Introduction to cloud computing

Sudhakaran Prabakaran & Matt Wayland

Lecture 1

Lecture 1: Introduction to cloud computing

1. Background

2. Why Cloud Computing?

Some history & background

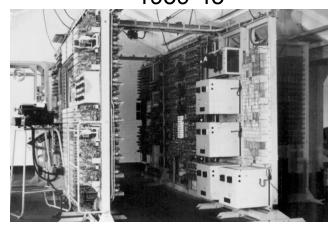
First computers!

1939-42



ABC computer that solved 29 problems at once

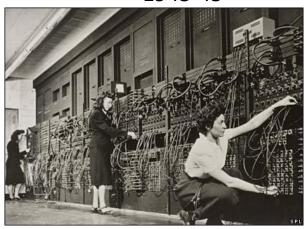
1939-45



British engineers built Colossus to crack WW2 codes

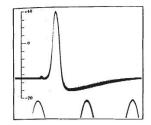
DNA the genetic material 1944

1943-45



ENIAC computer solved 1000s of MATH problem per second

Hodgkin-Huxley Model in 1952



1964



CDC 6600 can do 3 million tasks per second

Jacob and Monad Lac Operon Model in 1961





Recombinant DNA technology and automated sequencing



H. influenzae, first genome sequenced



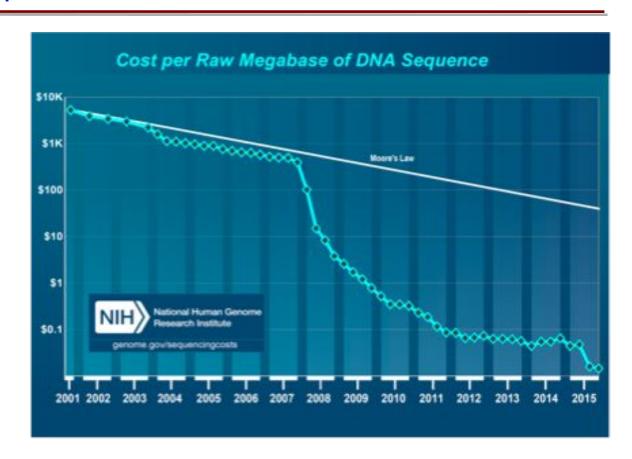


Human genome sequenced 13 years and 3 billion USDs

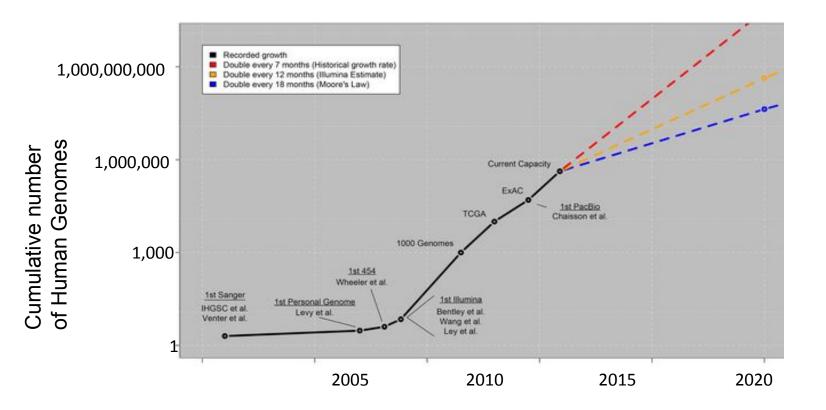
Sequencing data explosion: faster than moore's law over time

DNA sequencing has gone through technological S-curves

- In the early 2000's, improvements in Sanger sequencing produced a scaling pattern similar to Moore's law.
- The advent of NGS was a shift to a new technology with dramatic decrease in cost).



