

<http://nesusws.irb.hr/>

Big Data Analytics

3rd NESUS Winter School on Data Science & Heterogeneous Computing



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Parallel Computing and Optimization Group (PCOG),
University of Luxembourg (UL), Luxembourg

<http://nesusws-tutorials-BD-DL.rtfld.io>

Before the tutorial starts: Visit
<https://goo.gl/M5ABf7>
for *preliminary setup instructions!*

Jan. 23th, 2018, Zagreb, Croatia



<https://varrette.gforge.uni.lu>

- Permanent **Research Scientist** at **University of Luxembourg**
 - ↪ Part of the **PCOG Team** led by Prof. P. Bouvry since 2007
 - ↪ **Research interests:**
 - ✓ High Performance Computing
 - ✓ Security (crash/cheating faults, obfuscation, blockchains)
 - ✓ Performance of HPC/Cloud/IoT platforms and services

- Manager of the **UL HPC Facility** with Prof. P. Bouvry since 2007
 - ↪ \simeq 206.772 TFlops (2017), 7952.4 TB
 - ↪ expert UL HPC team (*S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot*)
- National / EU HPC projects:
 - ↪ ETP4HPC, EU COST NESUS...
 - ↪ PRACE[2] (acting Advisor)
 - ↪ EuroHPC / IPCEI on HPC and Big Data (BD) Applications

- 3rd NESUS WS on Data Science & Heterogeneous Computing

In this session: Tutorial on Big Data Analytics

- Focus on **practicals tools** rather than theoretical content
- starts with **daily data management** ...
 - ↪ ... before speaking about **Big** data management
 - ↪ in particular: data transfer (over **SSH**), data versioning with **Git**
- continue with **classical tools** and their usage in HPC
 - ↪ review HPC environments and the hands-on environment
 - ✓ reviewing **Environment Modules** and **Lmod**
 - ✓ introducing **Vagrant** and **Easybuild**
 - ↪ introduction to Big Data processing engines: **Hadoop**, **Spark**
 - ↪ introduction to **Tensorflow**, an ML/DL processing framework

Disclaimer: Acknowledgements

- Part of these slides were **courtesy** borrowed w. permission from:
 - ↳ Prof. **Martin Theobald** (*Big Data and Data Science Research Group*), UL
- Part of the slides material adapted from:
 - ↳ *Advanced Analytics with Spark*, O Reilly
 - ↳ *Data Analytics with HPC* courses
 - ✓ © CC AttributionNonCommercial-ShareAlike 4.0
- the hands-on material is adapted from several resources:
 - ↳ (of course) the **UL HPC School**, **credits**: UL HPC team
 - ✓ S. Varrette, V. Plugaru, S. Peter, H. Cartiaux, C. Parisot
 - ↳ similar Github projects:
 - ✓ Jonathan Dursi: [hadoop-for-hpcers-tutorial](#)



Lecture & hands-on:

Big Data Analytics: Overview and Practical Examples

<http://nesusws-tutorials-BD-DL.rtf.d.io>

Time	Session
09:00 - 09:30	Discover the Hands-on tool: Vagrant
09:30 - 10:00	HPC and Big Data (BD): Architectures and Trends
10:00 - 10:30	Interlude: Software Management in HPC systems
10:30 - 11:00	[Big] Data Management in HPC Environment: Overview and Challenges
11:00 - 11:15	Coffee Break
11:15 - 12:30	Big Data Analytics with Hadoop & Spark
12:30 - 13:00	Deep Learning Analytics with Tensorflow
13:00	Lunch



Summary

- 1 Introduction**
 - Before we start...
 - Overview of HPC & BD Trends
 - Main HPC and DB Components
- 2 Interlude: Software Management in HPC systems**
- 3 [Big] Data Management in HPC Environment: Overview and Challenges**
 - Performance Overview in Data transfer
 - Data transfer in practice
 - Sharing Data
- 4 Big Data Analytics with Hadoop & Spark**
 - Apache Hadoop
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Tutorial Pre-Requisites / Setup

<http://nesusws-tutorials-BD-DL.rtf.d.io/>

- Follow instructions on **Getting Started / Pre-requisites**
 - ↪ create (if needed) accounts: **Github, Vagrant Cloud, Docker Hub**
 - ↪ install **mandatory software**, *i.e.* (apart from Git):

Platform	Software	Description	Usage
Mac OS	Homebrew	The missing package manager for macOS	<code>brew install ...</code>
Mac OS	Brew Cask Plugin	Mac OS Apps install made easy	<code>brew cask install ...</code>
Mac OS	iTerm2	(optional) enhanced Terminal	
Windows	MobaXTERM	Terminal with tabbed SSH client	
Windows	Git for Windows	may be you guessed... .	
Windows	SourceTree	(optional) enhanced git GUI	
Windows/Linux	Virtual Box	Free hypervisor provider for Vagrant	
Windows/Linux	Vagrant	Reproducible environments made easy.	
Linux	Docker for Ubuntu	Lightweight Reproducible Containers	
Windows	Docker for Windows	Lightweight Reproducible Containers	

Discover the Hands-on Tool: Vagrant

<http://vagrantup.com/>



VMWARE INTEGRATION

DOWNLOADS DOCUMENTATION BLOG ABOUT

**Development
environments
made easy.**

Create and configure lightweight, reproducible,
and portable development environments.

DOWNLOAD

GET STARTED

What is Vagrant ?

Create and configure **lightweight**, **reproducible**, and **portable** development environments

- **Command line** tool vagrant [...]
- Easy and Automatic per-project VM management
 - ↳ Supports many hypervisors: **VirtualBox**, **VMWare**...
 - ↳ Easy text-based configuration (Ruby syntax) Vagrantfile
- Supports **provisioning** through configuration management tools
 - ↳ Shell
 - ↳ Puppet <https://puppet.com/>
 - ↳ Salt... <https://saltstack.com/>

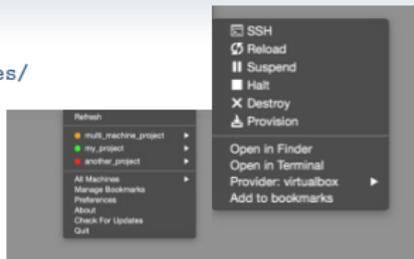
Cross-platform: runs on Linux, Windows, MacOS

Installation Notes

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/setup/preliminaries/>

- **Mac OS X:**

↪ best done using **Homebrew** and **Cask**



```
$> brew install caskroom/cask/brew-cask
$> brew cask install virtualbox # install virtualbox
$> brew cask install vagrant
$> brew cask install vagrant-manager # cf http://vagrantmanager.com/
```

- **Windows / Linux:**

↪ install **Oracle Virtualbox** and the **Extension Pack**

↪ install **Vagrant**



Why use Vagrant?

- Create new VMs quickly and easily: only one command!
 - ↳ `vagrant up`
- Keep the number of VMs under control
 - ↳ All configuration in `VagrantFile`
- **Reproducibility**
 - ↳ Identical environment in development and production
- **Portability**
 - ↳ **avoid** sharing 4 GB VM disks images
 - ↳ `Vagrant Cloud` to share your images
- **Collaboration made easy:**
 - \$> `git clone ...`
 - \$> `vagrant up`

Minimal default setup

```
$> vagrant init [-m] <user>/<name> # setup vagrant cloud image
```

- A Vagrantfile is configured for box <user>/<name>

- ↪ Find existing box: [Vagrant Cloud](https://vagrantcloud.com/) <https://vagrantcloud.com/>
- ↪ You can have multiple (named) box within the **same** Vagrantfile
 - ✓ See [ULHPC/puppet-sysadmins/Vagrantfile](#)
 - ✓ See [Falkor/tutorials-BD-ML/Vagrantfile](#)

```
Vagrant.configure(2) do |config|  
  config.vm.box = '<user>/<name>'  
  config.ssh.insert_key = false  
end
```

Box name	Description
ubuntu/trusty64	Ubuntu Server 14.04 LTS
debian/contrib-jessie64	Vanilla Debian 8 Jessie
centos/7	CentOS Linux 7 x86_64

Pulling and Running a Vagrant Box

```
$> vagrant up           # boot the box(es) set in the Vagrantfile
```

- Base box is downloaded and stored locally `~/.vagrant.d/boxes/`
- A new VM is created and configured with the base box as template
 - ↳ The VM is booted and (eventually) provisioned
 - ↳ Once within the box: `/vagrant` = directory hosting Vagrantfile



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```
$> vagrant status      # State of the vagrant box(es)
```



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```
$> vagrant status       # State of the vagrant box(es)
```

```
$> vagrant ssh          # connect inside it, CTRL-D to exit
```

Stopping Vagrant Box

```
$> vagrant { destroy | halt } # destroy / halt
```

- Once you have finished your work within a *running* box
 - ↪ save the state for later with `vagrant halt`
 - ↪ reset changes / tests / errors with `vagrant destroy`
 - ↪ commit changes by generating a new version of the box

Hands-on 0: Vagrant

- This tutorial heavily relies on **Vagrant**
↳ you will need to familiarize with the tool if not yet done

Your Turn!

Hands-on 0

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/vagrant/>

- **Clone** the tutorial repository Step 1
- **Basic Usage of Vagrant** Step 2



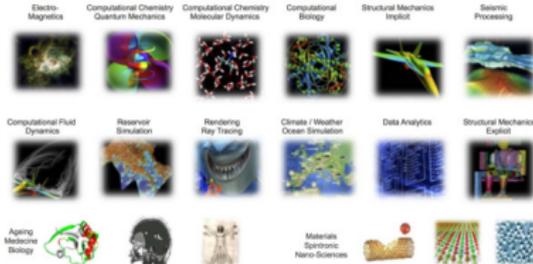
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Why HPC and BD ?

HPC: High Performance Computing
BD: Big Data



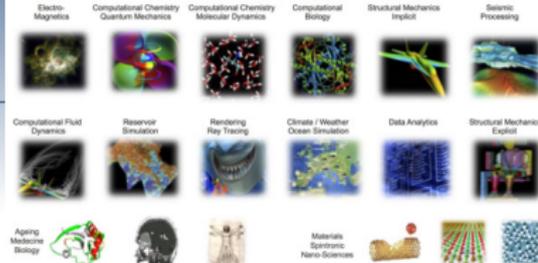
Andy Grant, Head of Big Data and HPC, Alcos UK&I

**To out-compete
you must out-compute**

Increasing competition, heightened customer expectations and shortening product development cycles are forcing the pace of acceleration across all industries



Why HPC and BD ?



HPC: High Performance Computing
BD: Big Data

- Essential tools for **Science, Society and Industry**
 - ↪ All scientific disciplines are becoming computational today
 - ✓ requires very high computing power, handles **huge** volumes of data
- **Industry, SMEs** increasingly relying on HPC
 - ↪ to invent innovative solutions
 - ↪ ... while reducing cost & decreasing time to market

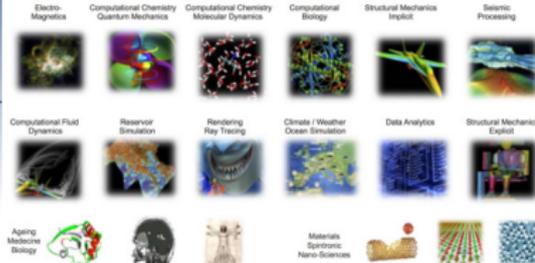
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- Essential tools for **Science, Society and Industry**
 - ↪ All scientific disciplines are becoming computational today
 - ✓ requires very high computing power, handles **huge** volumes of data
- **Industry, SMEs** increasingly relying on HPC
 - ↪ to invent innovative solutions
 - ↪ ... while reducing cost & decreasing time to market
- HPC = **global race** (strategic priority) - EU takes up the challenge:
 - ↪ EuroHPC / IPCEI on HPC and Big Data (BD) Applications

Andy Grant, Head of Big Data and HPC, Alcos UKGI

**To out-compete
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New Trends in HPC

- **Continued scaling** of scientific, industrial & financial applications
 - ↪ ... well beyond Exascale
- New trends changing the landscape for HPC
 - ↪ Emergence of **Big Data analytics**
 - ↪ Emergence of (**Hyperscale**) **Cloud Computing**
 - ↪ **Data intensive Internet of Things (IoT)** applications
 - ↪ **Deep learning & cognitive computing** paradigms

This study was carried out for RIKEN by



Special Study

Analysis of the Characteristics and Development Trends of the Next-Generation of Supercomputers in Foreign Countries

Earl C. Joseph, Ph.D.
Steve Conway

Robert Sorensen
Kevin Monroe

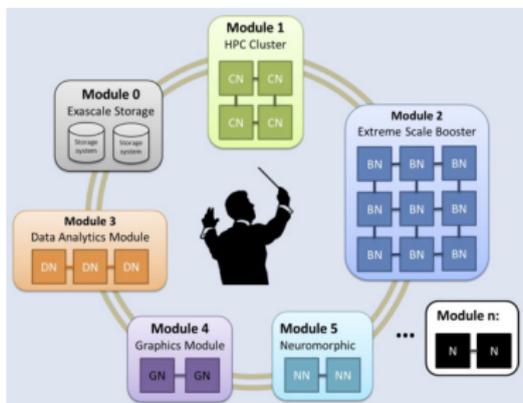
[Source : IDC RIKEN report, 2016]



[Source : EuroLab-4-HPC]

Toward Modular Computing

- Aiming at **scalable, flexible HPC infrastructures**
 - ↪ *Primary processing* on CPUs and accelerators
 - ✓ **HPC & Extreme Scale Booster** modules
 - ↪ *Specialized modules* for:
 - ✓ **HTC & I/O intensive** workloads;
 - ✓ **[Big] Data Analytics & AI**



[Source : "Towards Modular Supercomputing: The DEEP and DEEP-ER projects", 2016]

Prerequisites: Metrics

- **HPC: High Performance Computing**

BD: Big Data

Main HPC/BD Performance Metrics

- **Computing Capacity:** often measured in **flops** (or **flop/s**)
 - ↪ **Floating point operations per seconds** (often in DP)
 - ↪ **GFlops** = 10^9 **TFlops** = 10^{12} **PFlops** = 10^{15} **EFlops** = 10^{18}

Prerequisites: Metrics

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 - ↪ **GFlops** = 10^9 **TFlops** = 10^{12} **PFlops** = 10^{15} **EFlops** = 10^{18}
- **Storage Capacity**: measured in multiples of **bytes** = 8 **bits**
 - ↪ **GB** = 10^9 bytes **TB** = 10^{12} **PB** = 10^{15} **EB** = 10^{18}
 - ↪ **GiB** = 1024^3 bytes **TiB** = 1024^4 **PiB** = 1024^5 **EiB** = 1024^6
- **Transfer rate** on a medium measured in **Mb/s** or **MB/s**
- Other metrics: Sequential vs Random **R/W speed**, **IOPS** ...



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HPC Components: [GP]CPU

CPU

- Always multi-core
- Ex: Intel Core i7-7700K (Jan 2017) $R_{peak} \simeq 268.8$ GFlops (DP)
 - ↪ 4 cores @ 4.2GHz (14nm, 91W, 1.75 billion transistors)
 - ↪ + integrated graphics (24 EUs) $R_{peak} \simeq +441.6$ GFlops

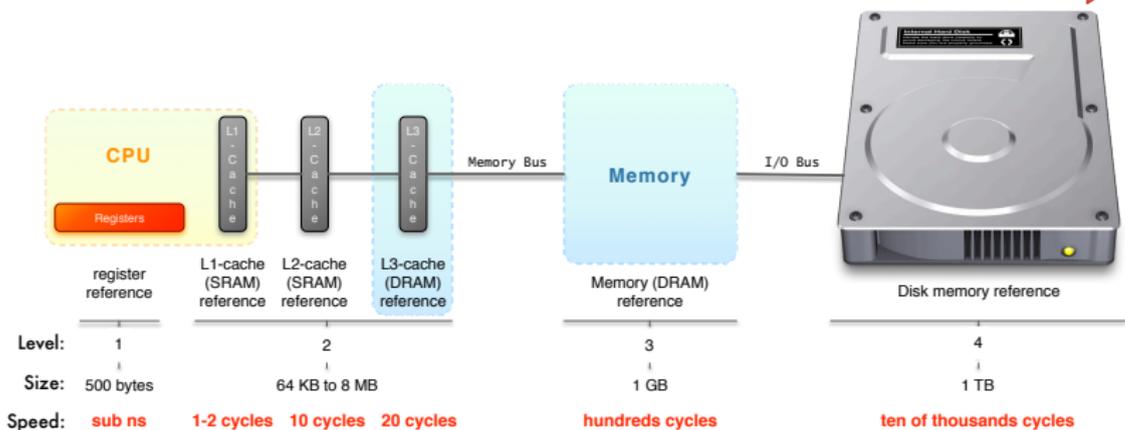
GPU / GPGPU

- Always multi-core, optimized for vector processing
- Ex: Nvidia Tesla V100 (Jun 2017) $R_{peak} \simeq 7$ TFlops (DP)
 - ↪ 5120 cores @ 1.3GHz (12nm, 250W, 21 billion transistors)
 - ↪ focus on Deep Learning workloads $R_{peak} \simeq 112$ TFLOPS (HP)

$\simeq 100$ Gflops for 130\$ (CPU), 214\$? (GPU)

HPC Components: Local Memory

Larger, slower and cheaper

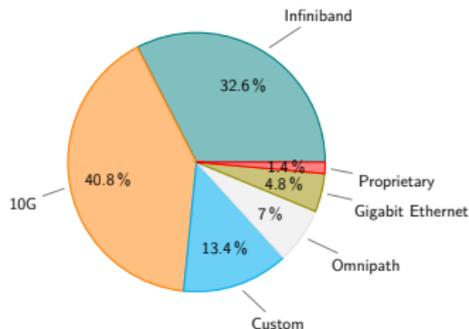


- SSD (SATA3) R/W: 550 MB/s; 100000 IOPS **450 €/TB**
- HDD (SATA3 @ 7,2 krpm) R/W: 227 MB/s; 85 IOPS **54 €/TB**

HPC Components: Interconnect

- **latency**: time to send a minimal (0 byte) message from A to B
- **bandwidth**: max amount of data communicated per unit of time

Technology	Effective Bandwidth		Latency
Gigabit Ethernet	1 Gb/s	125 MB/s	40 μ s to 300 μ s
10 Gigabit Ethernet	10 Gb/s	1.25 GB/s	4 μ s to 5 μ s
Infiniband QDR	40 Gb/s	5 GB/s	1.29 μ s to 2.6 μ s
Infiniband EDR	100 Gb/s	12.5 GB/s	0.61 μ s to 1.3 μ s
100 Gigabit Ethernet	100 Gb/s	1.25 GB/s	30 μ s
Intel Omnipath	100 Gb/s	12.5 GB/s	0.9 μ s

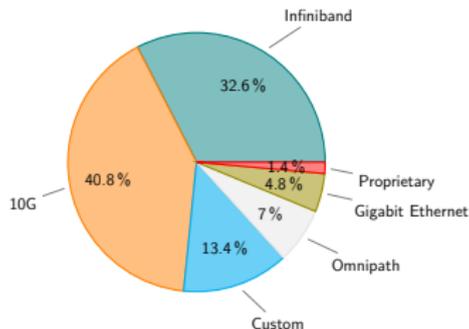


[Source : www.top500.org, Nov. 2017]

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Network Topologies

- **Direct** vs. **Indirect** interconnect

- ↪ *direct*: each network node attaches to at least one compute node
- ↪ *indirect*: compute nodes attached at the edge of the network only
 - ✓ many routers only connect to other routers.

