

CS3DP: Introduction to Distributed and Parallel Computing



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Learning Outcomes



After the session, a participant should be able to:

- Recite system characteristics for distributed/parallel/computational science
- Describe use-cases and challenges in the domain of D/P/S computing
- Sketch generic D/P system architectures
- Describe how the scientific method relies on D/P/S computing
- Name big data challenges and the typical workflow

Outline



- 1 Distributed Computing
- 2 Parallel Computing
- 3 Computational Science
- 4 BigData Challenges
- 5 Organization of the Module
- 6 Summary

Distributed Computing

Field in computer science that studies **distributed systems**¹

Definition

- System which components² are located on different networked computers
- Components communicate and coordinate actions by passing messages
- Components interact to achieve a common goal
- *In the wider sense*: autonomous processes coordinated by passing messages

Characteristics

- Distributed memory: components have their own (private) memory
- Concurrency of components: different components compute at the same time
- Lack of a global clock: clocks may diverge
- Independent failure of components, e.g., due to power outage

¹https://en.wikipedia.org/wiki/Distributed_computing

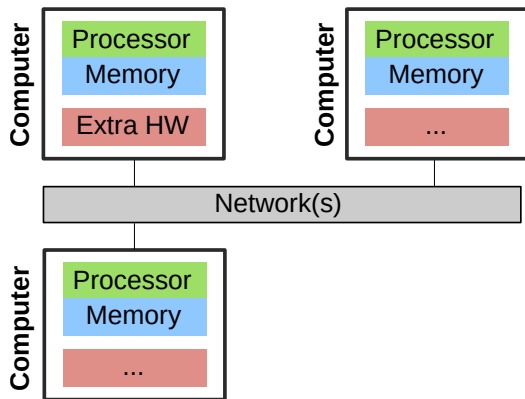
²In this context, means a component from a software architecture.

Example Distributed System and Distributed Program

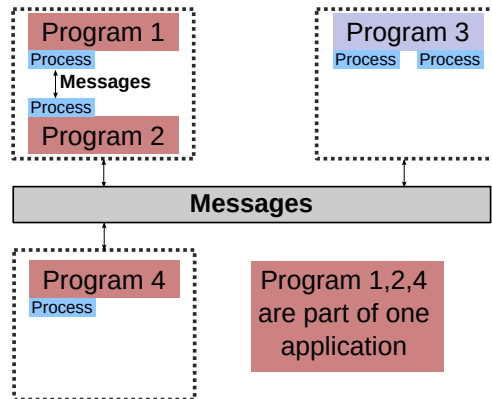


- A **distributed program** (DP) runs on a distributed system
 - Processes are instances of one program running on one computer
- A **distributed applications/algorithm** may involve various DPs/different vendors

Hardware perspective



Software perspective (mapped to hw)



Example Distributed Applications and Algorithms

Applications

- The Internet and telecommunication networks
- Cloud computing
- Wireless sensor networks
- The Internet of Things (IoT) – “everything is connected to the Internet”

Algorithms (selection from real world examples)

- Consensus: reliable agreement on a decision (malicious participants?)
- Leader election
- Reliable broadcast (of a message)
- Replication

Cloud Computing

Definition

- On-demand availability of computer system resources (data storage and computing)
 - ▶ Without direct active management by the user
- Typically relates to distributed resources
 - ▶ provided by data centers
 - ▶ to many users
 - ▶ over the Internet
- Fog/Edge Computing: brings cloud closer to user

Examples

- Applications: Dropbox, Google Mail, Office 365
- Infrastructure: Amazon, Google, Microsoft, Oracle

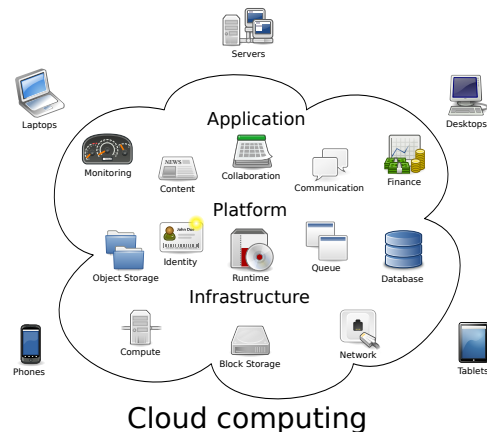


Image source: Frank, B. Wilson - CloudNINE, https://en.wikipedia.org/wiki/Cloud_computing