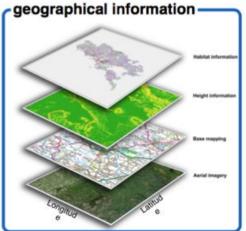
"More human genomes" creates more challenges



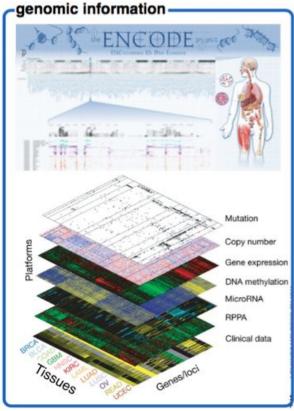
Between 2014-2018, production of new NGS data to exceed 2 Exabytes

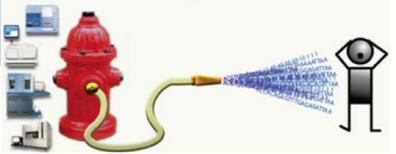
More and more data!

Human genome annotation — a non-intuitive map



- Large-scale organisation providing an overview of the genome
- · Integration of heterogeneous data

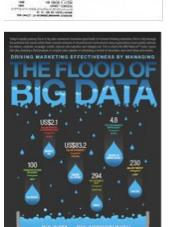




Big data world

IBM estimates that 90% of world's data has been created in the last two years









Commercial





Human brain 2.5 PB

Spotify

Ebay

Facebook 300 PB 15000 PB Google

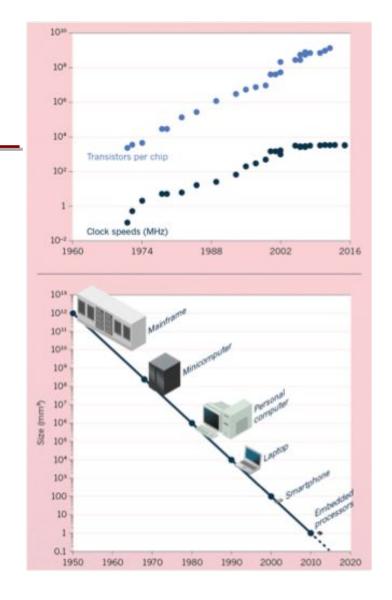
10 PB

90 PB

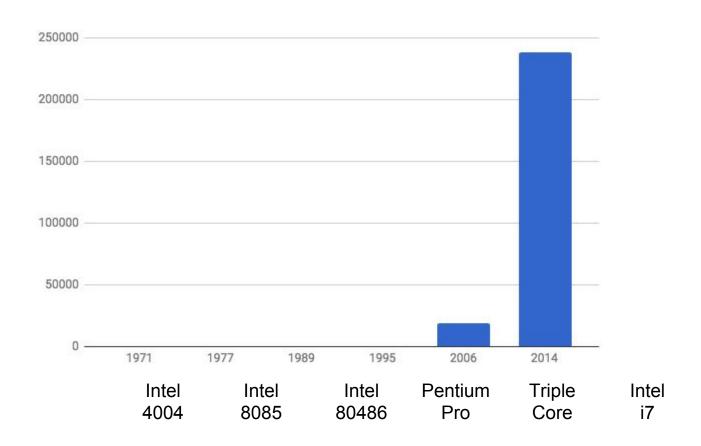
*Royal Society website

Moore's Law: Exponential Scaling of Computer Technology

- Exponential increase in the number of transistors per chip.
- Led to improvements in speed and miniaturization.
- Drove widespread adoption and novel applications of computer technology.