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Main HPC Topologies

- **CLOS Network / Fat-Trees** [Indirect]

- ↪ can be fully non-blocking (1:1) or blocking (x:1)
- ↪ typically enables **best performance**
 - ✓ Non blocking bandwidth, lowest network latency



Network Topologies

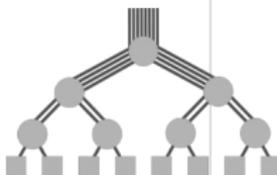
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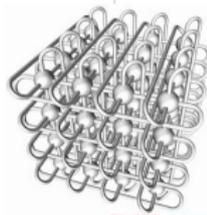
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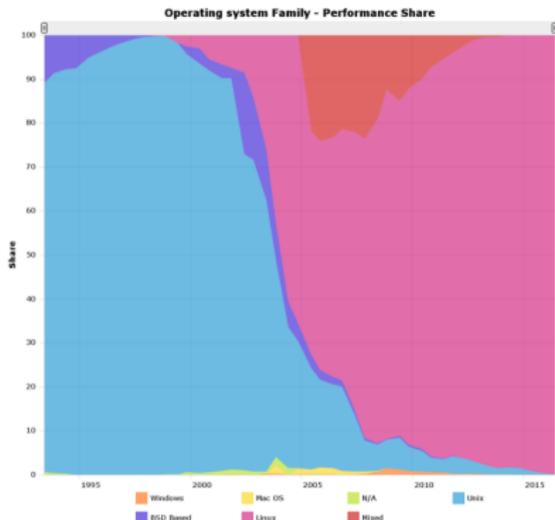


- **Mesh or 3D-torus** [Direct]

- ↳ Blocking network, cost-effective for systems at scale
- ↳ Great performance solutions for applications with locality
- ↳ Simple expansion for future growth

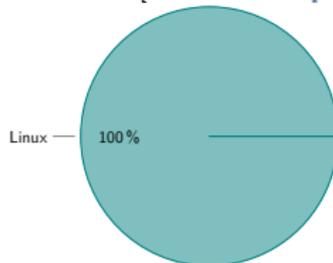


HPC Components: Operating System



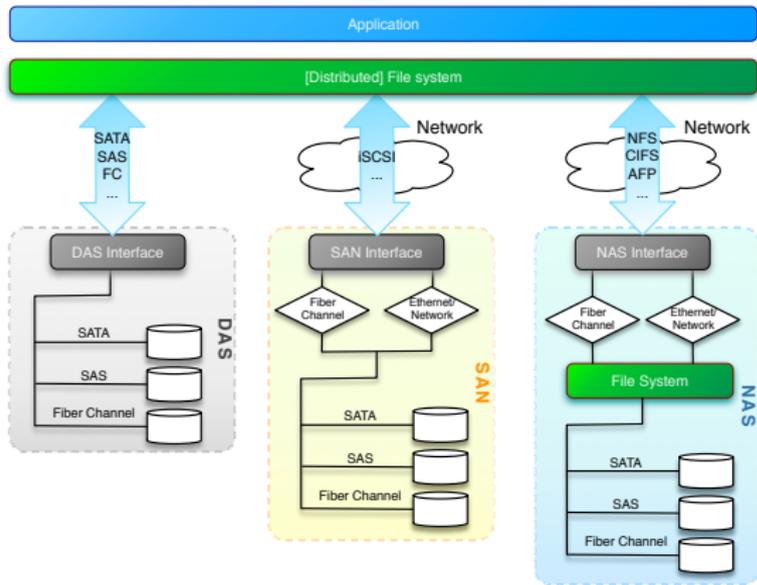
- Exclusively Linux-based (**really** 100%)
- Reasons:
 - ↔ stability
 - ↔ prone to devals

[Source : www.top500.org, Nov 2017]



[Big]Data Management

Storage architectural classes & I/O layers



[Big]Data Management: Disk Encl.



- \simeq 120 K€ - enclosure - 48-60 disks (4U)
↪ incl. redundant (i.e. 2) RAID controllers (master/slave)



[Big]Data Management: File Systems

File System (FS)

- Logical manner to **store, organize, manipulate & access** data

[Big]Data Management: File Systems

File System (FS)

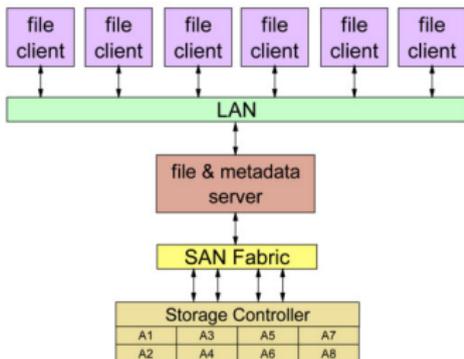
- Logical manner to **store, organize, manipulate & access** data
- (local) **Disk FS** : FAT32, NTFS, HFS+, ext{3,4}, {x,z,btr}fs...
 - ↳ manage data on permanent storage devices
 - ↳ *poor* perf. **read**: 100 → 400 MB/s | **write**: 10 → 200 MB/s

[Big]Data Management: File Systems

● Networked FS:

NFS, CIFS/SMB, AFP

- ↪ disk access from remote nodes via network access
- ↪ poorer performance for HPC jobs especially parallel I/O
 - ✓ **read**: only 381 MB/s on a system capable of 740MB/s (16 tasks)
 - ✓ **write**: only 90MB/s on system capable of 400MB/s (4 tasks)



[Source : LISA'09] Ray Paden: *How to Build a Petabyte Sized Storage System*

COMMENT:

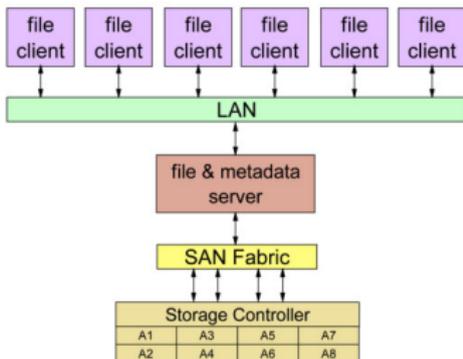
Traditionally, a single NFS/CIFS file server manages both user data and metadata operations which "gates" performance/scaling and presents a single point of failure risk. Products (e.g., CNFS) are available that provide multiple server designs to avoid this issue.

[Big]Data Management: File Systems

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- [scale-out] **NAS**

- ↳ aka Appliances OneFS...
- ↳ Focus on CIFS, NFS
- ↳ Integrated HW/SW
- ↳ **Ex: EMC (Isilon), IBM (SONAS), DDN...**

COMMENT:

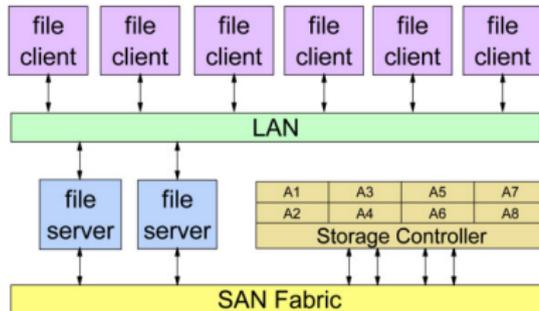
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[Big]Data Management: File Systems

● Basic Clustered FS

GPFS

- ↪ File access is parallel
- ↪ File System overhead operations is distributed and done in parallel
 - ✓ **no** metadata servers
- ↪ File clients access file data through file servers via the LAN



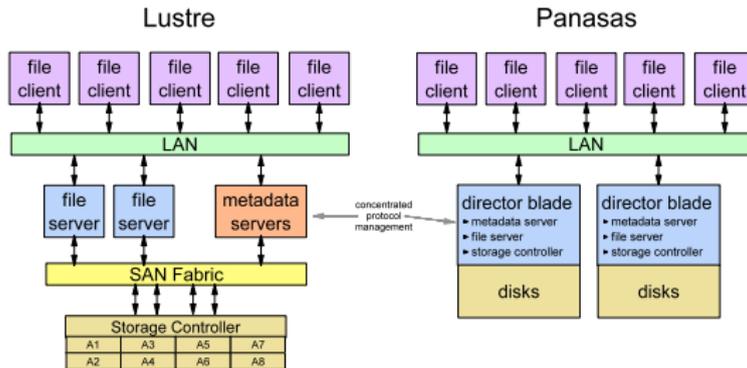
File system overhead operations are *distributed* across the entire cluster and is done in parallel; it is **not** concentrated in any given place. There is no single server bottleneck. User data and metadata flows between all nodes and all disks via the file servers.

[Big]Data Management: File Systems

- **Multi-Component Clustered FS**

Lustre, Panasas

- ↪ File access is parallel
- ↪ File System overhead operations on dedicated components
 - ✓ metadata server (Lustre) or director blades (Panasas)
- ↪ Multi-component architecture
- ↪ File clients access file data through file servers via the LAN





[Big]Data Management: FS Summary

- **File System (FS):** Logical manner to *store, organize & access* data
 - ↪ (local) **Disk FS** : FAT32, NTFS, HFS+, ext4, {x,z,btr}fs...
 - ↪ **Networked FS**: NFS, CIFS/SMB, AFP
 - ↪ **Parallel/Distributed FS**: SpectrumScale/GPFS, Lustre
 - ✓ typical FS for HPC / HTC (High Throughput Computing)

[Big]Data Management: FS Summary

- **File System (FS):** Logical manner to *store, organize & access* data
 - ↪ (local) **Disk FS** : FAT32, NTFS, HFS+, ext4, {x,z,btr}fs...
 - ↪ **Networked FS**: NFS, CIFS/SMB, AFP
 - ↪ **Parallel/Distributed FS**: SpectrumScale/GPFS, Lustre
 - ✓ typical FS for HPC / HTC (High Throughput Computing)

Main Characteristic of Parallel/Distributed File Systems

Capacity and Performance increase with #servers

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Main Characteristic of Parallel/Distributed File Systems

Capacity and Performance increase with #servers

Name	Type	Read* [GB/s]	Write* [GB/s]
ext4	Disk FS	0.426	0.212
nfs	Networked FS	0.381	0.090
gpfs (iris)	Parallel/Distributed FS	10.14	8.41
gpfs (gaia)	Parallel/Distributed FS	7.74	6.524
lustre	Parallel/Distributed FS	4.5	2.956

* maximum **random** read/write, per IOZone or IOR measures, using 15 concurrent nodes for networked FS.



HPC Components: Data Center

Definition (Data Center)

- Facility to house computer systems and associated components
 - ↳ Basic storage component: **rack** (height: 42 RU)

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Challenges: Power (UPS, battery), Cooling, Fire protection, Security

- Power/Heat dissipation per rack:
 - ↳ HPC **computing** racks: **30-120 kW**
 - ↳ **Storage** racks: **15 kW**
 - ↳ **Interconnect** racks: **5 kW**
- Various **Cooling** Technology
 - ↳ Airflow
 - ↳ Direct-Liquid Cooling, Immersion...

Power Usage Effectiveness

$$PUE = \frac{\text{Total facility power}}{\text{IT equipment power}}$$



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Software/Modules Management

<https://hpc.uni.lu/users/software/>

- Based on **Environment Modules / LMod**
 - ↪ convenient way to dynamically change the users environment \$PATH
 - ↪ permits to easily load software through `module` command
- Currently on **UL HPC**:
 - ↪ > **163 software packages**, in *multiple* versions, within **18 categ.**
 - ↪ reworked software set for `iris` cluster and now deployed everywhere
 - ✓ RESIF v2.0, allowing [real] semantic versioning of released builds
 - ↪ hierarchical organization **Ex:** `toolchain/{foss,intel}`

```
$> module avail # List available modules
```

```
$> module load <category>/<software>[/<version>]
```



Software/Modules Management

- Key module variable: `$MODULEPATH` / where to look for modules
↳ altered with `module use <path>`. **Ex:**

```
export EASYBUILD_PREFIX=$HOME/.local/easybuild
export LOCAL_MODULES=$EASYBUILD_PREFIX/modules/all
module use $LOCAL_MODULES
```

Software/Modules Management

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export LOCAL_MODULES=$EASYBUILD_PREFIX/modules/all
module use $LOCAL_MODULES
```

Main modules commands:

Command	Description
<code>module avail</code>	Lists all the modules which are available to be loaded
<code>module spider <pattern></code>	Search for among available modules (Lmod only)
<code>module load <mod1> [mod2...]</code>	Load a module
<code>module unload <module></code>	Unload a module
<code>module list</code>	List loaded modules
<code>module purge</code>	Unload all modules (purge)
<code>module display <module></code>	Display what a module does
<code>module use <path></code>	Prepend the directory to the <code>MODULEPATH</code> environment variable
<code>module unuse <path></code>	Remove the directory from the <code>MODULEPATH</code> environment variable

Software/Modules Management

<http://hpcugent.github.io/easybuild/>

- **Easybuild**: open-source framework to (automatically) build scientific software
- **Why?**: *"Could you please install this software on the cluster?"*
 - ↳ Scientific software is often **difficult** to build
 - ✓ non-standard build tools / incomplete build procedures
 - ✓ hardcoded parameters and/or poor/outdated documentation
 - ↳ EasyBuild helps to facilitate this task
 - ✓ **consistent** software **build and installation** framework
 - ✓ includes testing step that helps validate builds
 - ✓ **automatically generates LMod modulefiles**