Some Facts: Cloud Computing and Data Centers



- Server workload (VMs or hardware): 350 Million, about 10 instances per server
- Data Center storage capacity: 1,750 Exabyte (10^{18}), 720 Exabyte actually stored
 - ▶ 180 Exabyte from Big Data
- Global data center IP traffic: 14 Zettabyte (10^{21}), 440 Terabyte/s
 - ▶ 15% volume communicated to the user: 20 KB/s per human
- Power consumption: US data centers alone 40% UK or 3% of global energy³
 - ▶ 416 Terawatt = energy bill: 50 Billion £ (12 cents/kWh)
 - ▶ Estimate for 2025: 20% worldwide for all DCs?

³For 2017: <https://www.forbes.com/sites/forbestechcouncil/2017/12/15/why-energy-is-a-big-and-rapidly-growing-problem-for-data-centers/>

Estimate for 2019: <https://www.cisco.com/c/en/us/solutions/collateral/service-provider/global-cloud-index-gci/white-paper-c11-738085.pdf>

Challenges

- Programming: concurrency introduces new types of programming mistakes
 - ▶ It is difficult to think about all cases of concurrency
 - ▶ Must coordinate between programs
 - ▶ No global view and debugging
- Resource sharing: system shares resources between all users
- Scalability: system must be able to grow with the requirements
 - ▶ numbers of users/data volume/compute demand
 - ▶ retain performance level (response time)
 - ▶ requires to add hardware, though
- Fault handling: detect, mask, and recover from failures
 - ▶ Failures are inevitable and the normal mode of operation
- Heterogeneity: system consists of different hardware/software
- Transparency: Users do not care about how/where code/data is
- Security: Availability of services, confidentiality of data

Outline



1 Distributed Computing

2 Parallel Computing

- Overview
- Architectures
- High-Performance Computing
- Challenges

3 Computational Science

4 BigData Challenges

5 Organization of the Module

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Definition: Parallel Computing



Many calculations **or** the execution of processes are carried out simultaneously⁴

Characteristics

- Goal is to improve performance for an application
 - ▶ Either allowing to solve problems within a deadline or increased accuracy
- Application/System must coordinate the otherwise independent parallel processing
 - ▶ There are various programming models for parallel applications
- Different architectures to speed up computation: **may use** distributed systems

Levels of parallelism (from hardware perspective)

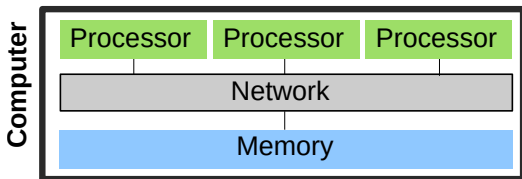
- Bit-level: process multiple bits concurrently (e.g., in an ALU)
- Instruction-level: process multiple instructions concurrently on a CPU
- Data: run the same computation on **different data**
- Task: run **different** computations concurrently

⁴https://en.wikipedia.org/wiki/Parallel_computing

Parallel Architectures

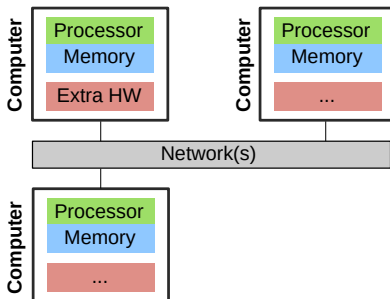
In practice, systems are a mix of two paradigms:

Shared memory



- Processors can access a joint memory
 - ▶ Enables communication/coordination
- Cannot be scaled up to any size
- Very expensive to build one big system

Distributed memory systems (again!)



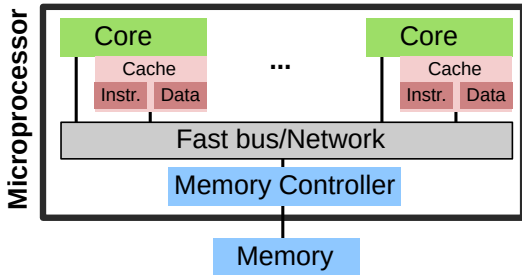
- Processor can only see own memory
- Performance of the network is key