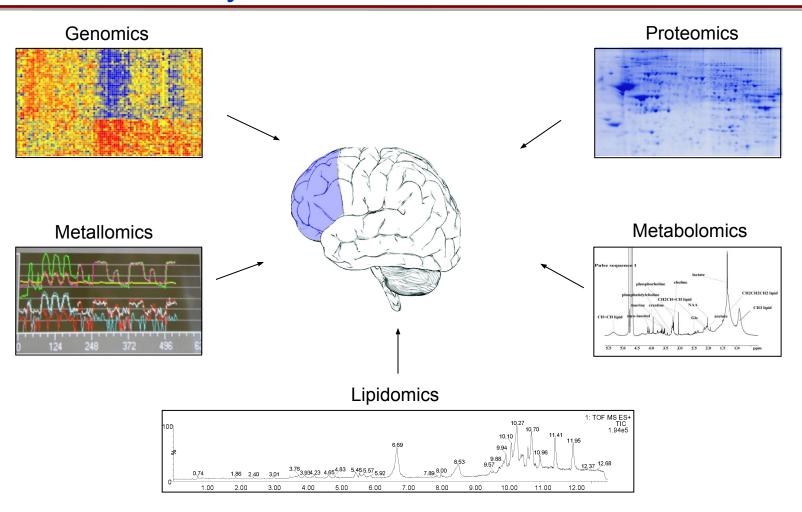


Processing speeds



My own path

Systems Neuroscience

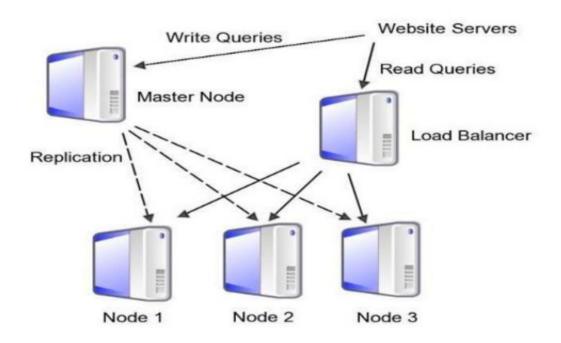


Prabakaran, S., et al. Mitochondrial dysfunction in schizophrenia: evidence for compromised brain metabolism and oxidative stress. *Mol Psychiatry*, 2004. 9, 684-97, 643.

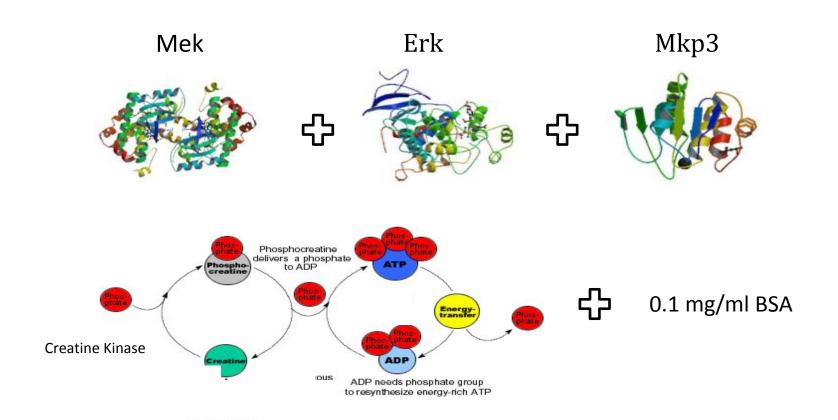
My Ph.D. work started with this one computer in 2002



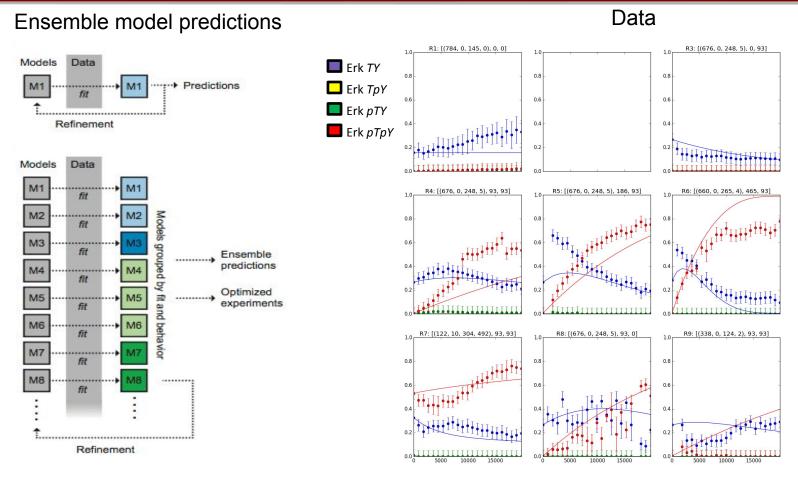
Soon became five computer study



Postdoctoral work:- Two site phosphorylation network



Ensemble modeling and Bayesian statistics



Prabakaran, S., Gyori, B. and Gunawardena, J. Regulation of Erk by multisite phosphorylation-a three body problem in biochemistry, Manuscript in preparation, 2016

Thousands of computers in the cluster





Please see our <u>Orchestra status</u> page for known issues.