```
$> module use $LOCAL_MODULES
$> module load tools/EasyBuild
$> eb -S HPL      # Search for recipes for HPL software
$> eb HPL-2.2-intel-2017a.eb # Install HPL 2.2 w. Intel toolchain
```

Hands-on 1: Modules & Easybuild

Your Turn!

Hands-on 1

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/easybuild/>

- **Discover** Environment Modules and Lmod Part 1
- Installation of EasyBuild Part 2 (a)
- **Local** vs. **Global** Usage Part 2 (b)
 - ↪ local installation of `zlib`
 - ↪ global installation of `snappy` and `protobuf`, needed later

Hands-on 2: Building Hadoop

- We will need to install the Hadoop MapReduce by Cloudera using EasyBuild.
 - ↪ this build is quite long (~**30 minutes on 4 cores**)
 - ↪ **Obj**: make it build while the keynote continues ;)

Hands-on 2

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/hadoop/install/>

- Pre-requisites
 - ↪ Installing **Java 1.7.0** (7u80) and **1.8.0** (8u152) Step 1
 - ↪ Installing **Maven 3.5.2** Step 1.a
 - ↪ Installing **Maven 3.5.2** Step 1.b
- Installing **Hadoop 2.6.0-cdh5.12.0** Step 2



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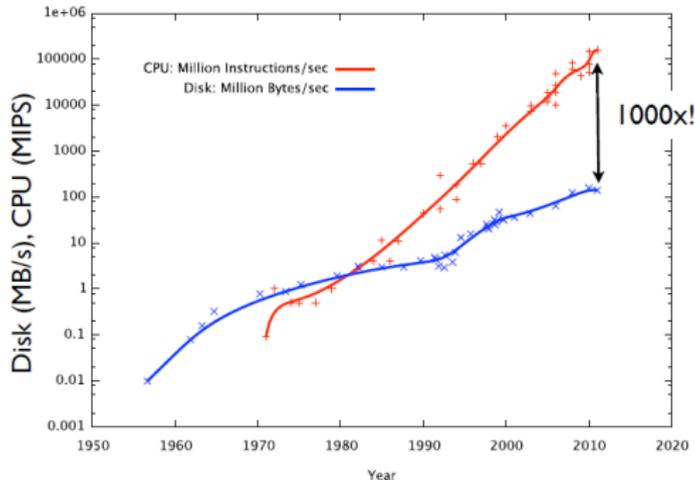


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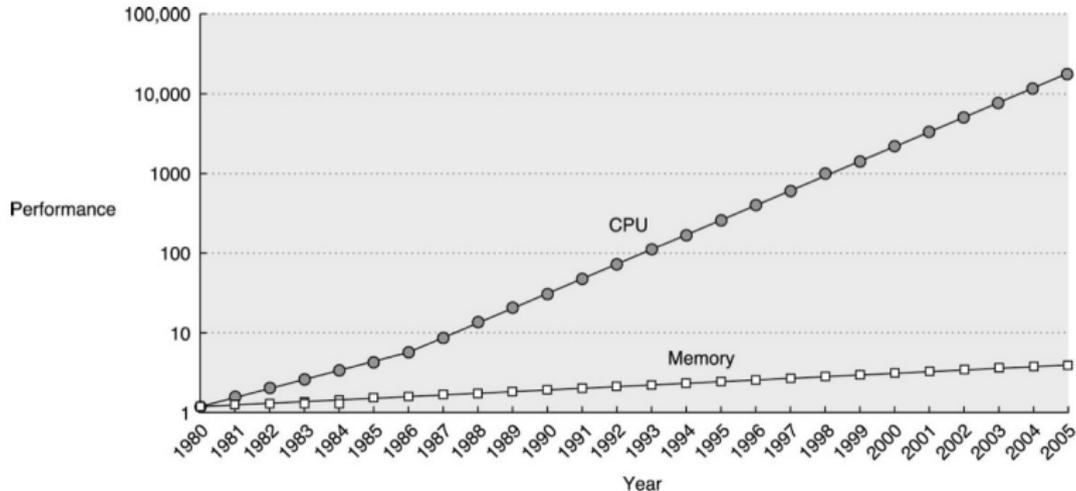
Data Intensive Computing

- Data volumes increasing massively
 - ↳ Clusters, storage capacity increasing massively
- Disk speeds are not keeping pace.
- Seek speeds even worse than read/write



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Speed Expectation on Data Transfer

<http://fasterdata.es.net/>

- How long to transfer **1 TB** of data across various speed networks?

Network	Time
10 Mbps	300 hrs (12.5 days)
100 Mbps	30 hrs
1 Gbps	3 hrs
10 Gbps	20 minutes

- **(Again)** small I/Os really **kill** performances
 - ↳ **Ex:** transferring 80 TB for the backup of ecosystem_biology
 - ↳ same rack, 10Gb/s. 4 weeks → 63TB transfer...

Speed Expectation on Data Transfer

<http://fasterdata.es.net/>

Data set size

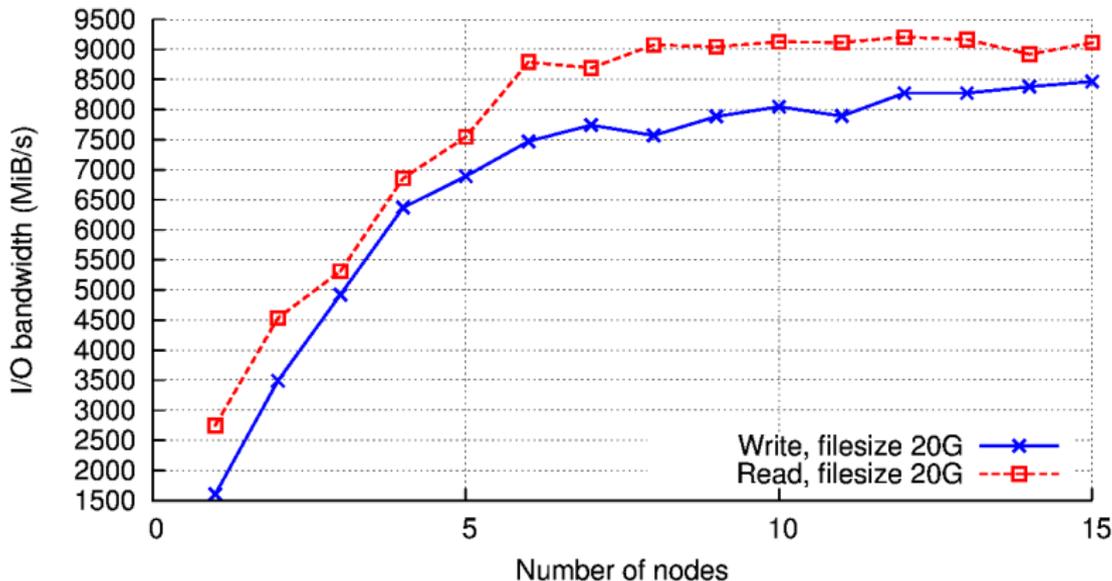
10PB	166.67 TB/sec	33.33 TB/sec	8.33 TB/sec	2.78 TB/sec
1PB	16.67 TB/sec	3.33 TB/sec	833.33 GB/sec	277.78 GB/sec
100TB	1.67 TB/sec	333.33 GB/sec	83.33 GB/sec	27.78 GB/sec
10TB	166.67 GB/sec	33.33 GB/sec	8.33 GB/sec	2.78 GB/sec
1TB	16.67 GB/sec	3.33 GB/sec	833.33 MB/sec	277.78 MB/sec
100GB	1.67 GB/sec	333.33 MB/sec	83.33 MB/sec	27.78 MB/sec
10GB	166.67 MB/sec	33.33 MB/sec	8.33 MB/sec	2.78 MB/sec
1GB	16.67 MB/sec	3.33 MB/sec	0.83 MB/sec	0.28 MB/sec
100MB	1.67 MB/sec	0.33 MB/sec	0.08 MB/sec	0.03 MB/sec
	1 Minute	5 Minutes	20 Minutes	1 Hour
	Time to transfer			

Speed Expectation on Data Transfer

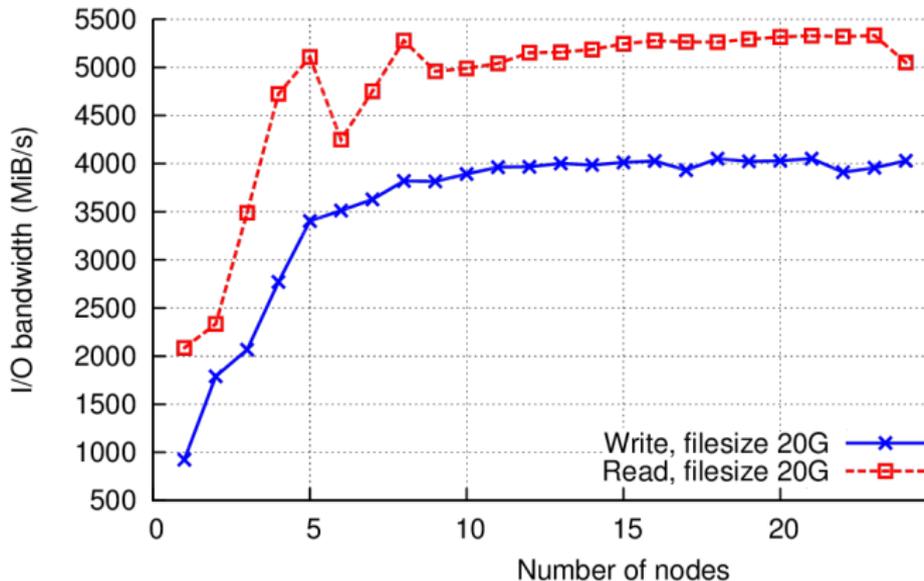
<http://fasterdata.es.net/>

Data set size	8 Hours	24 Hours	7 Days	30 Days
1XB	34.72 TB/sec	11.57 TB/sec	1.65 TB/sec	385.80 GB/sec
100PB	3.47 TB/sec	1.16 TB/sec	165.34 GB/sec	38.58 GB/sec
10PB	347.22 GB/sec	115.74 GB/sec	16.53 GB/sec	3.86 GB/sec
1PB	34.72 GB/sec	11.57 GB/sec	1.65 GB/sec	385.80 MB/sec
100TB	3.47 GB/sec	1.16 GB/sec	165.34 MB/sec	38.58 MB/sec
10TB	347.22 MB/sec	115.74 MB/sec	16.53 MB/sec	3.86 MB/sec
1TB	34.72 MB/sec	11.57 MB/sec	1.65 MB/sec	0.39 MB/sec
100GB	3.47 MB/sec	1.16 MB/sec	0.17 MB/sec	0.04 MB/sec
10GB	0.35 MB/sec	0.12 MB/sec	0.02 MB/sec	0.00 MB/sec
	8 Hours	24 Hours	7 Days	30 Days
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Storage Performances: GPFS



Storage Performances: Lustre

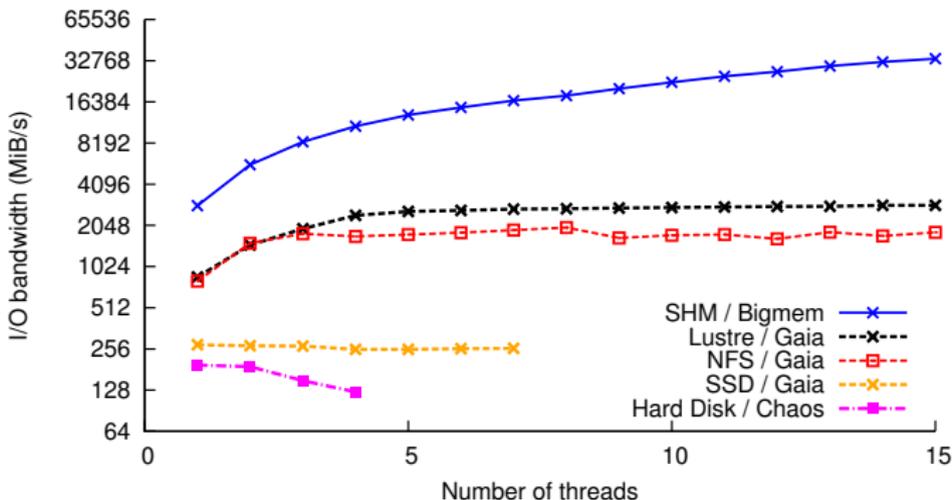


Storage Performances

- Based on IOR or IOZone, reference I/O benchmarks

Read

↳ tests performed in 2013

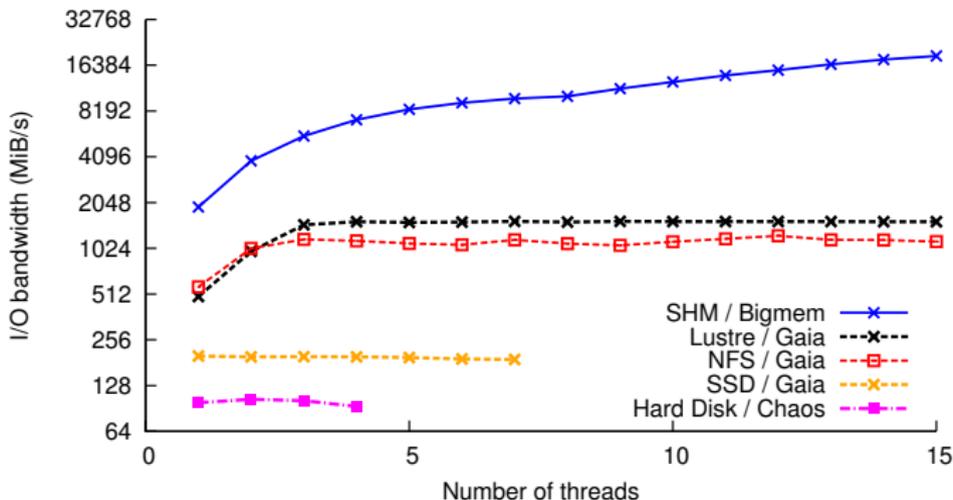


Storage Performances

- Based on IOR or IOZone, reference I/O benchmarks

Write

↳ tests performed in 2013



Understanding Your Storage Options

Where can I store and manipulate my data?

- **Shared storage**

- ↪ NFS - **not scalable** ≈ 1.5 GB/s (R) $\mathcal{O}(100$ TB)
- ↪ GPFS - **scalable** ≈ 10 GB/s (R) $\mathcal{O}(1$ PB)
- ↪ Lustre - **scalable** ≈ 5 GB/s (R) $\mathcal{O}(0.5$ PB)

- **Local storage**

- ↪ local file system (/tmp) $\mathcal{O}(200$ GB)
 - ✓ over HDD ≈ 100 MB/s, over SSD ≈ 400 MB/s
- ↪ RAM (/dev/shm) ≈ 30 GB/s (R) $\mathcal{O}(20$ GB)

- **Distributed storage**

- ↪ HDFS, Ceph, GlusterFS - **scalable** ≈ 1 GB/s

⇒ **In all cases: small I/Os really kill storage performances**



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Data Transfer in Practice

```
$> wget [-O <output>] <url>           # download file from <url>
```

```
$> curl [-o <output>] <url>          # download file from <url>
```

- Transfer **from** FTP/HTTP[S] wget or (better) curl
 - ↪ can also serve to send HTTP POST requests
 - ↪ support HTTP cookies (useful for JDK download)

Data Transfer in Practice

```
$> scp [-P <port>] <src> <user>@<host>:<path>
```

```
$> rsync -avzu [-e 'ssh -p <port>'] <src> <user>@<host>:<path>
```

- [Secure] Transfer **from/to** two remote machines over SSH
 - ↳ scp or (better) rsync (transfer **only** what is required)
- Assumes you have understood and configured appropriately SSH!

SSH: Secure Shell

- Ensure **secure** connection to remote (UL) server
 - ↪ establish **encrypted** tunnel using **asymmetric keys**
 - ✓ **Public** `id_rsa.pub` vs. **Private** `id_rsa` (**without** `.pub`)
 - ✓ typically on a non-standard port (**Ex:** 8022) *limits kiddie script*
 - ✓ Basic rule: 1 machine = 1 key pair
 - ↪ the private key is **SECRET**: **never** send it to anybody
 - ✓ Can be protected with a passphrase

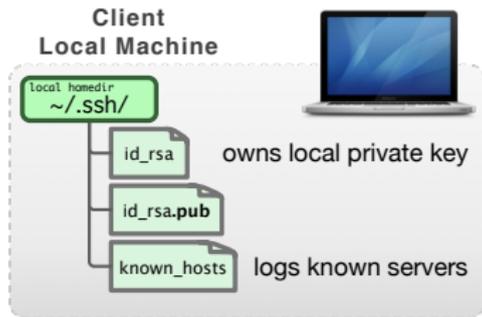
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- SSH is used as a secure backbone channel for **many** tools
 - ↪ Remote shell **i.e** remote command line
 - ↪ File transfer: `rsync`, `scp`, `sftp`
 - ↪ versioning synchronization (`svn`, `git`), `github`, `gitlab` etc.

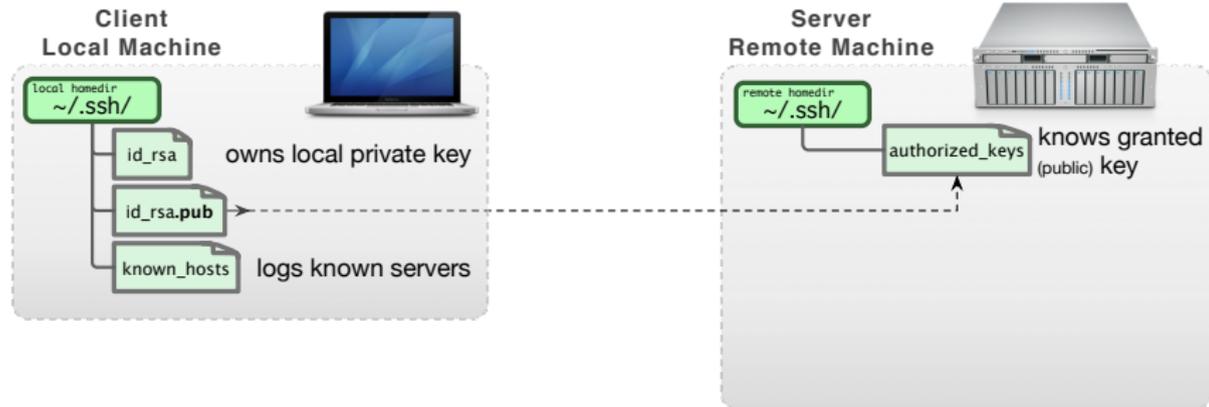
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- Authentication:
 - ↳ `password` (disable if possible)
 - ↳ (**better**) **public key authentication**

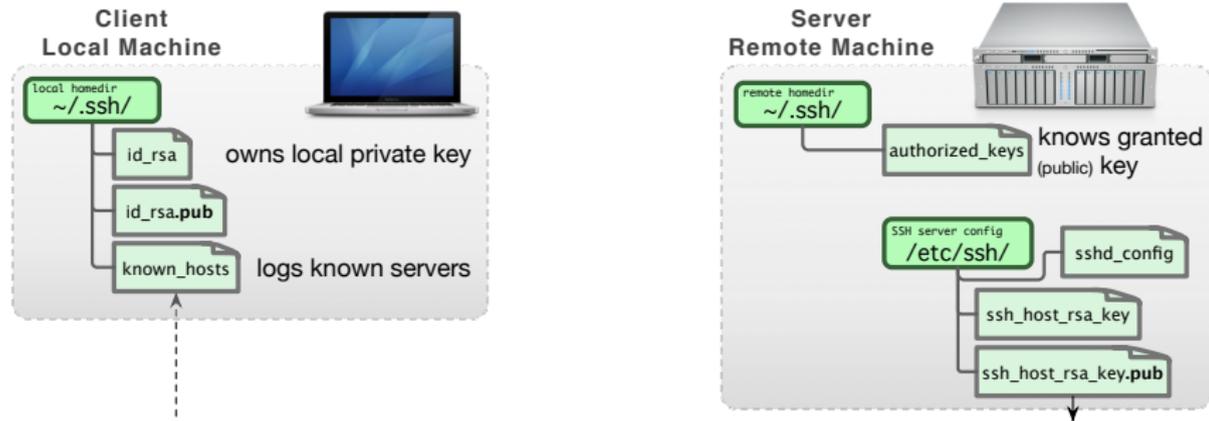
SSH: Public Key Authentication



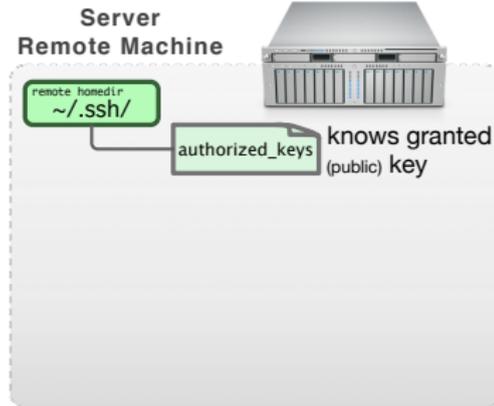
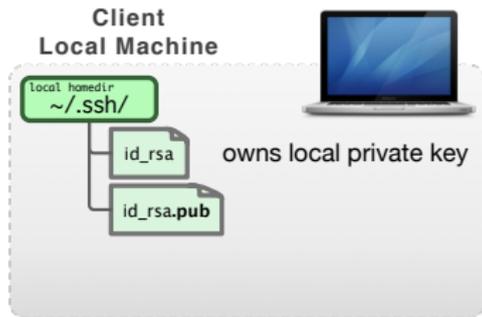
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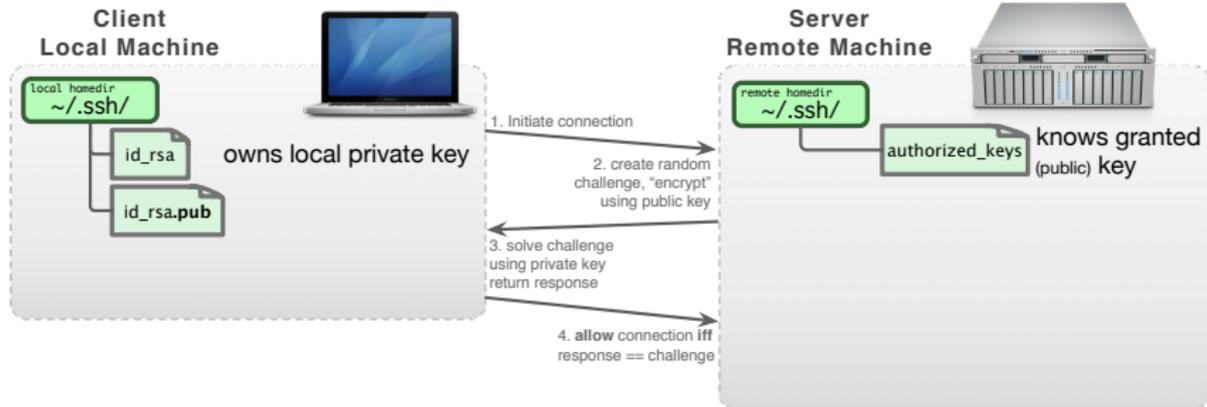
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SSH: Public Key Authentication



SSH: Public Key Authentication



- Restrict to public key authentication: `/etc/ssh/sshd_config`:

```
PermitRootLogin no
# Disable Passwords
PasswordAuthentication no
ChallengeResponseAuthentication no
```

```
# Enable Public key auth.
RSAAuthentication yes
PubkeyAuthentication yes
```

Hands-on 3: Data transfer over SSH

- Before doing **Big** Data, learn how to transfer data between 2 hosts
↳ do it securely over SSH