Parallel Programs

- A **parallel program** runs on parallel hardware

In the strict sense: A parallel application coordinates concurrent processing

Schema of a multicore processor



Processor provides all levels of parallelism

- Multiple ALU/other units
- Pipelining of processing stages
- SIMD: Single Instruction - Multiple Data
 - ▶ Same operation on multiple data
 - ▶ Instruction set: SSE, AVX
- Multiple cores
 - ▶ Each with own instruction pointer

<https://en.wikipedia.org/wiki/Microarchitecture>

High-Performance Computing



Definitions

- HPC: Field providing massive compute resources for a computational task
 - ▶ Task needs too much memory or time for a normal computer
 - ⇒ Enabler of complex challenging simulations, e.g., weather, astronomy
- Supercomputer: aggregates power of many compute devices
 - ▶ Nowadays: 100-1,000s of servers that are clustered together

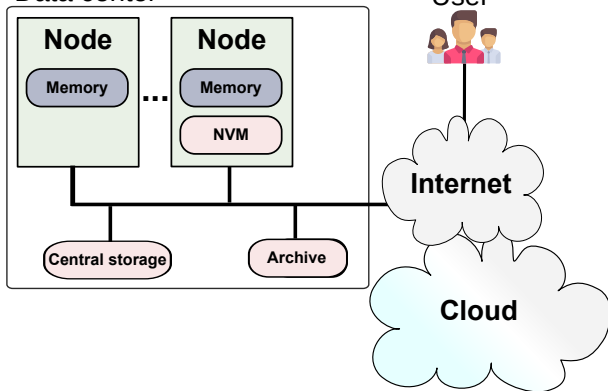
Example: Summit (Oak Ridge National Laboratories)

- Compute: 4,608 nodes; 2.4 Million cores
 - ▶ Peak 200 Petaflop/s (10^{15})
 - ▶ 2x IBM POWER9 22C 3.07GHz; 6x NVIDIA Volta V100 GPU
- 10 Petabyte memory (DRAM + HBM + GPU)
- Network: 100G Infiniband; 12.5 GB/s per node; 115 TB/s bisection bandwidth
- Storage: 32 PB capacity; 1 TB/s throughput

The **Top500** is a list of the most performant supercomputers

Supercomputers & Data Centers

Data center



Credits: STFC

JASMIN Cluster at RAL / STFC
Used for data analysis of the Centre for
Environmental Data Analysis (CEDA)

Challenges

- Programming: imports errors from distributed computed
 - ▶ Low-level APIs and code-optimization to achieve performance
 - ▶ Performance-optimized code is difficult to maintain
 - ▶ Expensive and challenging to debug 1'000 concurrently running processes
 - ▶ Utilizing all compute resources efficiently (load balancing)
 - ▶ Grand challenges are difficult to test, as nobody knows the true answer
- Scalability: stricter than distributed systems
 - ▶ Strong-scaling: same problem, more parallelism shall improve performance
 - ▶ Weak-scaling: data scales with processors, retain time-to-solution
- Environment: bleeding edge and varying hardware/software systems
 - ▶ Obscure special-purpose hardware (FPGA/ASIC Application-Specific Integrated Circuit)
 - ▶ Limited knowledge to administrate, use, and to compare performance

Outline



1 Distributed Computing

2 Parallel Computing

3 Computational Science

- Overview
- Scientific Method
- Relevance

4 BigData Challenges

5 Organization of the Module

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Computational Science



Definitions

- Multidisciplinary field using advanced computing capabilities to understand and solve complex problems
 - ▶ Typically using mathematical models and computer simulation
 - ▶ Problems are motivated by industrial or societal challenges
- May utilize single computer, distributed systems, or supercomputers

Examples utilizing distributed computing

- Finding the higgs boson (CERN)
- Bioinformatics applications, e.g., gene sequencing

Examples utilizing high-performance computing

- Computing the weather forecast for tomorrow / next week
- Simulating a tokamak fusion reactor

