to bid on spare Amazon EC2 computing capacity for up to 90% off the On-Demand price. Learn More.

Spot instances are recommended for:

- Applications that have flexible start and end times
- Applications that are only feasible at very low compute prices
- Users with urgent computing needs for large amounts of additional capacity

See Spot Pricing

Reserved Instances

Reserved Instances provide you with a significant discount (up to 75%) compared to On-Demand instance pricing. In addition, when Reserved Instances are assigned to a specific Availability Zone, they provide a capacity reservation, giving you additional confidence in your ability to launch instances when you need them.

For applications that have steady state or predictable usage, Reserved Instances can provide significant savings compared to using On-Demand instances. See How to Purchase Reserved Instances for more information.

Reserved Instances are recommended for:

- Applications with steady state usage
- Applications that may require reserved capacity
- Customers that can commit to using EC2 over a 1 or 3 year term to reduce their total computing costs

Dedicated Hosts

A Dedicated Host is a physical EC2 server dedicated for your use. Dedicated Hosts can help you reduce costs by allowing you to use your existing server-bound software licenses, including Windows Server, SQL Server, and SUSE Linux Enterprise Server (subject to your license terms), and can also help you meet compliance requirements. Learn more.

- Can be purchased On-Demand (hourly).
- Can be purchased as a Reservation for up to 70% off the On-Demand price.

Types of Cloud Services

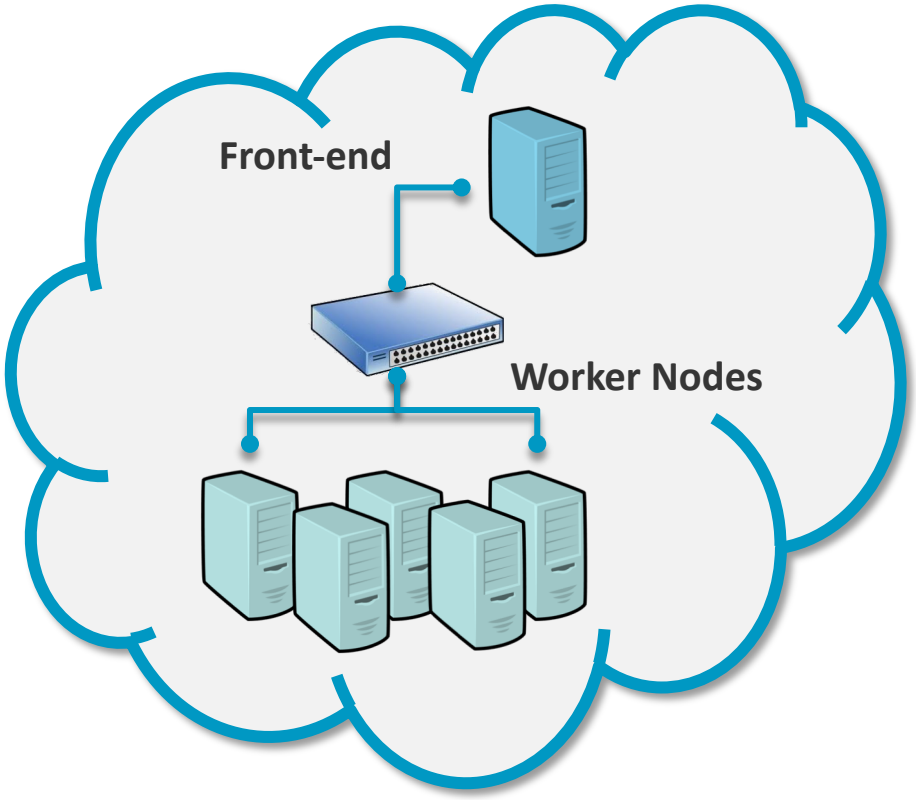
Infrastructure as a Service

amazon web services™

	vCPU	ECU	Memory (GiB)	Instance Storage (GB)	Linux/UNIX Usage
General Purpose - Current Generation					
t2.nano	1	Variable	0.5	EBS Only	$0.0059 per Hour
t2.micro	1	Variable	1	EBS Only	$0.012 per Hour
t2.small	1	Variable	2	EBS Only	$0.023 per Hour
t2.medium	2	Variable	4	EBS Only	$0.047 per Hour
t2.large	2	Variable	8	EBS Only	$0.094 per Hour
t2.xlarge	4	Variable	16	EBS Only	$0.188 per Hour
t2.2xlarge	8	Variable	32	EBS Only	$0.376 per Hour
m4.large	2	6.5	8	EBS Only	$0.1 per Hour
m4.xlarge	4	13	16	EBS Only	$0.2 per Hour
m4.2xlarge	8	26	32	EBS Only	$0.4 per Hour
m4.4xlarge	16	53.5	64	EBS Only	$0.8 per Hour
m4.10xlarge	40	124.5	160	EBS Only	$2 per Hour
m4.16xlarge	64	188	256	EBS Only	$3.2 per Hour