```
# Quickly generate a 10GB file  
$> dd if=/dev/zero of=/tmp/bigfile.txt bs=100M count=100  
# Now try to transfert it between the 2 Vagrant boxes ;)
```

Hands-on 3

<http://nesusws-tutorials-BD-DL.rtfid.io/en/latest/hands-on/data-transfer/>

- **Generate SSH Key Pair** and authorize the public part **Step 1**
- **Data transfer** over SSH with **scp** **Step 2.a**
- **Data transfer** over SSH with **rsync** **Step 2.b**



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Sharing Code and Data

- Before doing **Big** Data, manage and version correctly **normal** data

What kinds of systems are available?

- *Good*: NAS, Cloud Dropbox, Google Drive, Figshare. . .
- **Better** - **Version Control systems (VCS)**
↪ SVN, Git and Mercurial
- **Best** - **Version Control Systems** on the **Public/Private Cloud**
↪ GitHub, Bitbucket, Gitlab

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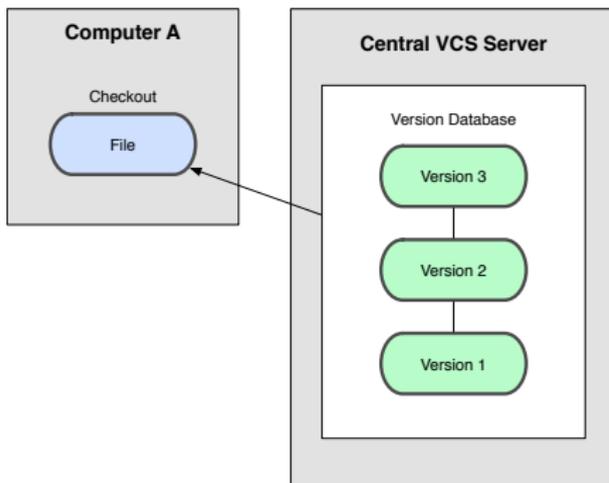
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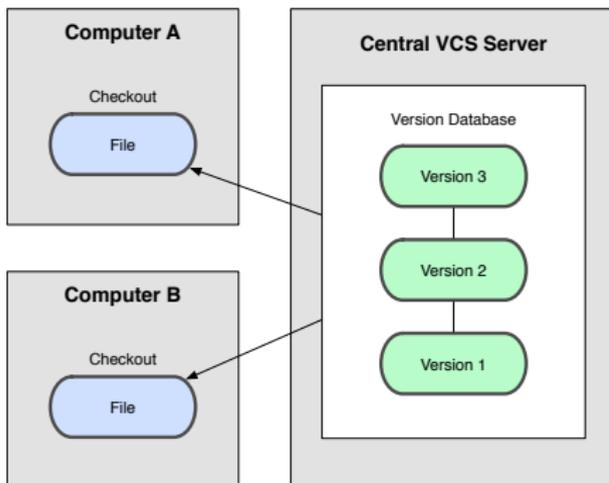
- **Which one?**

- ↪ Depends on the level of privacy you expect
 - ✓ . . . but you probably already know these tools ☺
- ↪ **Few handle GB files. . .**

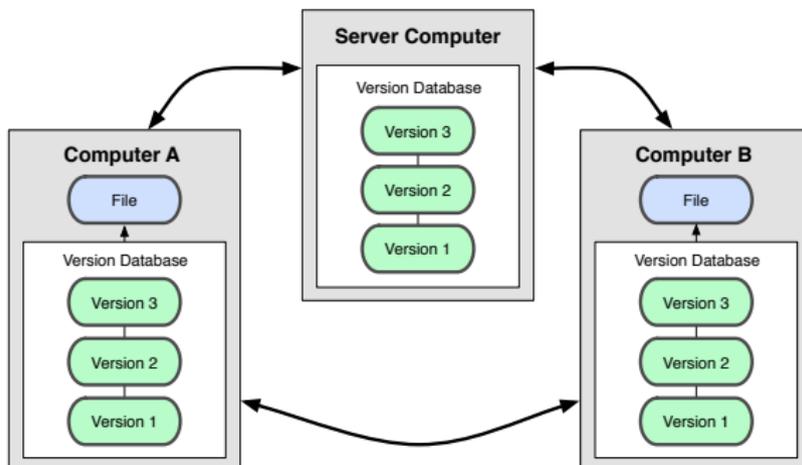
Centralized VCS - CVS, SVN



Centralized VCS - CVS, SVN

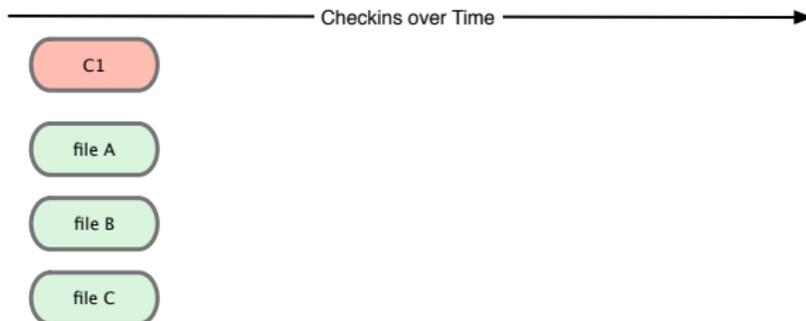


Distributed VCS - Git

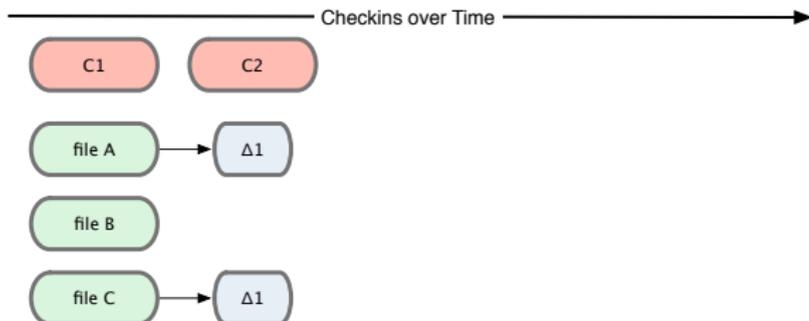


Everybody has the full history of commits

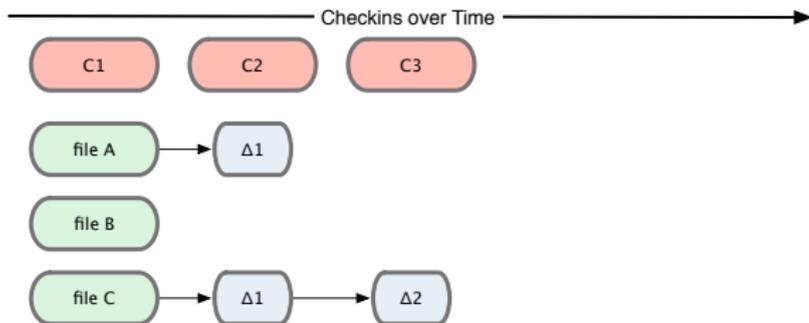
Tracking changes (most VCS)



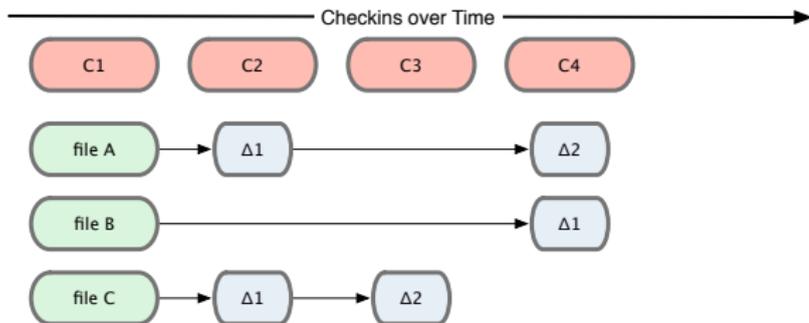
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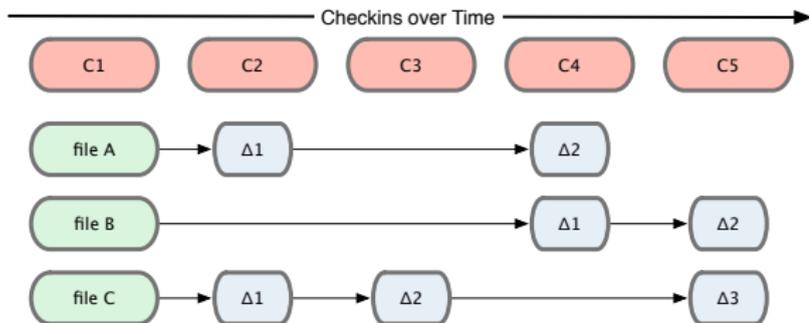
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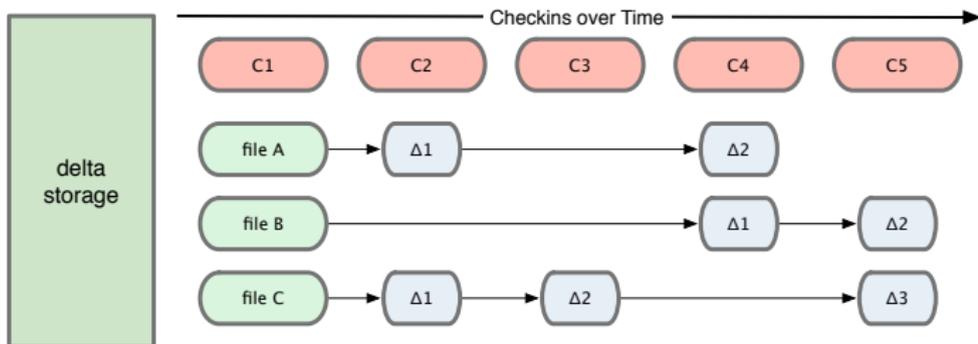
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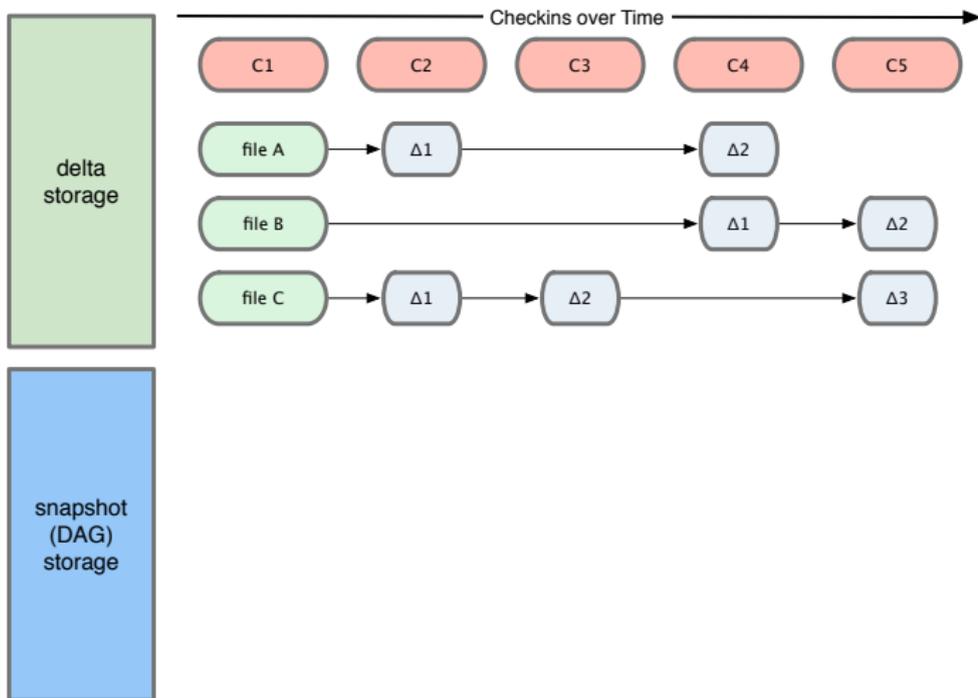
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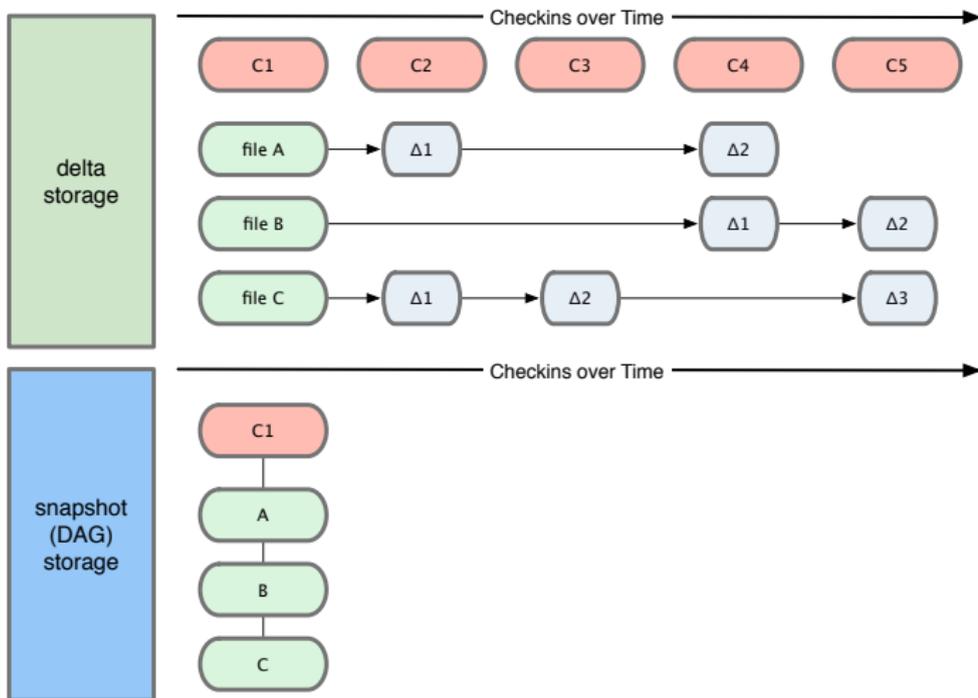
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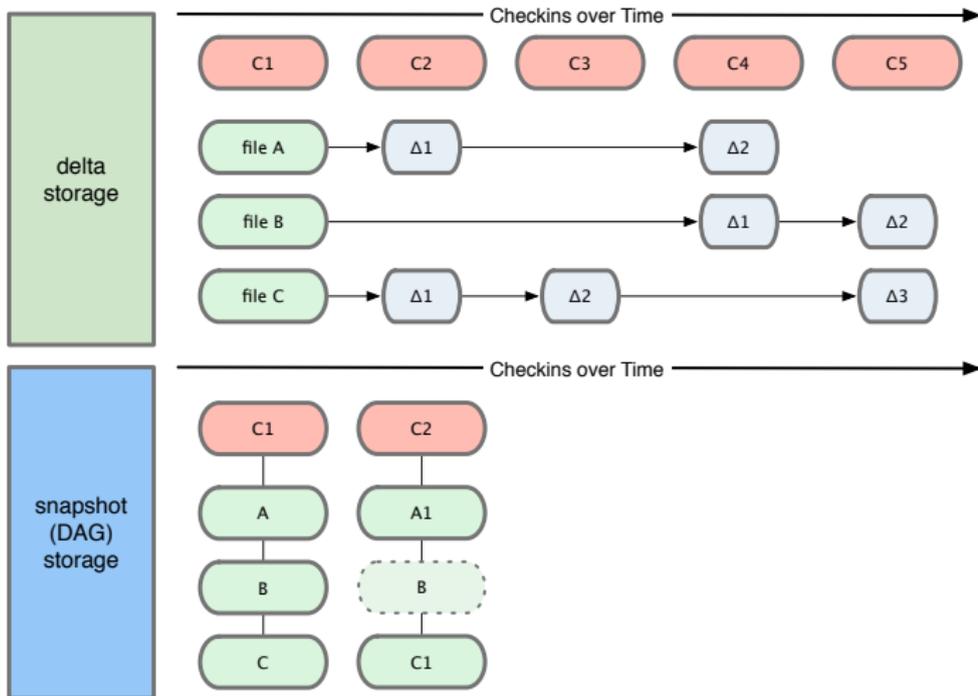
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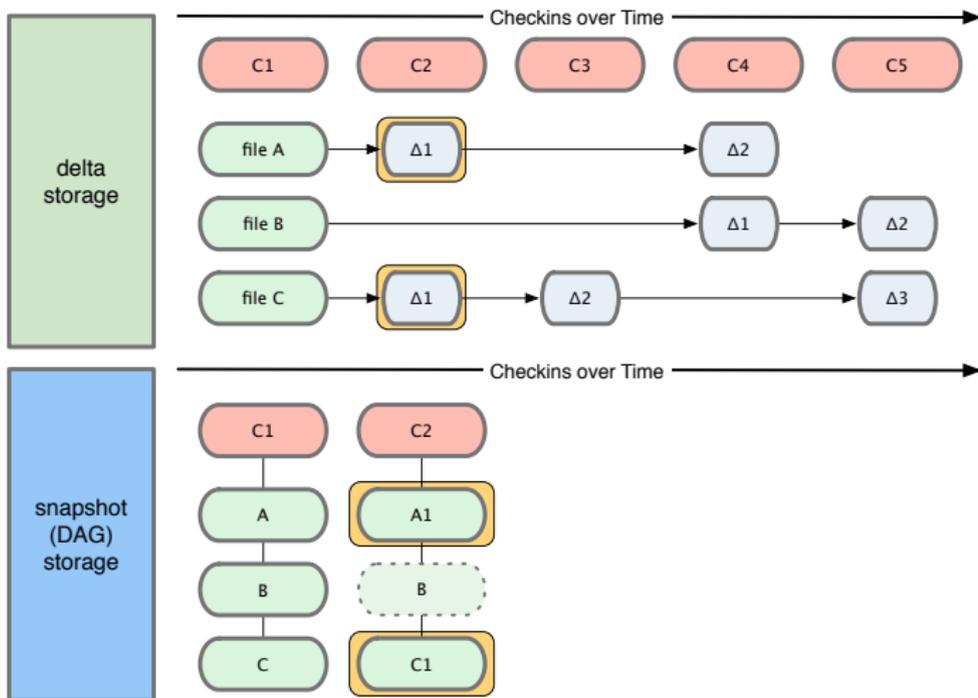
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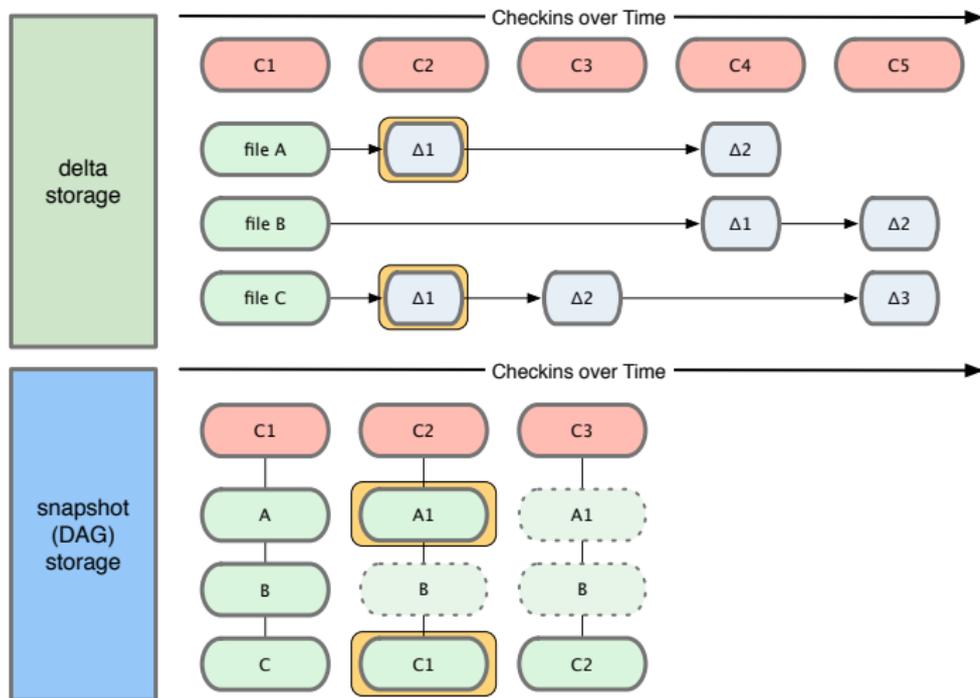
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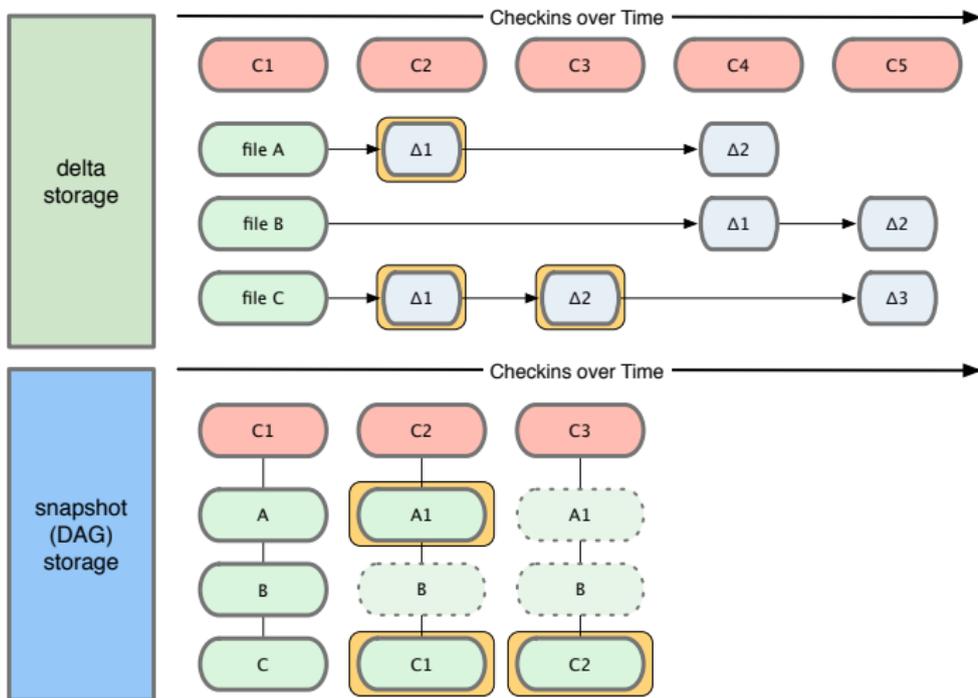
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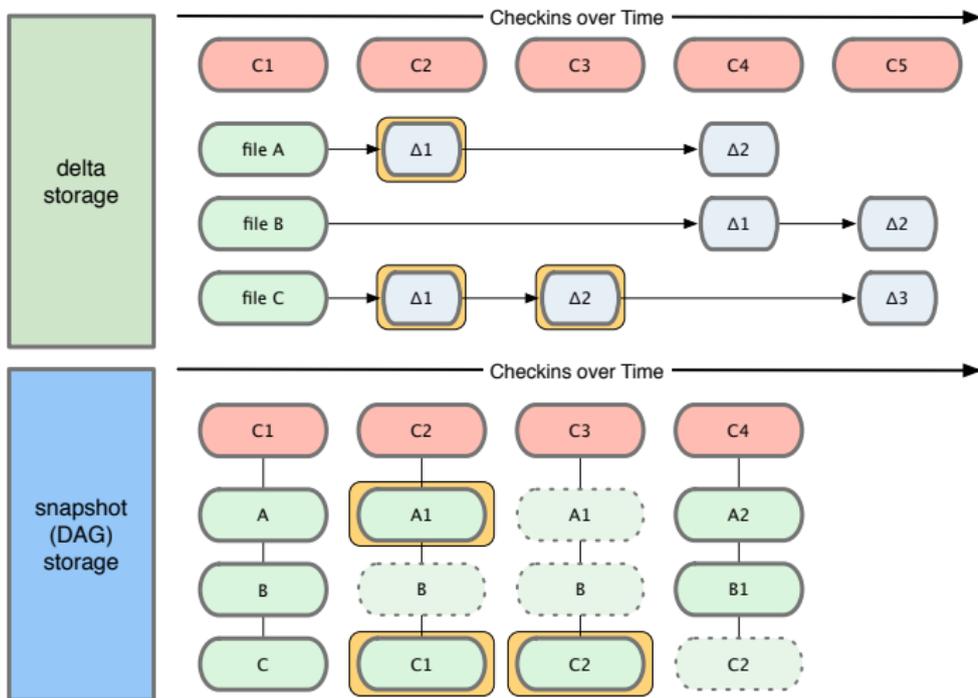
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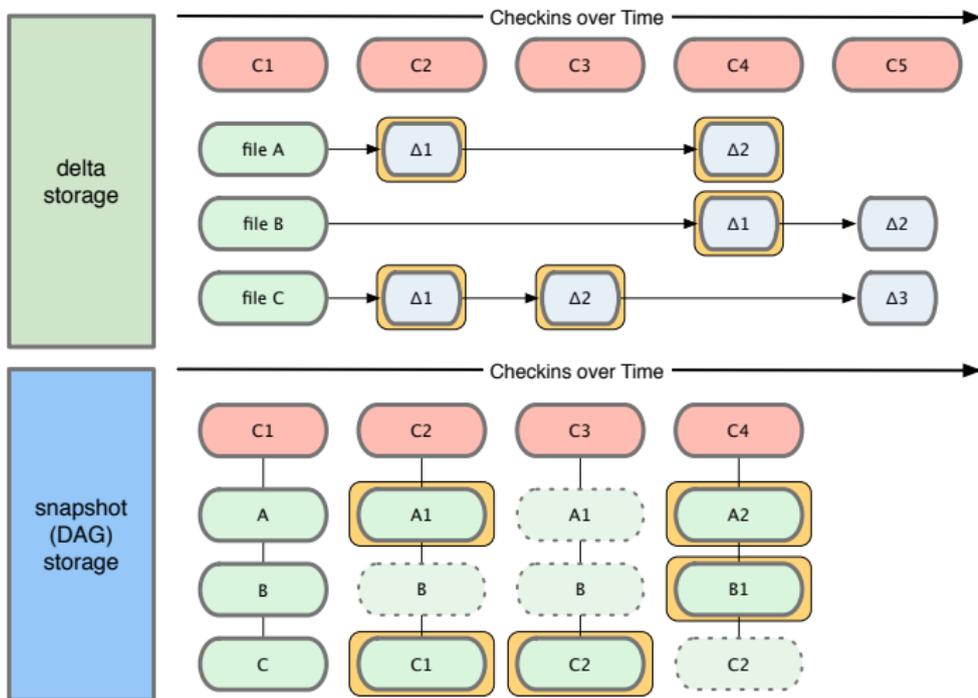
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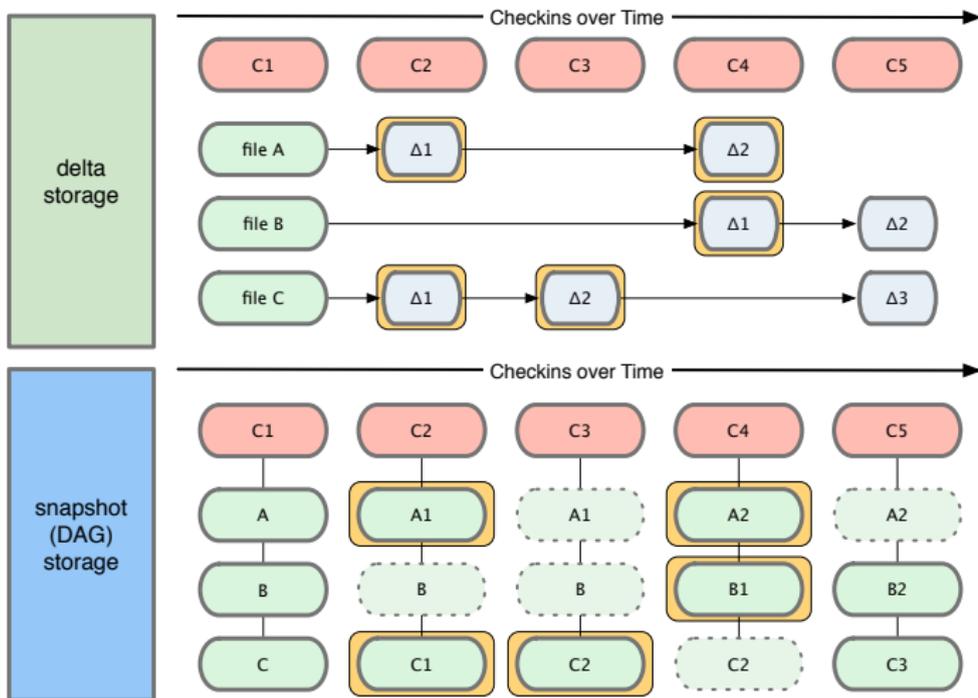
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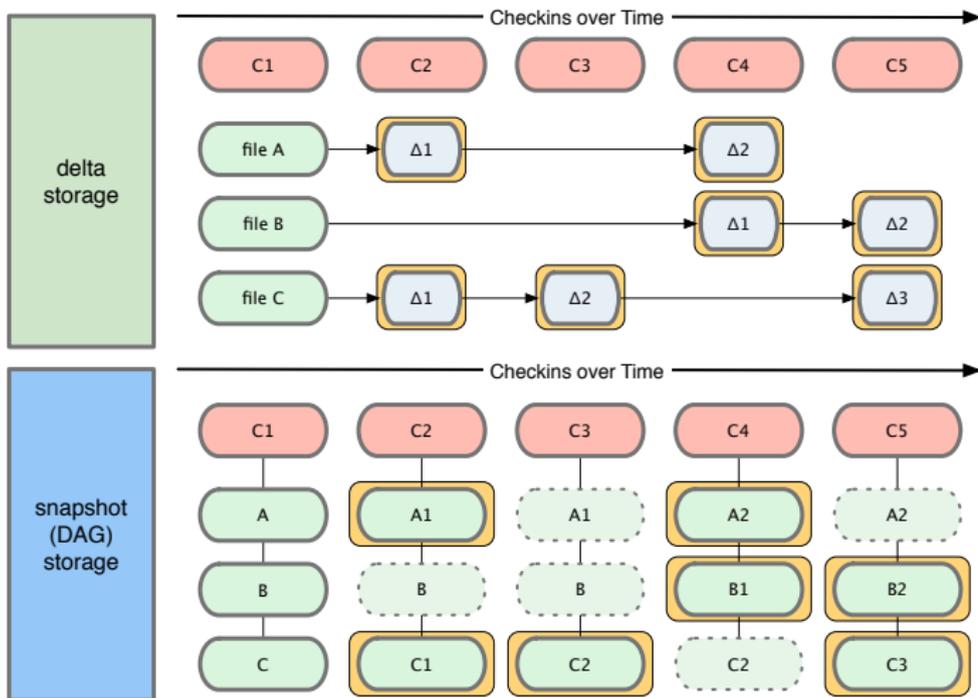
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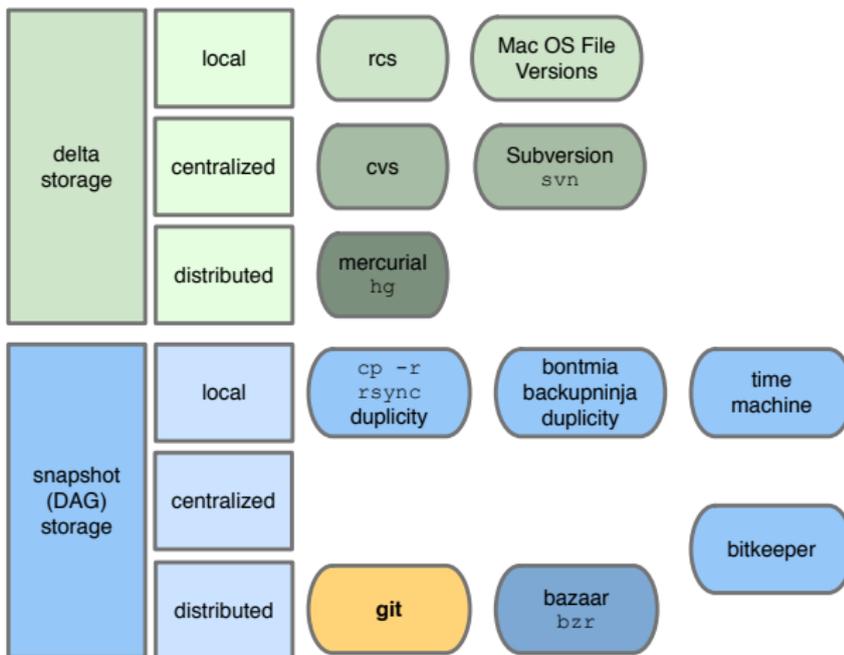
Tracking changes (Git)



Tracking changes (Git)



VCS Taxonomy



Git at the heart of BD

<http://git-scm.org>



Git on the Cloud: Github github.com

(Reference) web-based Git repository hosting service

Set up Git



Create Repository



Fork repository



Work together



So what makes Git so useful?

(almost) Everything is local

- everything is fast
- every clone is a backup
- you work **mainly offline**

Ultra Fast, Efficient & Robust

- Snapshots, not patches (deltas)
- **Cheap branching and merging**
 - ↳ Strong support for thousands of parallel branches
- Cryptographic integrity everywhere

Other Git features

- **Git does not delete**

- ↪ **Immutable** objects, Git generally only adds data
- ↪ If you mess up, you can usually recover your stuff
 - ✓ Recovery can be tricky though

Other Git features

- **Git does not delete**

- ↳ **Immutable** objects, Git generally only adds data
- ↳ If you mess up, you can usually recover your stuff
 - ✓ Recovery can be tricky though

Git Tools / Extension

- cf. **Git submodules** or **subtrees**

- **Introducing git-flow**

- ↳ workflow with a strict branching model
- ↳ offers the git commands to follow the workflow