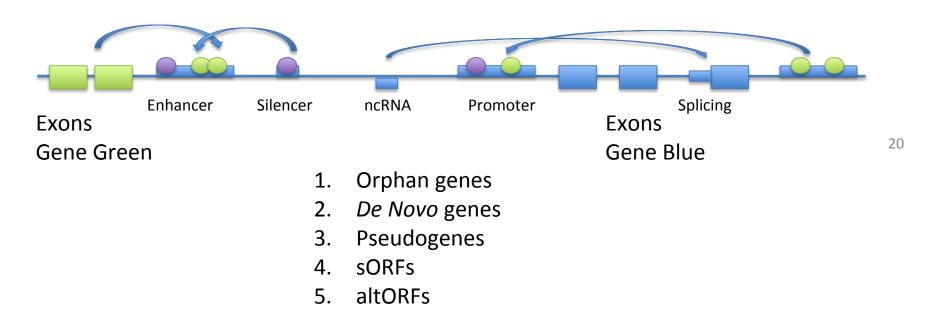
The **Orchestra** platform provides UNIX-based high performance computing, web hosting, and database hosting services at Harvard Medical School.

Orchestra and its associated services are managed by the Research Computing Group, part of the HMS Information Technology Department.



Current work

1. Identifying novel translation from noncoding regions using proteogenomics



2. Prioritizing variants in these regions using machine learning approaches

Inside TCGA

TCGA IS A TREMENDOUS GIFT TO THE CANCER RESEARCH COMMUNITY ...



More than 11,000 cases representing 33 cancer types

Data types in TCGA

TCGA Size & Complexity

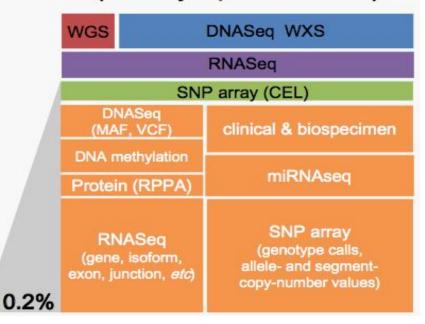
>1 PB of sequence data (controlled access)

DNASeq WXS

~4000 ~22,000 samples

RNASeq ~12,000 samples

~400,000 files of heterogeneous data (mostly open-access)



National and International sequencing projects

Examples of >100K projects already in progress

















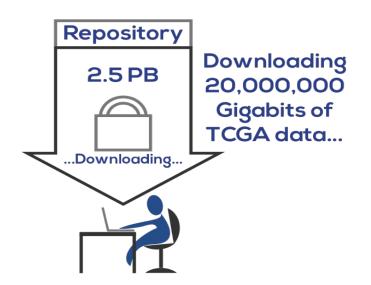




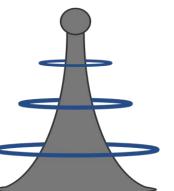




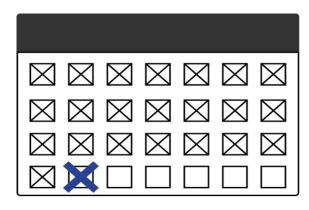
Accessing data at petabyte scale







...will take over <u>23 days</u>



Previous analysis methods



















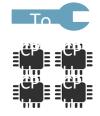


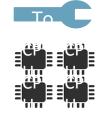






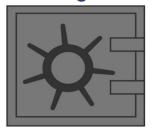




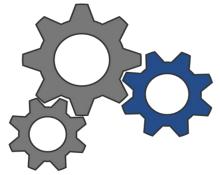


Cost of this model

\$2M/year in storage costs



Data is locked away and replicated unnecessarily across many institutions



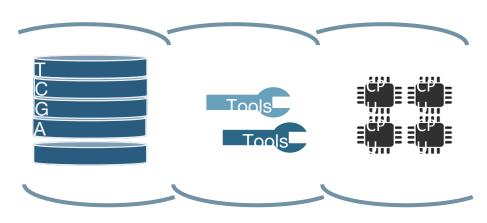
Requires significant computational resources



Collaborating in real-time and sharing reproducible results is challenging.