https://en.wikipedia.org/wiki/Computational_science

Scientific Method

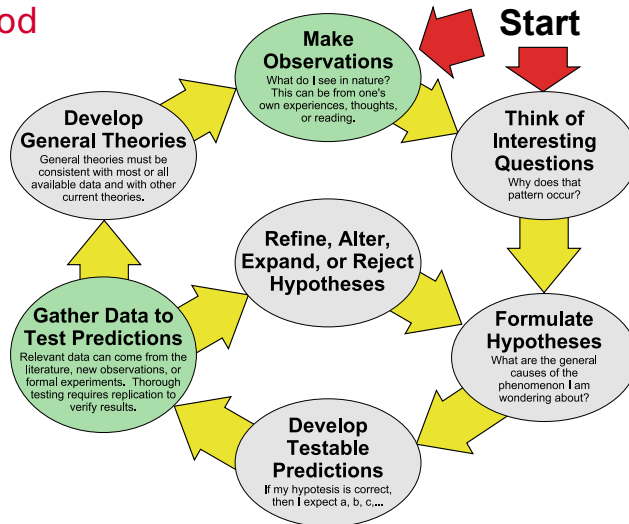
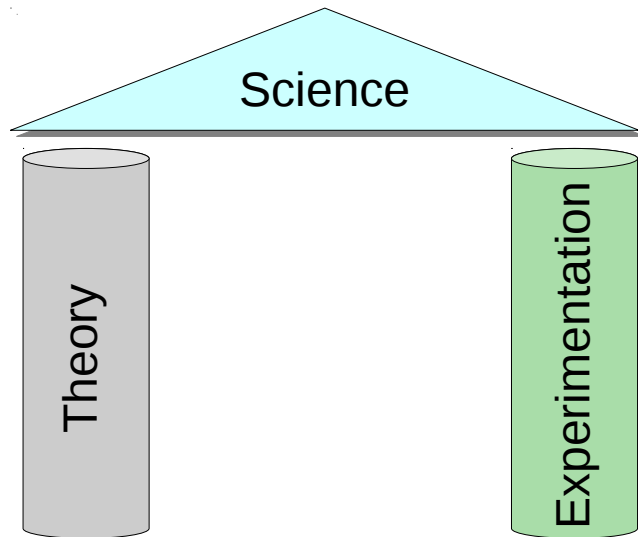
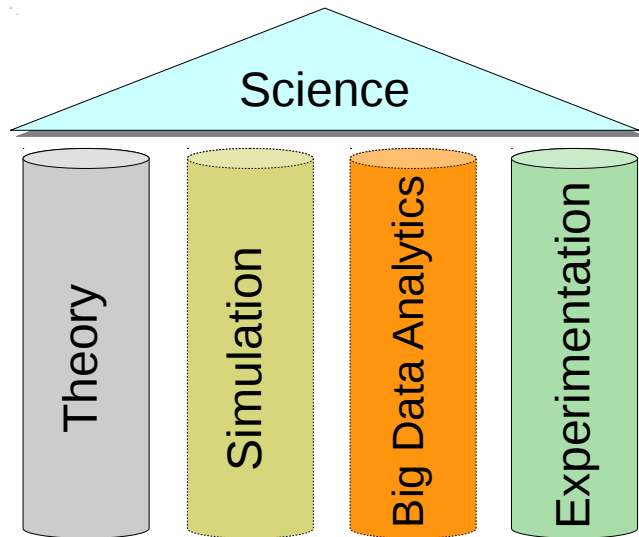


Figure: Based on “The Scientific Method as an Ongoing Process”, ArchonMagnus
https://en.wikipedia.org/wiki/Scientific_method

Pillars of the Scientific Method



Pillars of Science: **Modern Perspective**



Relation of the Scientific Method to D/P/S Computing



Simulation models real systems to gain new insight

- Instrument to make observations, e.g., high-resolution and fast timescale
- Typically used to validate/refine theories, identify new phenomenon
- Classical computational science: hard facts (based on models)
- The frontier of science needs massive computing resources on supercomputers
- Data-intensive sciences like climate imposes challenges to data handling, too

Big Data Analytics extracts insight from data

- Provides a data pool to identify/mine new insight and to validate theories
- In business often approximate insight is enough (a small advantage)
- Distributed and parallel systems are needed to manage and analyze the data
- Gained knowledge is often made available as part of the cloud (for money)...