```
$> git flow init
$> git flow feature { start, publish, finish } <name>
$> git flow release { start, publish, finish } <version>
```

Git in practice

Basic Workflow

- **Pull** latest changes `git pull`
- **Edit** files `vim / emacs / subl ...`
- **Stage** the changes `git add`
- **Review** your changes `git status`
- **Commit** the changes `git commit`

Git in practice

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- **Review** your changes `git status`
- **Commit** the changes `git commit`

For cheaters: A Basicer Workflow

- **Pull** latest changes `git pull`
- **Edit** files `vim / emacs / subl ...`
- **Stage & commit** all the changes `git commit -a`

Git Summary

- **Advices: Commit early, commit often!**

- ↪ commits = save points
 - ✓ use descriptive commit messages
- ↪ Do not get out of sync with your collaborators
- ↪ Commit the sources, not the derived files

- **Not covered here (by lack of time)**

- ↪ does not mean you should not dig into it!
- ↪ *Resources:*
 - ✓ <https://git-scm.com/>
 - ✓ tutorial: IT/Dev[op]s Army Knives Tools for the Researcher
 - ✓ tutorial: Reproducible Research at the Cloud Era



Summary

- 1 Introduction**
 - Before we start...
 - Overview of HPC & BD Trends
 - Main HPC and DB Components
- 2 Interlude: Software Management in HPC systems**
- 3 [Big] Data Management in HPC Environment: Overview and Challenges**
 - Performance Overview in Data transfer
 - Data transfer in practice
 - Sharing Data
- 4 Big Data Analytics with Hadoop & Spark**
 - Apache Hadoop
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What is a Distributed File System?

- Straightforward idea: **separate logical from physical storage.**
 - ↪ Not all files reside on a single physical disk,
 - ↪ or the same physical server,
 - ↪ or the same physical rack,
 - ↪ or the same geographical location,...
- **Distributed file system (DFS):**
 - ↪ virtual file system that enables clients to access files
 - ✓ ... as if they were stored locally.

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● Major DFS distributions:

- ↳ **NFS:** originally developed by Sun Microsystems, started in 1984
- ↳ **AFS/CODA:** originally prototypes at Carnegie Mellon University
- ↳ **GFS:** Google paper published in 2003, not available outside Google
- ↳ **HDFS:** designed after GFS, part of Apache Hadoop since 2006



Distributed File System Architecture?

Master-Slave Pattern

- Single (or few) **master** nodes maintain state info. about clients
- All clients R&W requests go through the global master node.
- **Ex:** GFS, HDFS

Distributed File System Architecture?

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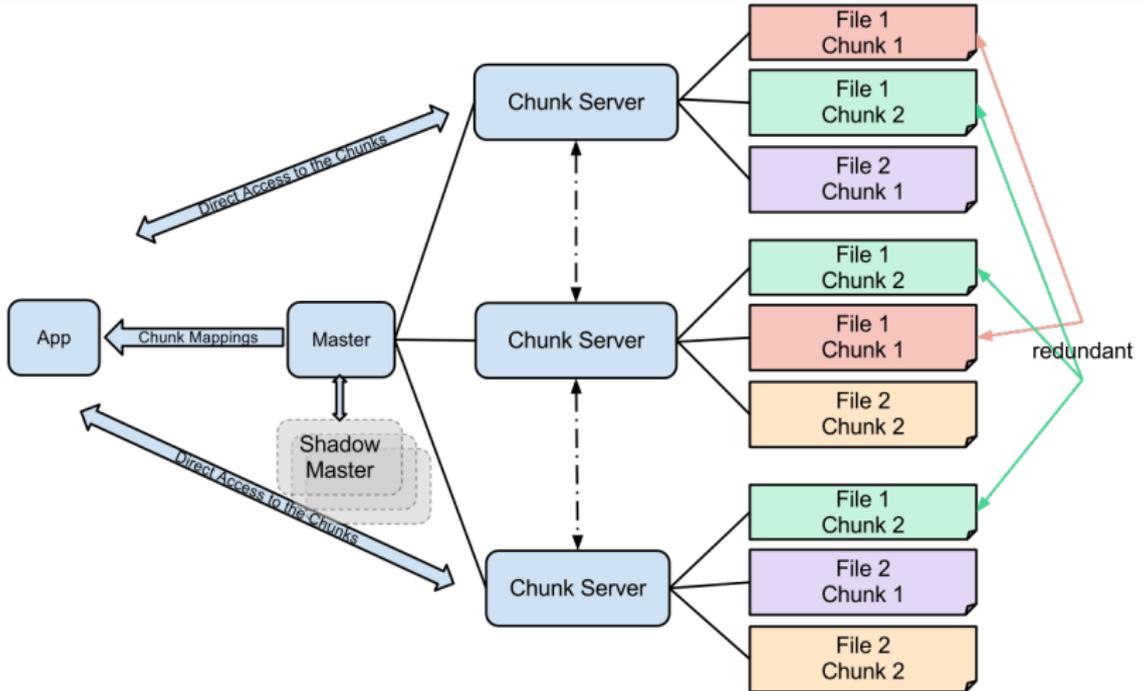
Peer-to-Peer Pattern

- No global state information.
- Each node may both serve and process data.

Google File System (GFS) (2003)

- Radically different architecture compared to NFS, AFS and CODA.
 - ↪ specifically tailored towards **large-scale** and **long-running analytical processing tasks**
 - ↪ over thousands of storage nodes.
- **Basic assumption:**
 - ↪ client nodes (aka. *chunk servers*) may fail any time!
 - ↪ Bugs or hardware failures.
 - ↪ Special tools for monitoring, periodic checks.
 - ↪ Large files (multiple GBs or even TBs) are split into 64 MB *chunks*.
 - ↪ Data modifications are mostly append operations to files.
 - ↪ Even the master node may fail any time!
 - ✓ Additional *shadow master* fallback with read-only data access.
- Two types of reads: Large sequential reads & small random reads

Google File System (GFS) (2003)



GFS Consistency Model

- **Atomic File Namespace Mutations**

- ↪ File creations/deletions centrally controlled by the master node.
- ↪ Clients typically create and write entire file,
 - ✓ then add the file name to the file namespace stored at the master.

- **Atomic Data Mutations**

- ↪ only 1 atomic modification of 1 replica (!) at a time is guaranteed.

- **Stateful Master**

- ↪ Master sends regular **heartbeat** messages to the chunk servers
- ↪ Master keeps chunk locations of all files (+ replicas) in memory.
- ↪ locations not stored persistently. . .
 - ✓ but polled from the clients at startup.

- **Session Semantics**

- ↪ Weak consistency model for file replicas and client caches only.
- ↪ Multiple clients may read and/or write the same file concurrently.
- ↪ The client that last writes to a file **wins**.

Fault Tolerance & Fault Detection

● Fast Recovery

- ↪ master & chunk servers can restore their states and (re-)start in s.
 - ✓ regardless of previous termination conditions.

● Master Replication

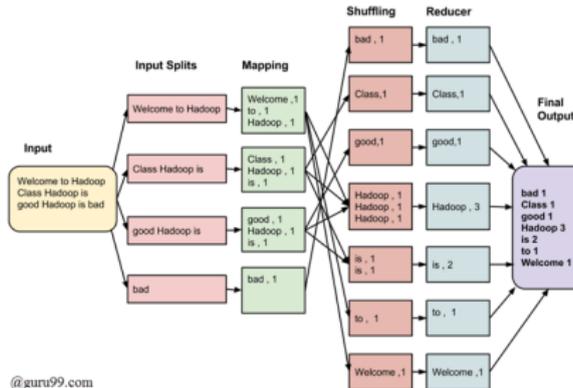
- ↪ *shadow master* provides RO access when primary master is down.
 - ✓ Switches back to read/write mode when primary master is back.
- ↪ Master node does not keep a persistent state info. of its clients,
 - ✓ rather polls clients for their states when started.

● Chunk Replication & Integrity Checks

- ↪ chunk divided into 64 KB blocks, each with its own 32-bit checksum
 - ✓ verified at read and write times.
- ↪ Higher replication factors for more intensively requested chunks (**hotspots**) can be configured.

Map-Reduce

- Breaks the processing into two main phases:
 1. the **map** phase
 2. the **reduce** phase.
- Each phase has key-value pairs as input and output,
 - ↳ the types of which may be chosen by the programmer.
 - ↳ the programmer also specifies the **map** and **reduce** functions



Hadoop



- Initially started as a student project at Yahoo! labs in 2006
 - ↳ Open-source Java implem. of GFS and MapReduce frameworks
- Switched to Apache in 2009. Now consists of three main modules:
 1. **HDFS**: Hadoop distributed file system
 2. **YARN**: Hadoop job scheduling and resource allocation
 3. **MapReduce**: Hadoop adaptation of the MapReduce principle

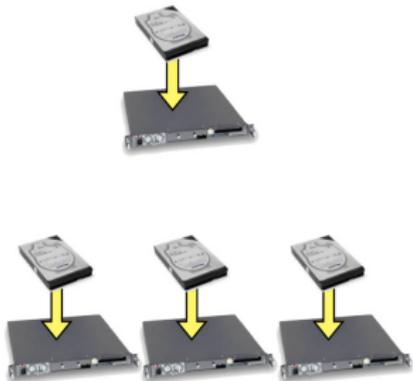
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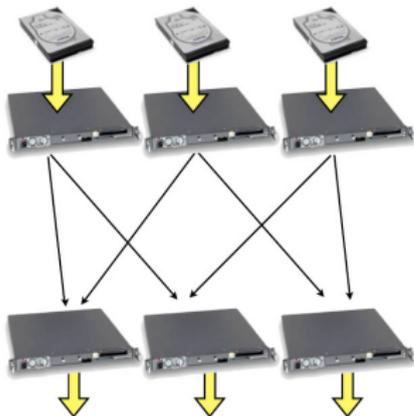
- Basis for many other open-source Apache toolkits:
 - ↪ **PIG/PigLatin**: file-oriented data storage & script-based query language
 - ↪ **HIVE**: distributed SQL-style data warehouse
 - ↪ **HBase**: distributed key-value store
 - ↪ **Cassandra**: fault-tolerant distributed database, etc.
- HDFS still mostly follows the original GFS architecture.

Scale-Out Design



- HDD streaming speed $\sim 50\text{MB/s}$
 - ↪ $3\text{TB} = 17.5\text{ hrs}$
 - ↪ $1\text{PB} = 8\text{ months}$
- Scale-out (weak scaling)
 - ↪ **FS distributes data on ingest**
- Seeking too slow
 - ↪ $\sim 10\text{ms}$ for a seek
 - ↪ Enough time to read half a megabyte
- **Batch processing**
- Go through entire data set in one (or small number) of passes

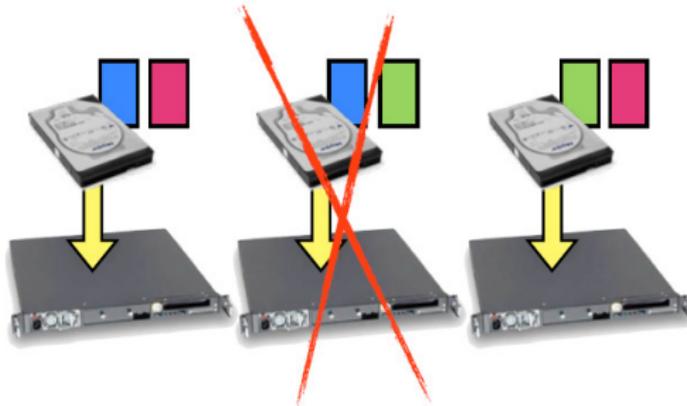
Combining Results



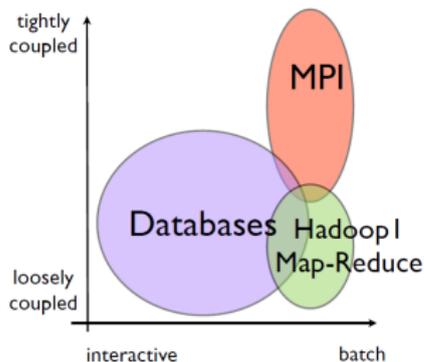
- Each node preprocesses its local data
 - ↳ Shuffles its data to a small number of other nodes
- Final processing, output is done there

Fault Tolerance

- Data also replicated upon ingest
- Runtime watches for dead tasks, restarts them on live nodes
- Re-replicates

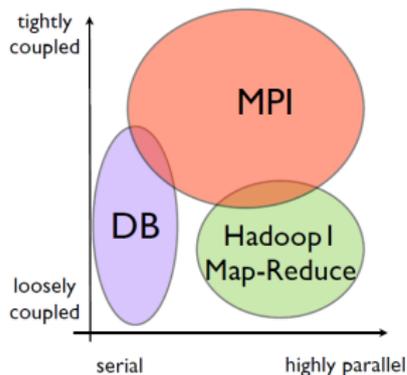


Hadoop: What is it Good At?



- **Classic Hadoop 1.x is all about batch processing** of massive amounts of data
 - ↳ Not much point below ~1TB
- Map-Reduce is relatively loosely coupled;
 - ↳ one **shuffle** phase.
- Very strong weak scaling in this model
 - ↳ more data, more nodes.
- **Batch:**
 - ↳ process all data in one go
 - ✓ w/classic Map Reduce
 - ↳ Current Hadoop has many other capabilities besides batch - **more later**

Hadoop: What is it Good At?



- **Compare with databases**

- ↪ very good at working on small subsets of large databases
 - ✓ DBs: very interactive for many tasks
 - ✓ ... yet have been difficult to scale

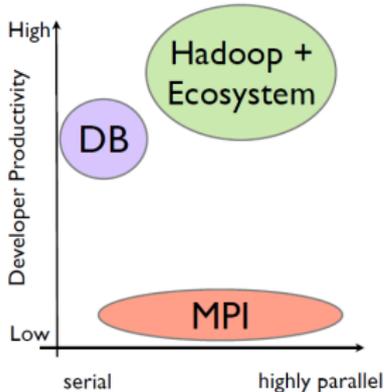
- **Compare with HPC (MPI)**

- ↪ Also typically batch
- ↪ Can (and does) go up to enormous scales

- Works extremely well for very tightly coupled problems:

- ↪ zillions of iterations/timesteps/ exchanges.

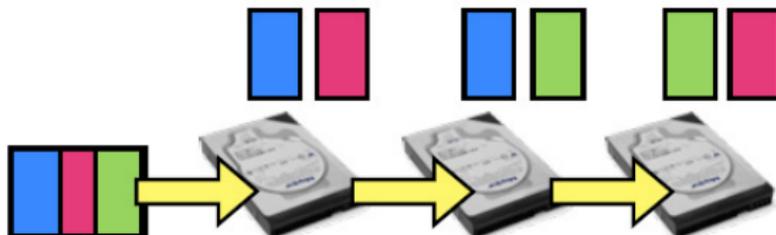
Hadoop vs HPC



- We HPC users might be tempted to an unseemly smugness
 - ↳ *They solved the problem of disk-limited, loosely-coupled, data analysis by throwing more disks at it and weak scaling?*
Ooooooooooh
- **We would be wrong.**
 - ↳ A single novice developer can write:
 - ✓ real, scalable,
 - ✓ 1000+ node data-processing tasks in Hadoop-family tools in an afternoon.
 - ↳ In MPI... less likely...

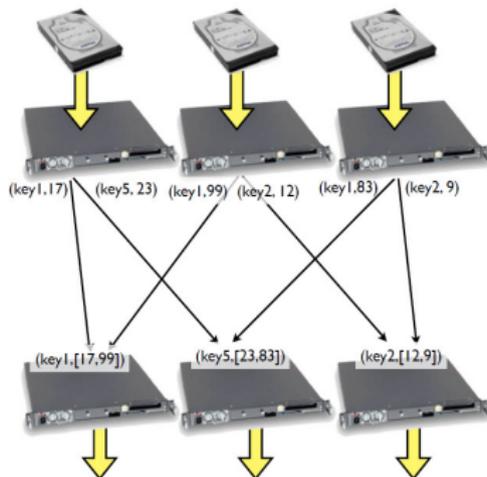
Data Distribution: Disk

- Hadoop & al. arch. handle the hardest part of parallelism for you
 - ↳ aka **data distribution**.
- **On disk:**
 - ↳ HDFS distributes, replicates data as it comes in
 - ↳ Keeps track of computations local to data



Data Distribution: Network

- **On network: Map Reduce** (eg) works in terms of key-value pairs.
 - ↪ Preprocessing (map) phase ingests data, emits (k, v) pairs
 - ↪ Shuffle phase assigns reducers,
 - ✓ gets all pairs with same key onto that reducer.
 - ↪ Programmer does not have to design communication patterns





Makes the problem easier

- **Hardest parts of parallel programming with HPC tools**

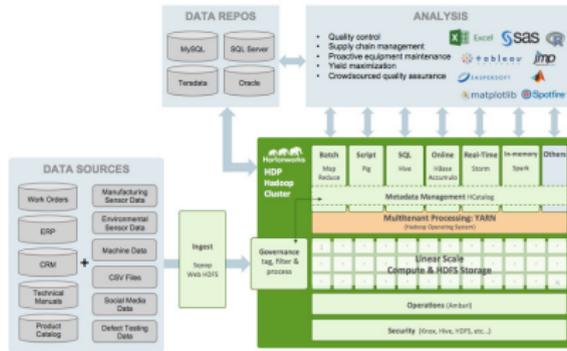
- ↪ Decomposing the problem, and,
- ↪ Getting the intermediate data where it needs to go,

- **Hadoop does that for you**

- ↪ automatically
- ↪ for a wide range of problems.

Built a reusable substrate

- HDFS and the MapReduce layer were very well architected.
 - ↳ Enables many higher-level tools
 - ↳ Data analysis, machine learning, NoSQL DBs,...
- Extremely productive environment
 - ↳ And Hadoop 2.x (YARN) is now much much more than just MapReduce



Hadoop and HPC

- **Not either-or anyway**

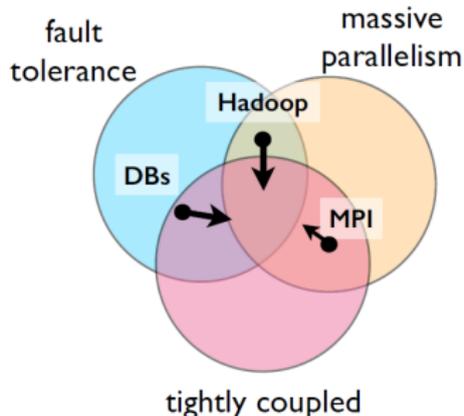
- ↪ Use HPC to generate big / many simulations,

- ↪ Use Hadoop to analyze results

- ✓ **Ex:** Use Hadoop to preprocess huge input data sets (ETL),

- ✓ ... and HPC to do the tightly coupled computation afterwards.

- **In all cases:** Everything is Converging



The Hadoop Filesystem

- **HDFS is a distributed parallel filesystem**
 - ↪ Not a general purpose file system
 - ✓ does not implement posix
 - ✓ cannot just mount it and view files
- Access via `hdfs fs` commands or programatic APIs
- Security slowly improving