Biological questions come to data

Current data analysis model













Tools to the data

AS THE AMOUNT OF DATA HAS GROWN, SO TOO HAS THE NUMBER OF TOOLS AVAILABLE TO ANALYZE IT.

1,000+-omics data analysis tools*

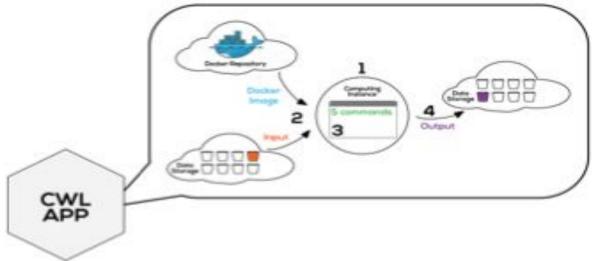
(each with many versions)

50+ used in a single TCGA marker paper

*omictools.com

Cloud computing to the rescue





Today the data comes to computation



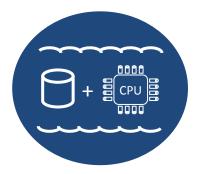


Research Centre 1





Millions of genomes will shift how computation will be done



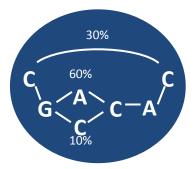
COMPUTATION CENTERS

replace data repositories



PORTABLE WORKFLOWS replace

data transfers



ADVANCED DATA STRUCTURES

replace static flat files

image source: Seven Bridges website

Introduction to cloud computing

Lecture 2

What is cloud?

Cloud is not a Buzzword

Web 2.0, Internet of Things are a buzzword! in fact Big Data is a buzzword

it is not a computer in some else's datacenter

NIST definition of cloud computing

Cloud computing is a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g., networks, servers, storage, applications, and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction. This cloud model is composed of five essential characteristics, three service models, and four deployment models.

Why Cloud Computing?

- Small as well as some large IT companies follows the traditional methods to provide the IT infrastructure. That means for any IT company, we need a **Server Room** that is the basic need of IT companies.
- In that server room, there should be a database server, mail server, firewalls, routers, modem, switches and the maintenance engineers.
- To establish such IT infrastructure, we need to spend lots of money. To overcome all these problems and to reduce the IT infrastructure cost, Cloud Computing came into existence.

What was used before?

1st Generation Business Computing: Mainframes

Upfront costs: High (millions of dollars)

Users: specialized IT operators

I/O: Punched card and Printer



2nd Generation Business Computing: Midrange

Upfront costs: Moderate (hundreds of thousands of dollars)

Users: Specialized IT Operators and specialized end-users

I/O: Keyboard and screen



3rd Generation Business Computing: Client Server

Upfront costs: Low (thousands of dollars)

Users: Specialized IT Operators and general end-user I/O: Keyboard, mouse and Graphical user interface



4th Generation Business Computing: The Cloud

Upfront costs: Very low or nothing

Users: IT operators, general end-users, consumers

I/O: Intelligent devices

Cloud computing service providers





vmware









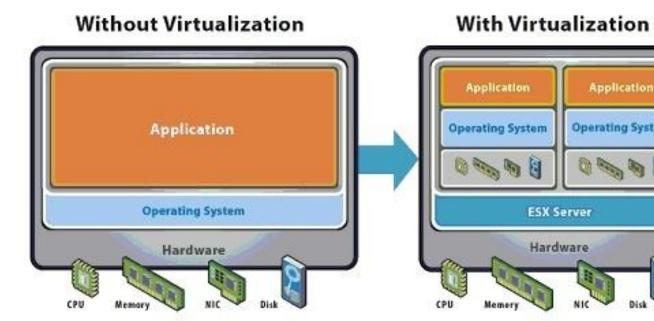




What makes cloud computing possible?

- Virtualization of workloads
- Storage
- Networking

What is virtualisation?