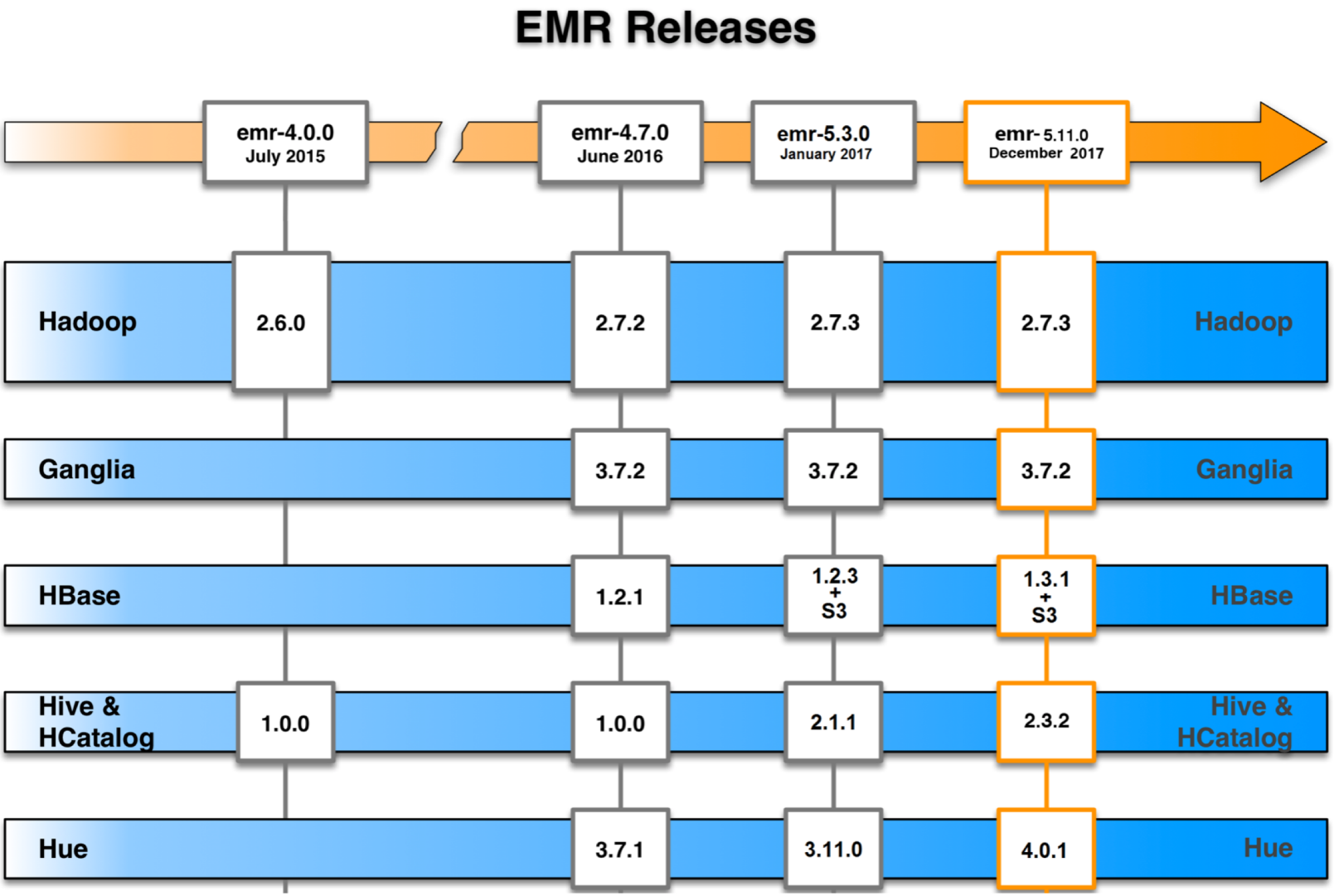
Cloud Services for Parallel Processing

Cloud as a Provisioning Tool: AWS - DIY



Cloud Services for Parallel Processing

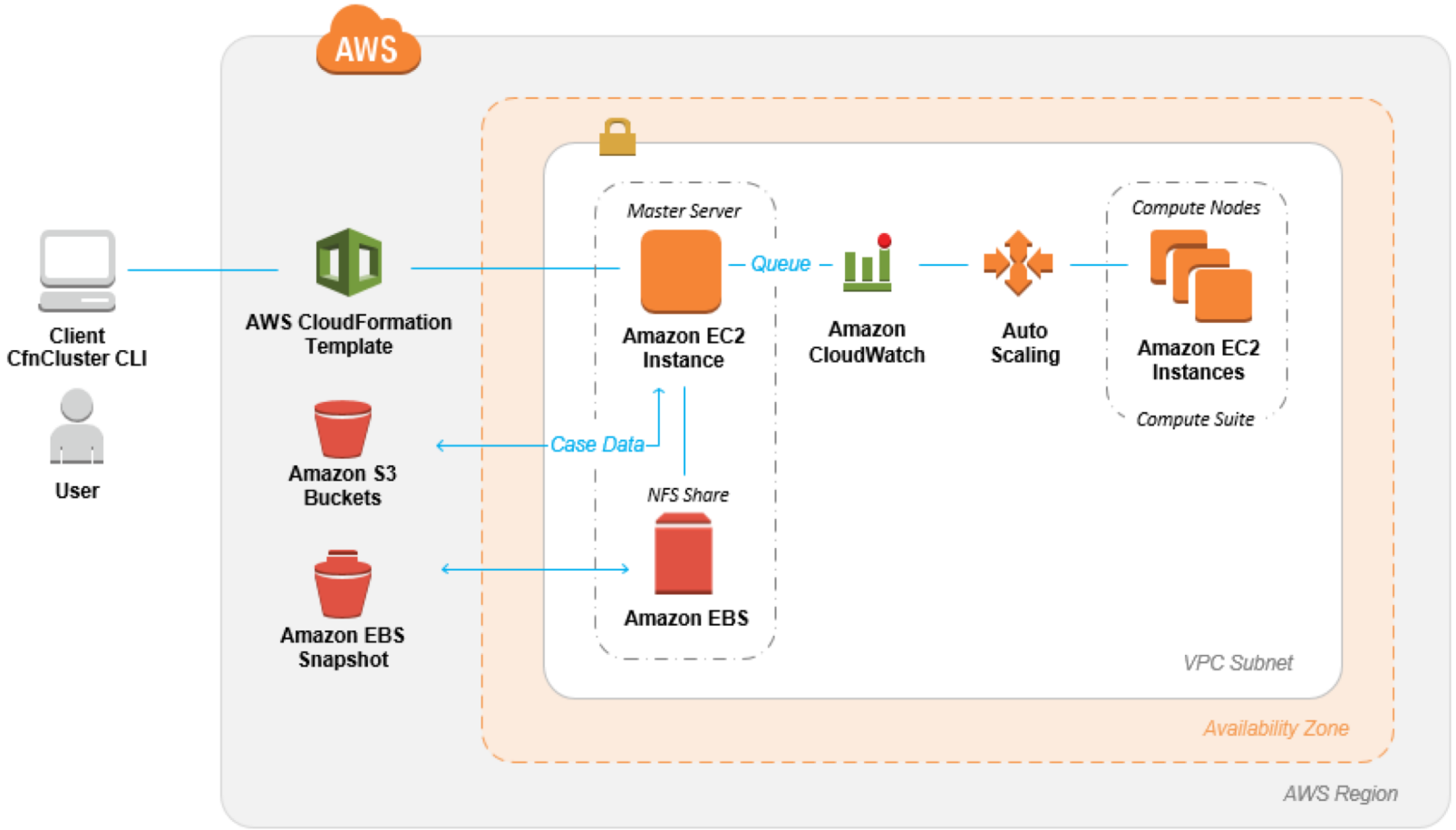
Cloud as Infrastructure Tool: AWS - EMR



Cloud Services for Parallel Processing

Cloud as Infrastructure Tool: AWS – HPC

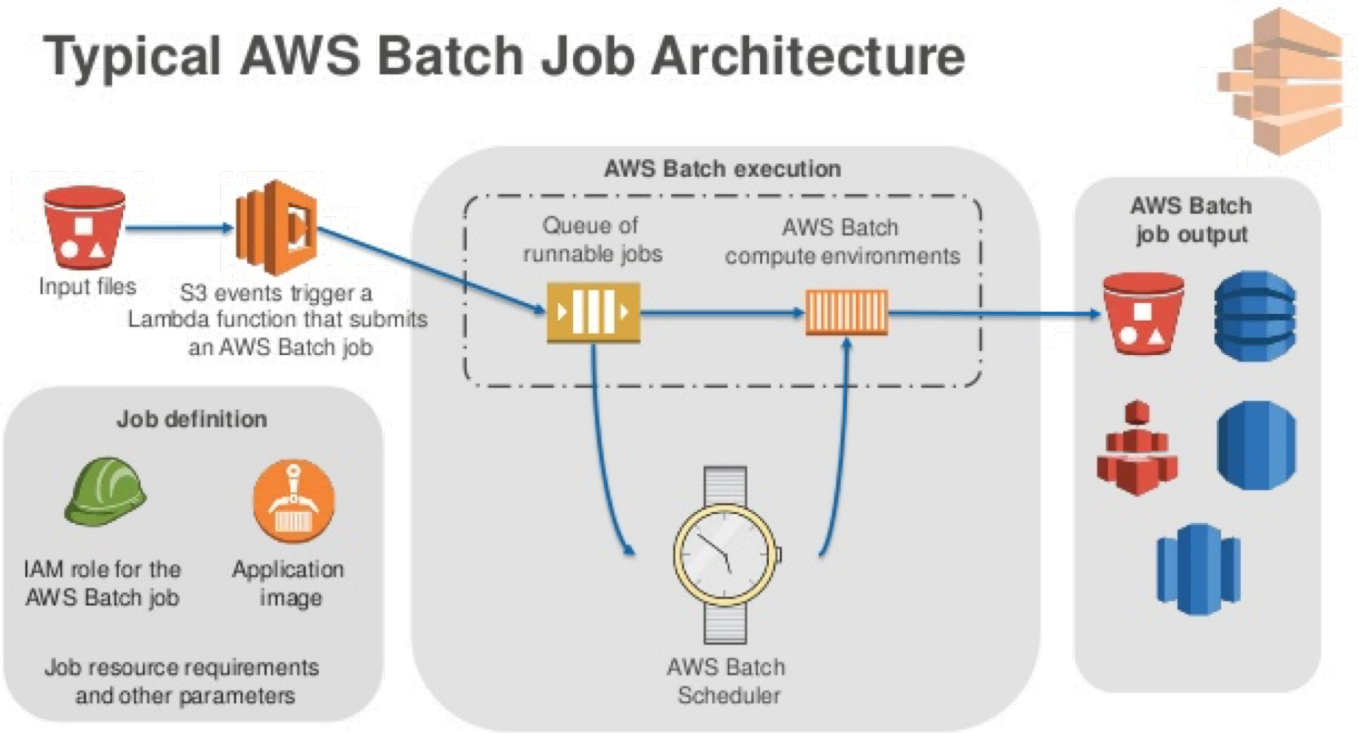
- Enhanced networking (20 Gigabit)
- Different high performance storage solution to build the cluster
- Managed by Engine Frame (CfnCluster)



Cloud Services for Parallel Processing

Cloud as Infrastructure Tool: AWS - Batch

- Fully-managed batch system for HTC (including DAG-based workflows)
- “Containerized” jobs (unit of execution), queues and environments
- Job definition includes container properties, capacity req., variables…
- Jobs reside in queues until they are executed (priorities)
- Jobs are mapped into computing environments (EC2 instances)