```
$> hdfs fs -[cmd]
```

cat	chgrp
chmod	chown
copyFromLocal	copyToLocal
cp	du
dus	expunge
get	getmerge
ls	lsr
mkdir	movefromLocal
mv	put
rm	rmr
setrep	stat
tail	test
text	touchz

The Hadoop Filesystem

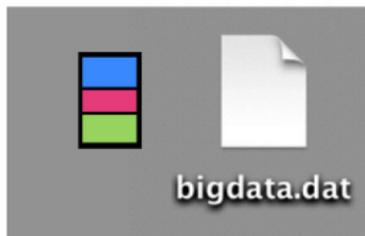
- **Required** to be:

- ↪ able to deal with large files, large amounts of data
- ↪ scalable & reliable in the presence of failures
- ↪ fast at reading contiguous streams of data
- ↪ only need to write to new files or append to files
- ↪ require only commodity hardware

- **As a result:**

- ↪ Replication
- ↪ Supports mainly high bandwidth, **not** especially low latency
- ↪ No caching
 - ✓ what is the point if primarily for streaming reads?
 - ✓ Poor support for seeking around files
 - ✓ Poor support for zillions of files
- ↪ Have to use separate API to see filesystem
- ↪ Modelled after Google File System (2004 Map Reduce paper)

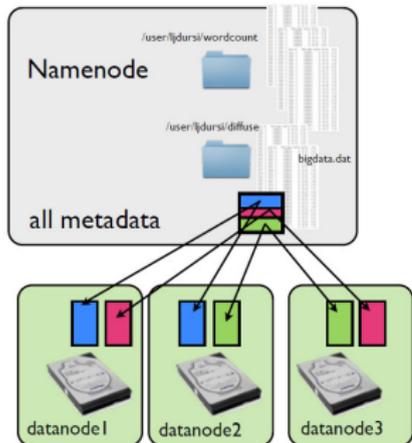
Hadoop vs HPC



- HDFS is a **block-based** FS
 - ↪ A file is broken into blocks,
 - ↪ these blocks are distributed across nodes
- **Blocks are large;**
 - ↪ 64MB is default,
 - ↪ many installations use 128MB or larger
- Large block size
 - ↪ time to stream a block much larger than time disk time to access the block.