Act of creating something virtual

Actual physical resources are hidden from users

operating system directly talking to hardware

hypevisor (ESX server): an intermediate layer between operting system and hardware will present the hardware as a virtual resource

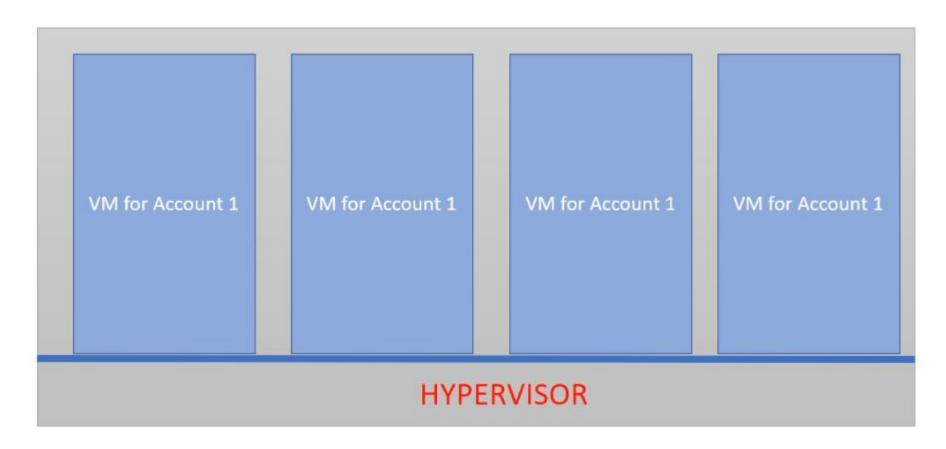
ESX Server

Hardware

Operating System

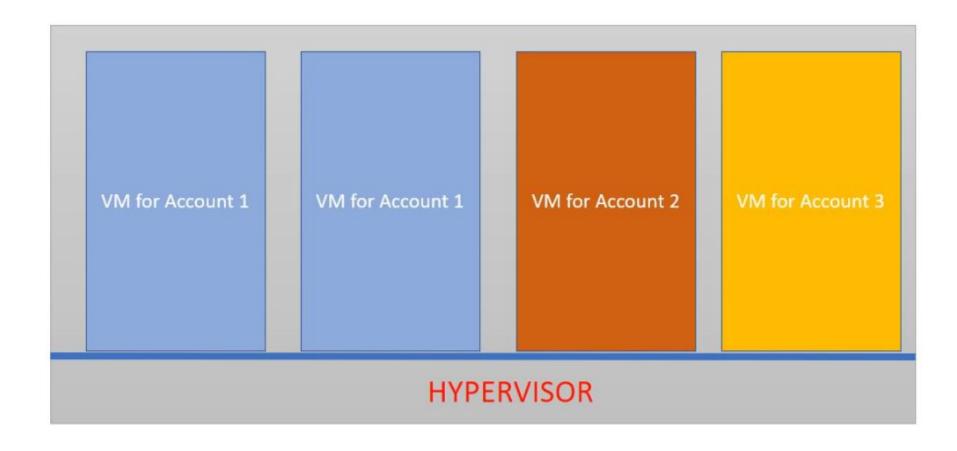
image source: VMware website

Single tenancy

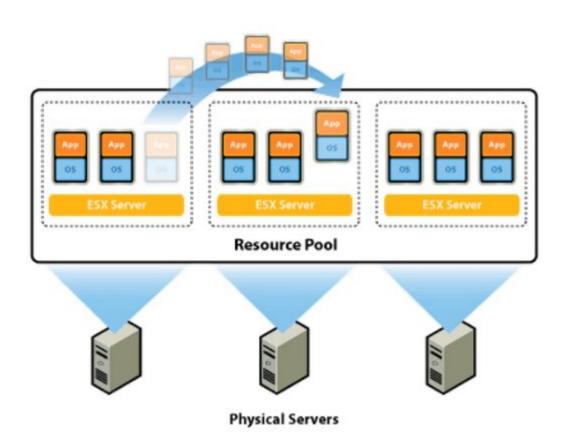


Each VM is an instance

Multi tenancy



Fault tolerant

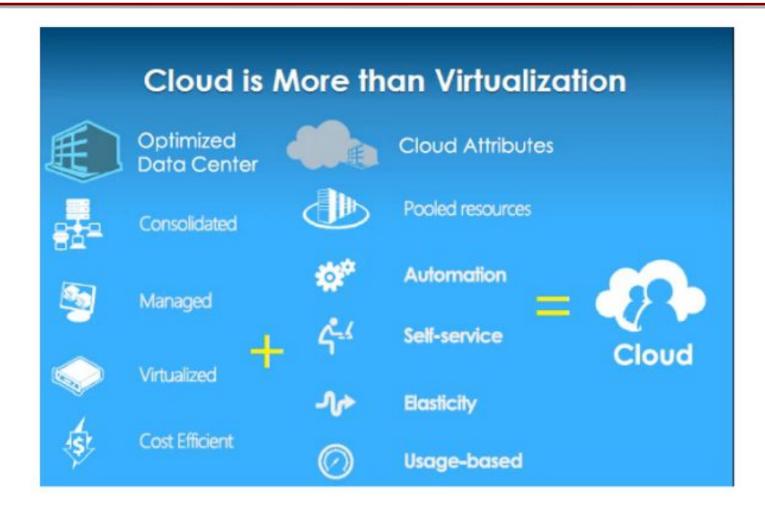


VM can be moved seamlessly if a certain physical machine fails

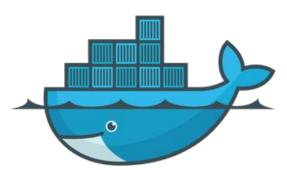
Advantages of VMs

- Optimal use of server resources (cost saving)
- Better fault tolerant
- Easy cloning
- Optimised load distribution

Data Centers



Docker and containerized workflow



Docker is a tool to create, deploy, and run applications by using containers.

Containers allow a developer to package up an application with all of the parts it needs, such as libraries and other dependencies, and ship it all out as one package. By doing so, thanks to the container, the developer can rest assured that the application will run on any other Linux machine regardless of any customized settings that machine might have that could differ from the machine used for writing and testing the code.

In a way, Docker is a bit like a virtual machine. But unlike a virtual machine, rather than creating a whole virtual operating system, Docker allows applications to use the same Linux kernel as the system that they're running on and only requires applications be shipped with things not already running on the host computer. This gives a significant performance boost and reduces the size of the application.

Common Workflow Language

 Common Workflow Language: An standard for describing a pipeline object model: Data, tools, pipelines, parameters

https://github.com/common-workflow-language/common-workflow-language

RABIX: Seven Bridges' open-source implementation of the CWL + custom extensions

http://rabix.io/

 Nextflow enables scalable and reproducible scientific workflows using software containers. It allows the adaptation of pipelines written in the most common scripting languages. (non containerised)

https://www.nextflow.io/

Key advantages of cloud computing

Cost planning

companies simply pay for what they use. As long as the company has the network capacity, they don't have to buy any hardware or other infrastructure to support the solution.

Enterprise level systems

enterprise level systems, which contain all the platform features and scalability needed by large organizations to run their businesses.

Faster go live

Cloud computing eliminates this worry because it is very easy to just select a virtual machine or component from your cloud provider and be up and running in seconds or minutes.

Agile and elastic capacity

It means the solution you deploy in the cloud does not have to stay the way you deployed it. So, elasticity means you can change your capacity requirements, and agility means you can do it as often as you like.

Key advantages of cloud computing

Out of the box integration

High Availability and disaster recovery

high availability (HA) & Disaster recovery (DR) are important features of the cloud