Big Data Analytics



Definition

- Extracting insight from data to support decisions
 - ▶ Vast amounts of data are available
 - ▶ Many different/heterogene data sources that can be correlated
 - ▶ Raw data is of low value (fine grained)

Analytics

- Analyzing data \Rightarrow Insight == value
 - ▶ For academia: knowledge
 - ▶ For industry: business advantage and money
- Levels of insight – primary abstraction levels of analytics
 - ▶ **Exploration**: study data and identify properties of (subsets) of data
 - ▶ **Induction/Inference**: infer properties of the full population
- Big data tools allow to construct a theory/model and validate it with data
 - ▶ **Statistics** and **machine learning** provide **algorithms and models**
 - ▶ Visual methods support data exploration and analysis

Relevance of Big Data and Parallel Computing



- Big Data Analytics is emerging, relevance increases compared to supercomputing
- Nowadays all processors provide parallelism, thus, experts are needed

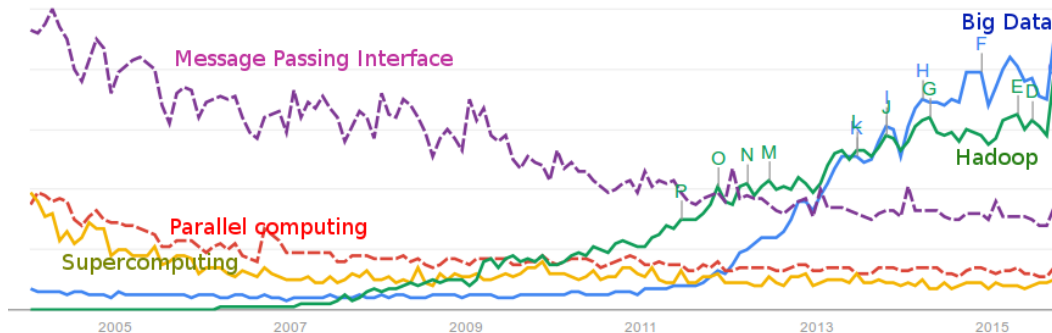


Figure: Google Search Trends, relative searches

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1 Distributed Computing

2 Parallel Computing

3 Computational Science

4 **BigData Challenges**

- Overview
- Volume
- Velocity
- Variety
- Veracity
- Value
- Value Chain
- Data Lake

BigData Challenges & Characteristics

Dealing with large data is challenging in Big Data Analytics but also in Computational Science

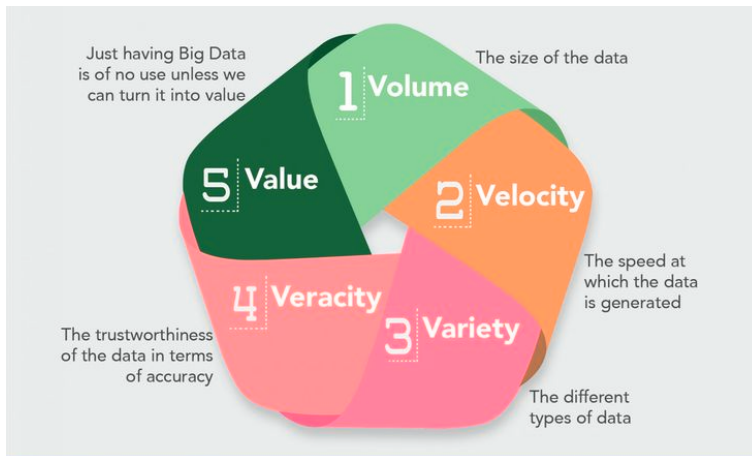


Figure: Source: MarianVesper (Forrester Big Data Webinar. Holger Kisker, Martha Bennet. Big Data: Gold Rush Or Illusion?)

Volume: The size of the Data

What is Big Data

Terrabytes to 10s of petabytes

What is not Big Data

A few gigabytes

Examples

- Wikipedia corpus with history ca. 10 TByte
- Wikimedia commons ca. 23 TByte
- Google search index ca. 46 Gigawebpages⁵
- YouTube per year 76 PByte (2012⁶)

⁵<http://www.worldwidewebsize.com/>

⁶<https://sumanrs.wordpress.com/2012/04/14/youtube-yearly-costs-for-storagenetworking-estimate/>

Velocity: Data Volume per Time



What is Big Data

30 KiB to 30 GiB per second
(902 GiB/year to 902 PiB/year)

What is not Big Data

A never changing data set

Examples

- LHC (Cern) with all experiments about 25 GB/s ⁷
- Square Kilometre Array 700 TB/s (in 2018) ⁸
- 50k Google searches per s ⁹
- Facebook 30 Billion content pieces shared per month ¹⁰

⁷<http://home.web.cern.ch/about/computing/processing-what-record>

⁸<http://venturebeat.com/2014/10/05/how-big-data-is-fueling-a-new-age-in-space-exploration/>