```
# Lists all blocks in all files:  
$> hdfs fsck / -files -blocks
```

Datanodes and Namenode



Two types of nodes in the filesystem:

1. Namenode

- ↪ stores all metadata / block locations in memory
- ↪ Metadata updates stored to persistent journal

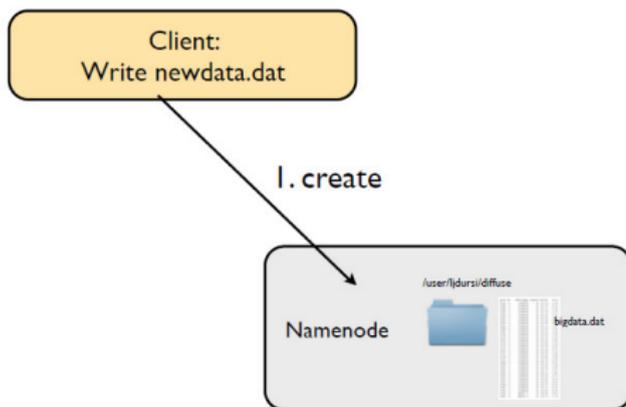
2. Datanodes

- ↪ store/retrieve blocks for client/namenode

- Newer versions of Hadoop: federation

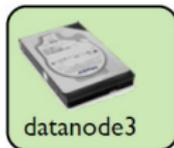
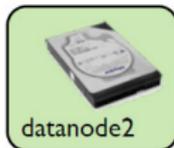
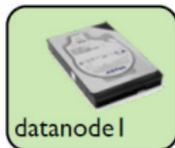
- ↪ \neq namenodes for `/user`, `/data`...
- ↪ High Availability namenode pairs

Writing a file

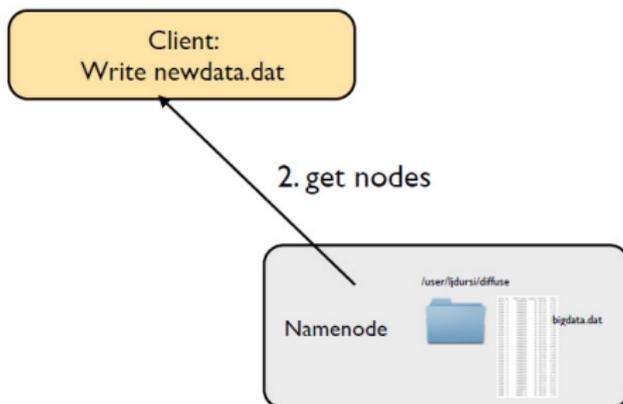


- **Writing a file** multiple stage process:

- ↪ Create file
- ↪ Get nodes for blocks
- ↪ Start writing
- ↪ Data nodes coordinate replication
- ↪ Get ack back
- ↪ Complete

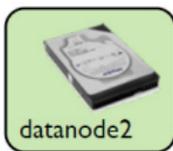
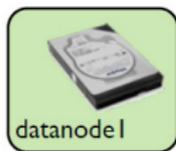


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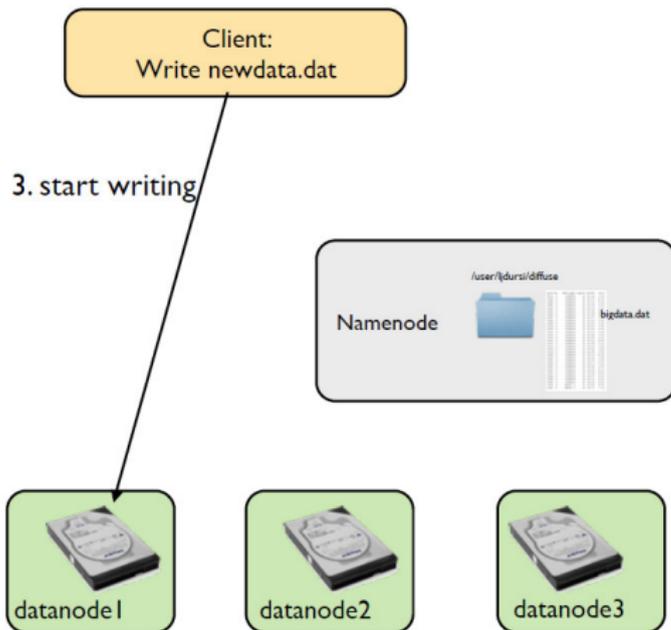


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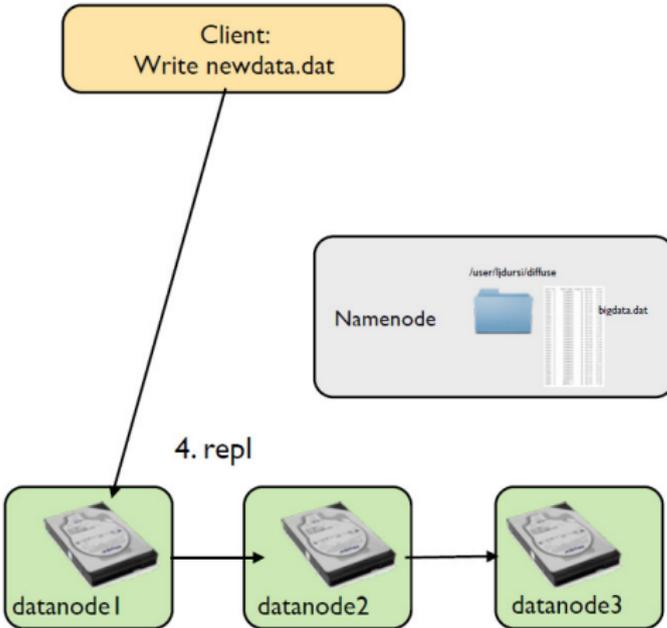


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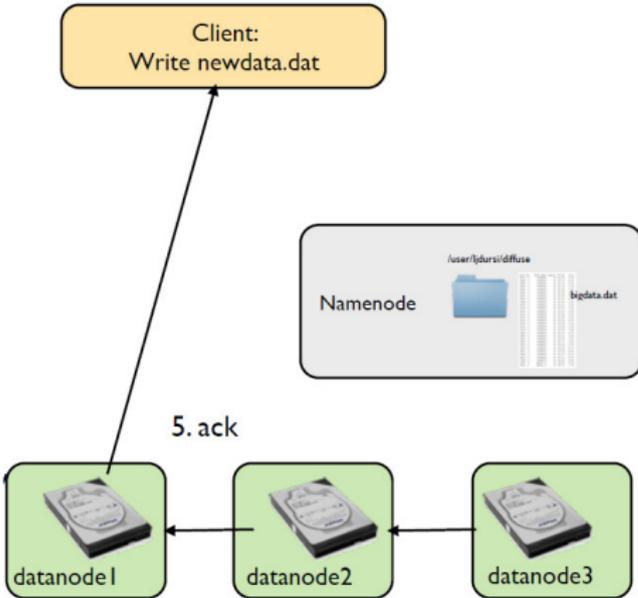
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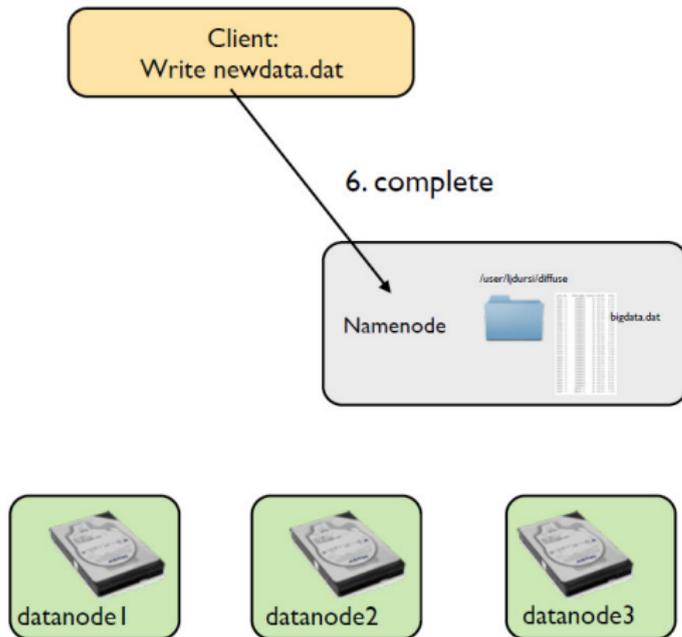
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 - ↪ Complete

Writing a file

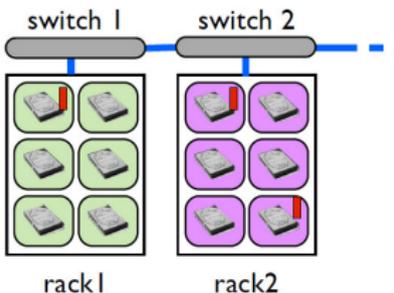


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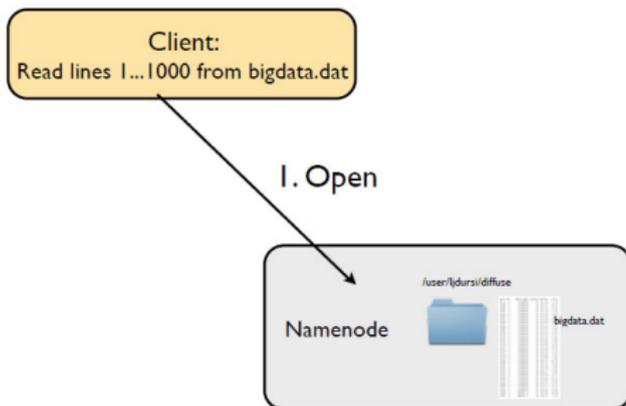
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- ↪ Get nodes for blocks
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- ↪ Get ack back (**while writing**)
- ↪ Complete

Where to Replicate?

- **Tradeoff** to choosing replication locations
 - ↪ **Close**: faster updates, less network bandwidth
 - ↪ **Further**: better failure tolerance
- **Default strategy**:
 1. copy on different location on same node
 2. second on different *rack*(switch),
 3. third on same rack location, different node.
- Strategy configurable.
 - ↪ Need to configure Hadoop file system to know location of nodes

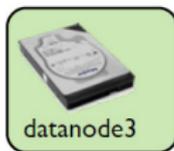
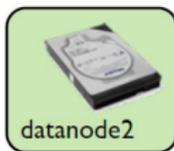
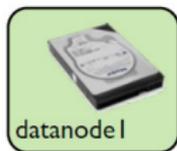


Reading a file

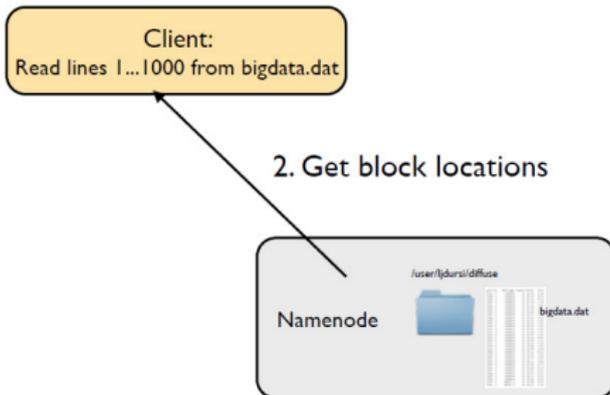


- **Reading** a file

- ↪ Open call
- ↪ Get block locations
- ↪ Read from a replica

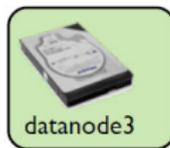
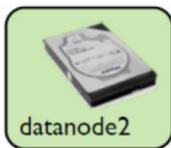
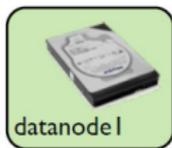


Reading a file



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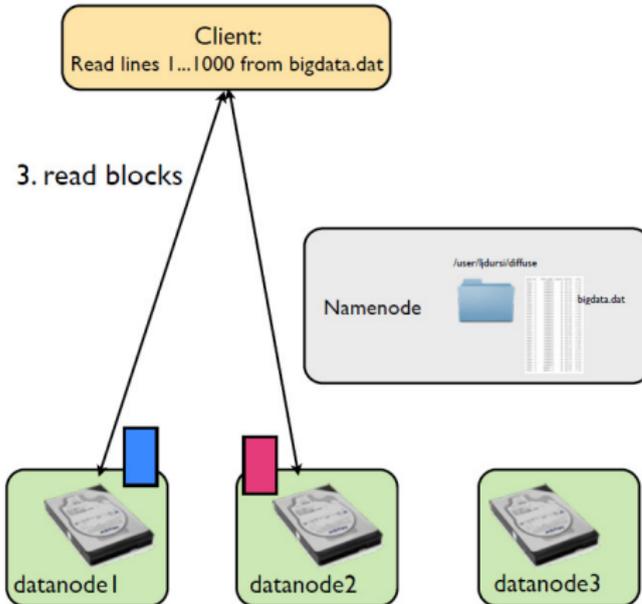
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Reading a file

- **Reading** a file

- ↪ Open call
- ↪ Get block locations
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Configuring HDFS

- Need to tell HDFS how to set up filesystem
 - ↳ `data.dir, name.dir`
 - ✓ where on local system (eg, local disk) to write data
 - ↳ parameters like replication
 - ✓ how many copies to make
 - ↳ default name - default file system to use
 - ↳ Can specify multiple FSs

Configuring HDFS

```
<!-- $HADOOP_PREFIX/etc/hadoop/core-site.xml -->
<configuration>
  <property>
    <name>fs.defaultFS</name>
    <value>hdfs://<server>:9000</value>
  </property>
  <property>
    <name>dfs.data.dir</name>
    <value>/home/username/hdfs/data</value>
  </property>
  <property>
    <name>dfs.name.dir</name>
    <value>/home/username/hdfs/name</value>
  </property>
  <property>
    <name>dfs.replication</name>
    <value>3</value>
  </property>
</configuration>
```

Configuring HDFS

- In Practice, in single mode
 - ↪ Only one node to be used, the VM
 - ↪ **default server**: localhost
 - ↪ Since only one node:
 - ✓ need to specify replication factor of 1, or will always fail

```
<property>
  <name>fs.defaultFS</name>
  <value>hdfs://localhost:9000</value>
</property>
[...]
```

```
<property>
  <name>dfs.replication</name>
  <value>1</value>
</property>
```



Configuring HDFS

- You will need to make sure that environment variables are set
 - ↪ path to Java, path to Hadoop. . .
 - ↪ Easybuild does **most** of the job for you
- You will need passwordless SSH access across all nodes
- You can then start processes on various FS nodes

Configuring HDFS

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 - ↳ path to Java, path to Hadoop. . .
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- Once configuration files are set up,
 - ↳ you can format the namenode like so
 - ↳ you can start up just the file systems

```
$> hdfs namenode -format  
$> start-dfs.sh
```

Using HDFS

- Once the file system is up and running,
↳ ... you can copy files back and forth

```
$> hadoop fs -{get|put|copyFromLocal|copyToLocal} [...]
```

- Default directory is /user/\${username}
↳ **Nothing like a cd**

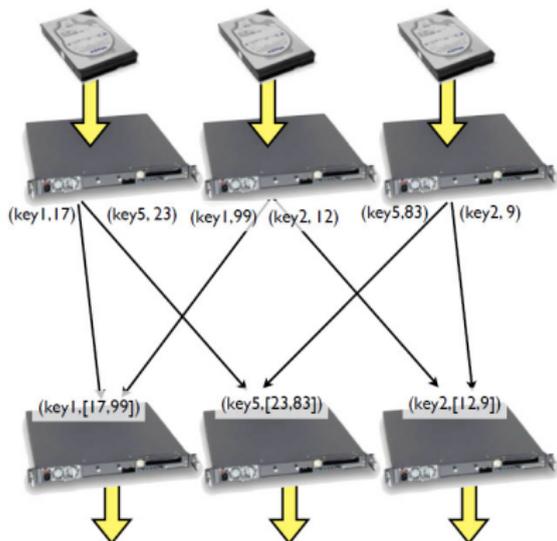
```
$> hdfs fs -mkdir /home/vagrant/hdfs-test  
$> hdfs fs -ls /home/vagrant  
$> hdfs fs -ls /home/vagrant/hdfs-test  
$> hdfs fs -put data.dat /home/vagrant/hdfs-test  
$> hdfs fs -ls /home/vagrant/hdfs-test
```



Using HDFS

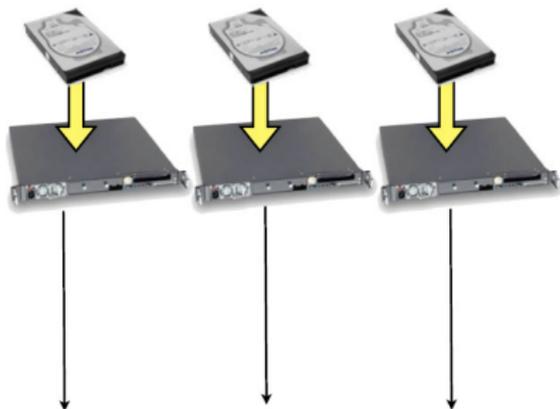
- In general, the data files you send to HDFS will be **large**
 - ↳ or else why bother with Hadoop.
- Do not want to be constantly copying back and forth
 - ↳ **view, append *in place***
- Several APIs to accessing the HDFS
 - ↳ Java, C++, Python
- Here, we use one to get a file status, and read some data from it at some given offset

Back to Map-Reduce



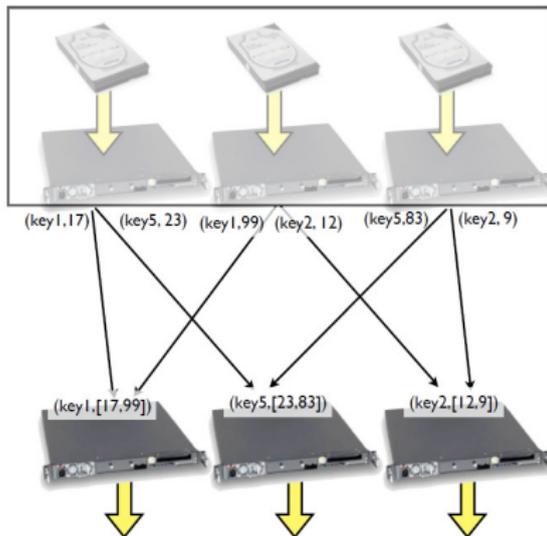
- Map processes **one element at a time**
 - ↪ emits results as (key, value) pairs.
- All results with **same key are gathered to the same reducers**
 - ↪ Reducers process list of values
 - ↪ emit results as (key, value) pairs

Map



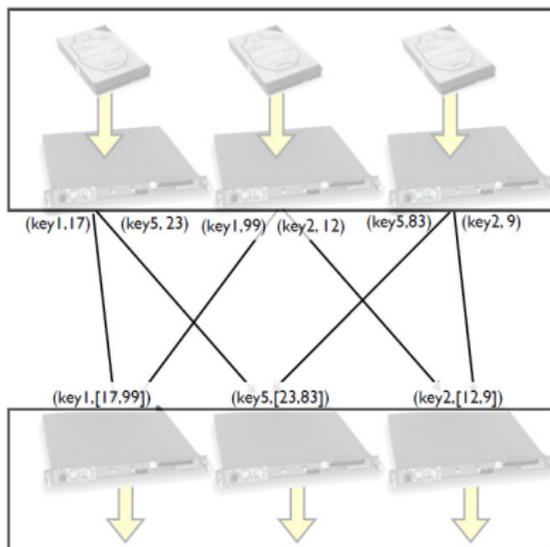
- All coupling done during **shuffle** phase
 - ↪ Embarrassingly parallel task
 - ↪ all map
- Take input, map it to output, done.
- **Famous case**
 - ↪ NYT using Hadoop to convert 11 million image files to PDFs
 - ✓ almost pure serial farm job

Reduce



- Reducing gives the coupling
- In the case of the NYT task:
 - ↪ not quite embarrassingly parallel:
 - ✓ images from multi-page articles
 - ✓ Convert a page at a time,
 - ✓ gather images with same article id onto node for conversion

Shuffle



- **shuffle is part of the Hadoop magic**

- ↳ By default, keys are hashed
- ↳ hash space is partitioned between reducers

- **On reducer:**

- ↳ gathered (k,v) pairs from mappers are sorted by key,
- ↳ then merged together by key
- ↳ Reducer then runs on one (k,[v]) tuple at a time

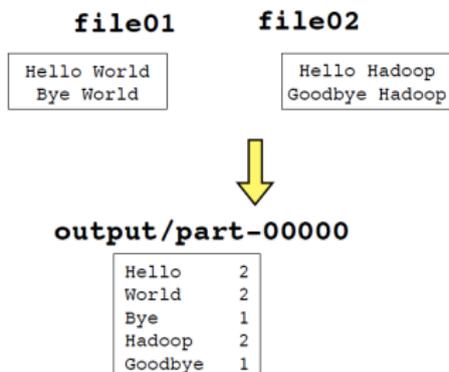
- **you can supply your own partitioner**

- ↳ Assign **similar** keys to same node
- ↳ Reducer still only sees one (k, [v]) tuple at a time.

Example: Wordcount

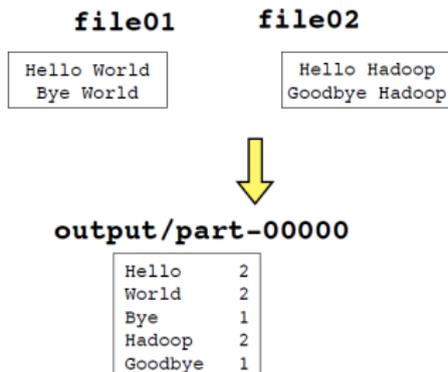
- Was used as an example in the original MapReduce paper
↳ Now basically the **hello world** of map reduce

- Problem description:** Given a **set** of documents:
↳ **count occurrences of words** within these documents



Example: Wordcount

- How would you do this with a huge document?
 - ↪ Each time you see a word:
 - ✓ if it is a new word, add a tick mark beside it,
 - ✓ otherwise add a new word with a tick
- ... But hard to parallelize
 - ↪ pb when updating the list



Example: Wordcount

file01