Enhanced security

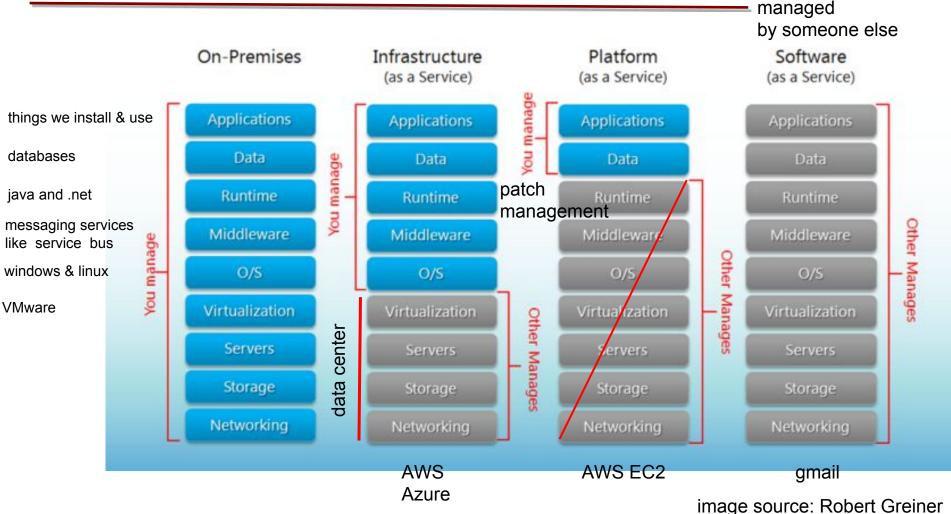
A cloud platform can offer a range of security features to detect or prevent attacks from the outside, which may be very expensive for smaller companies to implement. This again makes the IT systems in the cloud much more secure than they used to be in-house

Compliance

Many companies must comply with various laws and regulations based on the country/region or industry they work in. These include regulations such as Sarbanes-Oxley (SOX), HIPPA or GDPR. It can be very expensive to put the necessary infrastructure, processes, and management tools in place to ensure the company follow the laws of their government. When companies grow and they want to operate in other countries/regions, they also must adhere to the laws of those countries/regions. This will again mean more costs and management tools for the company. Cloud companies themselves must also follow these regulations and can therefore offer the same capabilities, management tools, and compliance certificates to the companies that use their cloud.



entire stack is



Essential characteristics of cloud computing

On-demand self-service:

A consumer can unilaterally provision computing capabilities, such as server time and network storage, as needed <u>automatically</u> without requiring human interaction with each service provider.

Broad network access:

Capabilities are available over the network & accessed through standard mechanisms that promote the use by heterogeneous thin or thick client platforms eg. mobile phones, laptops and workstations

Resource pooling:

The provider's computing resources are pooled to serve multiple consumers using a multi-tenant model, with different physical and virtual resources dynamically assigned and reassigned according to consumer demand. There is a sense of location independence in that the customer generally has no control or knowledge over the exact location of the provided resources but may be able to specify location at a higher level of abstraction (e.g., country, state, or datacenter). Examples of resources include storage, processing, memory, and network bandwidth.

Essential characteristics of cloud computing

Rapid elasticity:

Capabilities can be elastically provisioned and released, in some cases automatically, to scale rapidly outward and inward commensurate with demand. To the consumer, the capabilities available for provisioning often appear to be unlimited and can be appropriated in any quantity at any time.

Save money

Measured service:

Cloud systems automatically control and optimize resource use by leveraging a metering capability at some level of abstraction appropriate to the type of service (e.g., storage, processing, bandwidth, and active user accounts). Resource usage can be monitored, controlled, and reported, providing transparency for both the provider and consumer of the utilized service.

source: NIST

Deployment Models

Private cloud: The cloud infrastructure is provisioned for exclusive use by a single organization comprising multiple consumers (e.g., business units). It may be owned, managed, and operated by the organization, a third party, or some combination of them, and it may exist on or off premises.

Community cloud: The cloud infrastructure is provisioned for exclusive use by a specific community of consumers from organizations that have shared concerns (e.g., mission, security requirements, policy, and compliance considerations). It may be owned, managed, and operated by one or more of the organizations in the community, a third party, or some combination of them, and it may exist on or off premises.

Public cloud: The cloud infrastructure is provisioned for open use by the general public. It may be owned, managed, and operated by a business, academic, or government organization, or some combination of them. It exists on the premises of the cloud provider.

Hybrid cloud: The cloud infrastructure is a composition of two or more distinct cloud infrastructures (private, community, or public) that remain unique entities, but are bound together by standardized or proprietary technology that enables data and application portability (e.g., cloud bursting for load balancing between clouds).

Pros and Cons of Cloud Computing

Pros of Cloud Computing

- Lower cost computer for users
- Lower IT infrastructure cost
- Fewer maintenance cost
- Increased computing Power
- Unlimited storage capacity

Cons of Cloud Computing

- Require a constant Internet Connection
- Require High Speed Internet connection

Summary