- Basic scheduler and simple job life-cycle



Cloud Services for Parallel Processing

Performance Penalty as a Small Tax You Have to Pay

Overhead in Computing
- Single node has processor performance penalty between 1% and 5%
- NASA reported an overhead between 9% and 25% (HPCC and NPB)[1]
- Growing number of clouds using containers (OpenVZ and LXC)

Overhead in Input/Output
- Growing number of Big Data apps
- Support for multiple system datastores including automatic scheduling

Need for Low-Latency High-Bandwidth Interconnection
- Lower performance, 10 GigE typically, used in clouds has a significant negative (x2-x10, especially latency) impact on HPC applications[1]
- PCI passthrough available for VMs that need consumption of raw GPU devices and Infiniband access
- FermiCloud has reported MPI performance (HPL benchmark) on VMs and SR-IOV/Infiniband with only a 4% overhead[2]

(1) An Application-Based Performance Evaluation of Cloud Computing, NASA Ames, 2013
(2) FermiCloud Update, Keith Chadwick, Fermilab, HePIX Spring Workshop 2013

Reading Assignments / Open Discussion

Potential of Cloud for Scientific Applications

I. Sadooghi et al, *"Understanding the Performance and Potential of Cloud Computing for Scientific Applications"*,
IEEE TCC, Issue No. 02 - April-June (2017 vol. 5)

What is the aim of the study?

Which infrastructures are compared?

What is the methodology?

What is the overhead in the memory, network, compute and storage components?

Next Steps

- **Lab session** this week:
  Help with HWA or Infrastructure Guide
  "First Access to AWS"?

- Get ready for **next lecture**:
  A.3. Practical Aspects of Cloud Computing

- **Reading Assignment**:

J. Riley, J. Noss, W. Dillingham, J. Cuff, I. M. Llorente, "*A High-Availability Cloud for Research Computing*", IEEE Computer, Volume: 50, Issue: 6, 2017

Questions

Large-Scale Parallel Processing on the Cloud