```
Hello World  
Bye World
```

file02

```
Hello Hadoop  
Goodbye Hadoop
```



output/part-00000

```
Hello      2  
World      2  
Bye        1  
Hadoop     2  
Goodbye    1
```

- **MapReduce way**

- ↪ all hard work done automatically by shuffle

- **Map:**

- ↪ just emit a 1 for each word you see

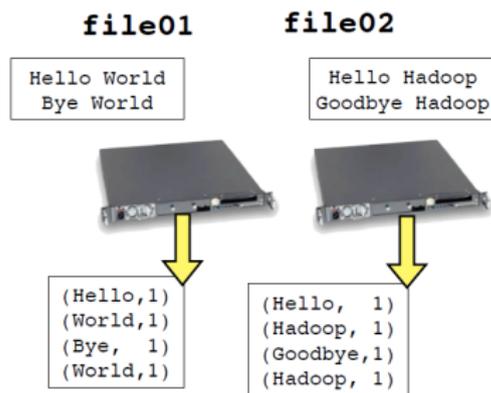
- **Shuffle:**

- ↪ assigns keys (words) to each reducer,
- ↪ sends (k,v) pairs to appropriate reducer

- **Reducer**

- ↪ just has to sum up the ones

Example: Wordcount



- **MapReduce way**

- ↪ all hard work done automatically by shuffle

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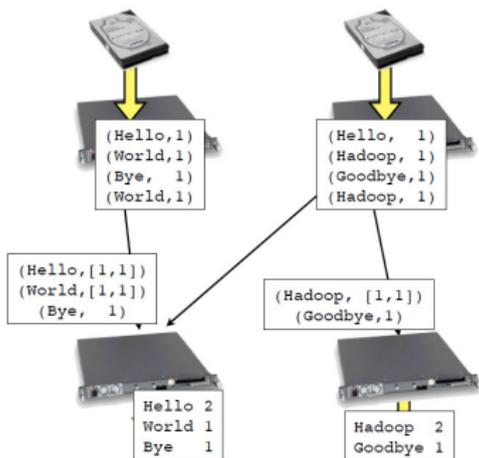
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Example: Wordcount



- **MapReduce way**

- ↪ all hard work done automatically by shuffle

- **Map:**

- ↪ just emit a 1 for each word you see

- **Shuffle:**

- ↪ assigns keys (words) to each reducer,
 - ↪ sends (k,v) pairs to appropriate reducer

- **Reducer**

- ↪ just has to sum up the ones

Hands-on 4: Playing with Hadoop

Your Turn!

- Now you are ready to play with the installed Hadoop

Hands-on 4

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/hadoop/wordcount>

- Test the tools/Hadoop modules in Single mode Step 1
 ↪ setup the wordcount example
- Enable a Cluster Setup Step 2

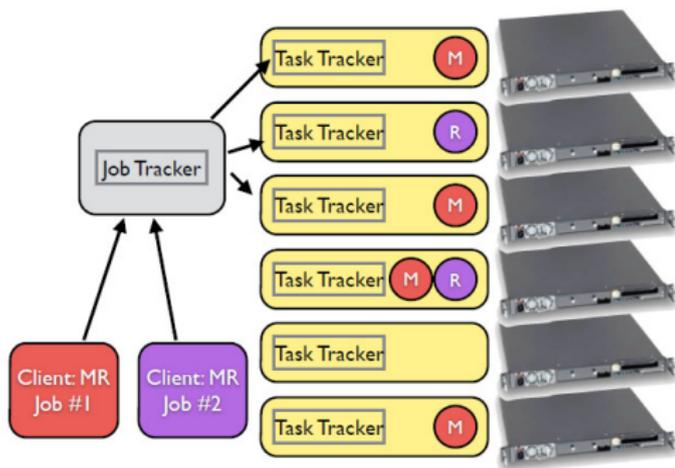


Summary

- 1 Introduction**
 - Before we start...
 - Overview of HPC & BD Trends
 - Main HPC and DB Components
- 2 Interlude: Software Management in HPC systems**
- 3 [Big] Data Management in HPC Environment: Overview and Challenges**
 - Performance Overview in Data transfer
 - Data transfer in practice
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- 4 Big Data Analytics with Hadoop & Spark**
 - Apache Hadoop
 - Apache Spark
- 5 Deep Learning Analytics with Tensorflow**

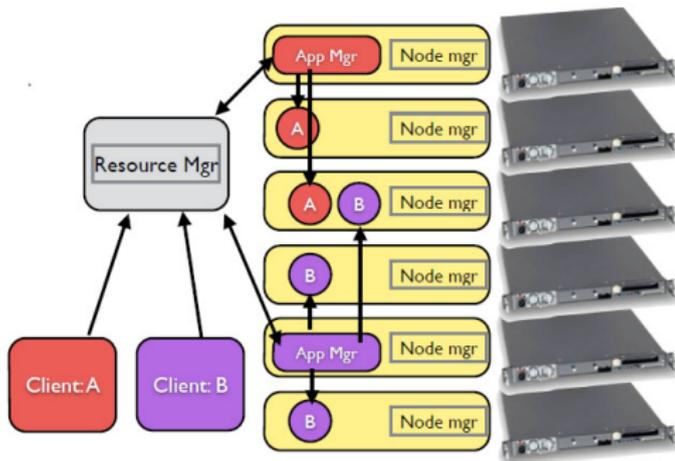
Hadoop 0.1x

- Original Hadoop was basically HDFS + infra. for MapReduce
 - ↳ Very faithful implementation of Google MapReduce paper.
 - ↳ Job tracking, orchestration all very tied to M/R model
- Made it difficult to run other sorts of jobs



YARN and Hadoop 2

- **YARN**: Yet Another Resource Negotiator
 - ↪ Looks a lot more like a cluster scheduler/resource manager
 - ↪ Allows arbitrary jobs.
- Allow for new compute/data tools. **Ex**: streaming with Spark



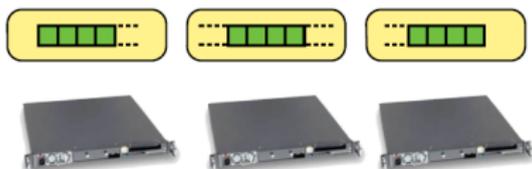
- Spark is (yet) a(-nother) distributed, **Big Data** processing platform.
↳ Everything you can do in Hadoop, you can also do in Spark.

In contrast to Hadoop

- Spark computation paradigm is not **just** MapReduce job
- Key feature - **in-memory analyses**.
↳ **multi-stage, in-memory dataflow graph** based on **Resilient Distributed Datasets (RDDs)**.

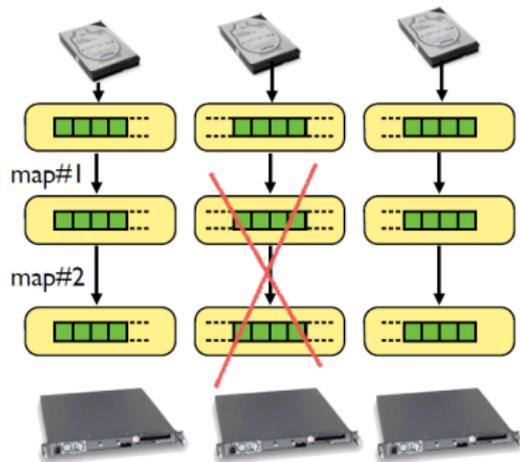
- Spark is implemented in Scala, running in a Java Virtual Machine.
 - ↳ Spark supports different languages for application development:
 - ✓ Java, Scala, Python, R, and SQL.
- Originally developed in AMPLab (UC Berkeley) from 2009,
 - ↳ donated to the Apache Software Foundation in 2013,
 - ↳ top-level project as of 2014.
- **Latest release:** 2.2.1 (Dec. 2017)

RDD



- Resilient Distributed Dataset (RDD)
 - ↪ Partitioned collections (lists, maps..) across nodes
 - ↪ Set of well-defined operations (incl map, reduce) defined on these RDDs.

RDD



- Fault tolerance works three ways:
 - ↪ Storing, reconstructing lineage
 - ↪ Replication (optional)
 - ↪ Persistence to disk (optional)



RDD Lineage

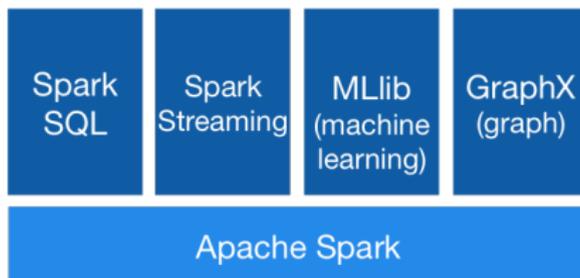
- Map Reduce implemented FT by outputting everything to disk always.
 - ↪ Effective but extremely costly.
 - ↪ **How to maintain fault tolerance without sacrificing in-memory performance?**
 - ✓ for truly large-scale analyses

RDD Lineage

- Map Reduce implemented FT by outputting everything to disk always.
 - ↪ Effective but extremely costly.
 - ↪ **How to maintain fault tolerance without sacrificing in-memory performance?**
 - ✓ for truly large-scale analyses
- **Solution:**
 - ↪ Record lineage of an RDD (think version control)
 - ↪ If container, node goes down, reconstruct RDD from scratch
 - ✓ Either from beginning,
 - ✓ or from (occasional) checkpoints which user has some control over.
 - ↪ User can suggest caching current state of RDD in memory,
 - ✓ or persisting it to disk, or both.
 - ↪ You can also save RDD to disk, or replicate partitions across nodes for other forms of fault tolerance.

Main Building Blocks

- The **Spark Core API** provides the general execution layer on top of which all other functionality is built upon.
- Four higher-level components (in the _Spark ecosystem):
 1. **Spark SQL** (formerly **Shark**),
 2. **Streaming**, to build scalable fault-tolerant streaming applications.
 3. **MLlib** for machine learning
 4. GraphX, the API for graphs and graph-parallel computation



Hands-on 5: Spark installation

Your Turn!

Hands-on 5

<http://nesusws-tutorials-BD-DL.rtfid.io/en/latest/hands-on/spark/install/>

- Use **EasyBuild** to search for a Recipy for **Apache Spark**
- Install it and check the installed software

Hands-on 6: Spark Usage

Your Turn!

Hands-on 6

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/spark/usage/>

- Check a single interactive run Step 1
 - ↪ PySpark, the Spark Python API Step 1.a.
 - ↪ Scala Spark Shell Step 1.b.
 - ↪ R Spark Shell **will not be reviewed** here.
- Running Spark standalone cluster Step 2
 - ↪ In particular, illustrated on Pi estimation.



Summary

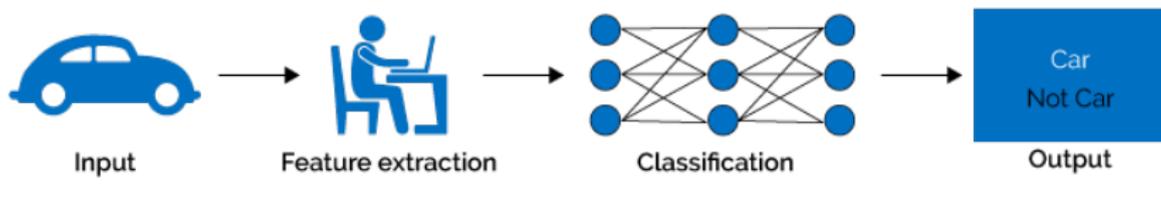
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Big data and Machine/Deep Learning

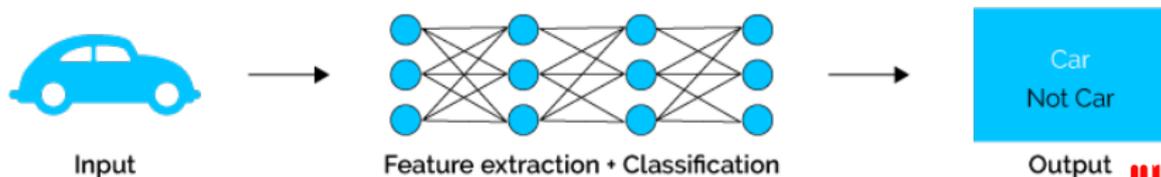
- **Out-of-scope of this tutorial:**

↪ Machine Learning (ML) / Deep Learning theoretical basis

Machine Learning



Deep Learning



Machine Learning Cheat sheet

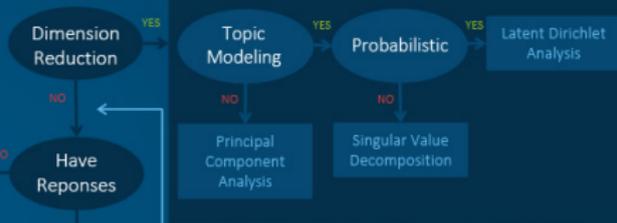
Machine Learning Algorithms Cheat Sheet

Unsupervised Learning: Clustering



Unsupervised Learning: Dimension Reduction

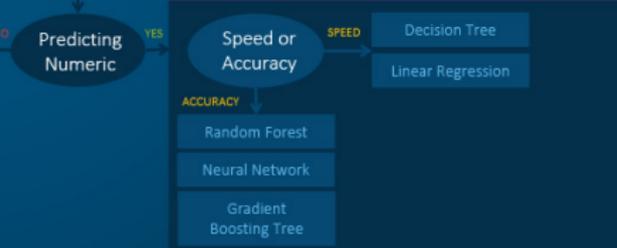
START



Supervised Learning: Classification



Supervised Learning: Regression



Machine/Deep-Learning Frameworks

- Pytorch

- ↪ Python version of Torch open-sourced by Facebook in 2017.
- ↪ Torch is a computational framework with an API written in Lua that supports machine-learning algorithms.
- ↪ PyTorch offers dynamic computation graphs, which let you process variable-length inputs and outputs.

- TensorFlow

- ↪ open source software library from Google for numerical computation using data flow graphs,
- ↪ thus close to the [Deep Learning book](#) way of thinking about neural networks.

- Keras,

- ↪ high-level neural networks API,
- ↪ written in Python and capable of running on top of TensorFlow.

- Caffe

- ↪ a well-known and widely used machine-vision library that ported

Matlabs implementation of fast convolutional nets to C and C++

- ↪ You also have to consider its successor, Caffe 2,

Machine/Deep-Learning Frameworks

- Offer various **Package Design Choices**
 - ↪ **Model specification:**
 - ✓ Configuration file (Caffe, DistBelief, CNTK) vs. programmatic generation (Torch, Theano, Tensorflow)
 - ↪ For programmatic models, choice of high-level language:
 - ✓ Lua (Torch)
 - ✓ vs. Python (Theano, Tensorflow)
 - ✓ vs others (Go etc.)

In this talk

- We chose to work with python because of rich community and library infrastructure.



TensorFlow vs. Theano

- Theano is another deep-learning library with pythonwrapper
 - ↳ was inspiration for Tensorflow
- Theano and TensorFlow are very similar systems.
 - ↳ TensorFlow has better support for distributed systems though,
 - ↳ development funded by Google, while Theano is an academic project.



What is TensorFlow ?

- TensorFlow is a deep learning library recently open-sourced by Google.
 - ↪ library for numerical computation using **data flow graphs**.
 - ✓ **Nodes** represent mathematical operations,
 - ✓ **edges** represent the multidimensional data arrays (**tensors**) communicated between them.
- Flexible architecture allowing to deploy computation anywhere:
 - ↪ to one or more CPUs or GPUs in a desktop, server,
 - ↪ or mobile device with a single API.
- TensorFlow was originally developed within the Google Brain Team

Hands-on 7: Installing Tensorflow

- **Without further development**

- ↪ you are ready to play with tensorflow
- ↪ provided tutorial is self-explicit and make use of Jupyter Notebook

Hands-on 7

<http://nesusws-tutorials-BD-DL.rtfid.io/en/latest/hands-on/tensorflow/install/>

- Preparation of a Python sand-boxed environment Step 1
 - ↪ using `pyenv` and `virtualenv`
- Tensorflow installation using `pip` Step 2
- Installation of jupyter **Jupyter Notebook** Step 3

Hands-on 8: Playing with Tensorflow

Your Turn!

Hands-on 8

<http://nesusws-tutorials-BD-DL.rtf.d.io/en/latest/hands-on/tensorflow/mnist/>

- Run a very simple **MNIST** classifier **Step 1**
 - ↪ MNIST: computer vision dataset (images of handwritten digits)
- Run a deep MNIST classifier using convolutional layers **Step 2**
 - ↪ compare results with **best models**

Questions?

<http://hpc.uni.lu>

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mail: sebastien.varrette@uni.lu



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