⁹<http://www.internetlivestats.com/google-search-statistics/>

¹⁰<https://blog.kissmetrics.com/facebook-statistics/>

Data Sources



Enterprise data

- Serves business objectives, well defined
- Customer information
- Transactions, e.g., purchases

Experimental/Observational data (EOD)

- Created by machines from sensors/devices
- Trading systems, satellites
- Microscopes, video streams, smart meters

Social media

- Created by humans
- Messages, posts, blogs, Wikis

Variety: Types of Data

■ Structured data

- ▶ Like tables with fixed attributes
- ▶ Traditionally handled by relational databases

■ Unstructured data

- ▶ Usually generated by humans
- ▶ Examples: natural language, voice, Wikipedia, Twitter posts
- ▶ Must be processed into (semi-structured) data to gain value

■ Semi-structured data

- ▶ Has some structure in tags but it changes with documents
- ▶ Examples: HTML, XML, JSON files, server logs

What is Big Data

- Use data from multiple sources and in multiple forms
- Involve unstructured and semi-structured data

Veracity: Trustworthiness of Data



What is Big Data

- Data involves some uncertainty and ambiguities
- Mistakes can be introduced by humans and machines
- Examples
 - ▶ People sharing accounts
 - ▶ Like sth. today, dislike it tomorrow
 - ▶ Wrong system timestamps

Data Quality is vital!

Analytics and conclusions rely on good data quality

- Garbage data + perfect model => garbage results
- Perfect data + garbage model => garbage results

GIGO paradigm: *Garbage In – Garbage Out*

Value of Data

What is Big Data

- Raw data of Big Data is of low value
 - ▶ For example, single observations of the weather, a bill
- The output of a large scale climate simulation that cost 10k to run
 - ▶ It still needs to be analyzed to come to conclusions!

Analytics and theory about the data increases the value

- Analytics transform big data into smart (valuable) data!

Abstraction Levels of Analytics and the Value of Data

5. Prescriptive analytics

- ▶ “What should we do and why?”

4. Predictive analytics

- ▶ “What will happen?”

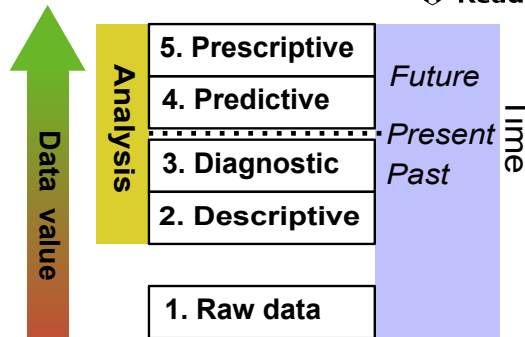
3. Diagnostic analytics

- ▶ “What went wrong?”
- ▶ “Why did this happen?”

2. Descriptive analytics¹¹

- ▶ “What happened?”

1. Raw (observed) data



Relation to Computational Science

- These analysis steps are still done just by running computational experiments
- Also the output of the simulation must be analyzed

¹¹Decriptive and diagnostic analysis are like forensics

Analytics Abstraction Level

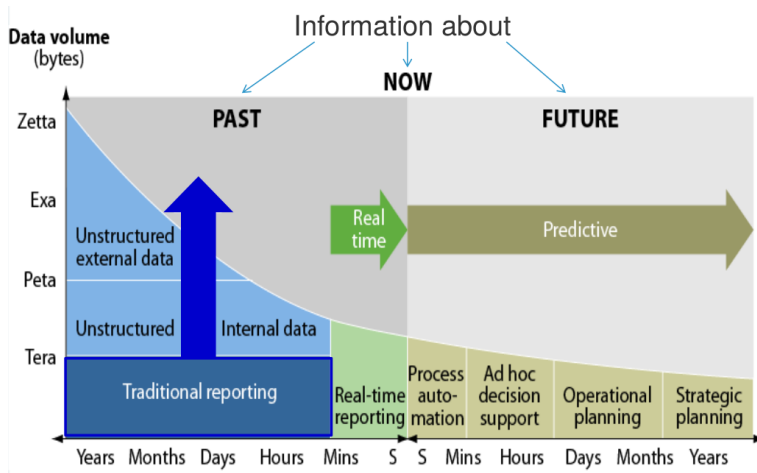


Figure: Source: Forrester report. Understanding The Business Intelligence Growth Opportunity. 20-08-2011

Data Analysis Workflow

The traditional approach proceeds in phases:

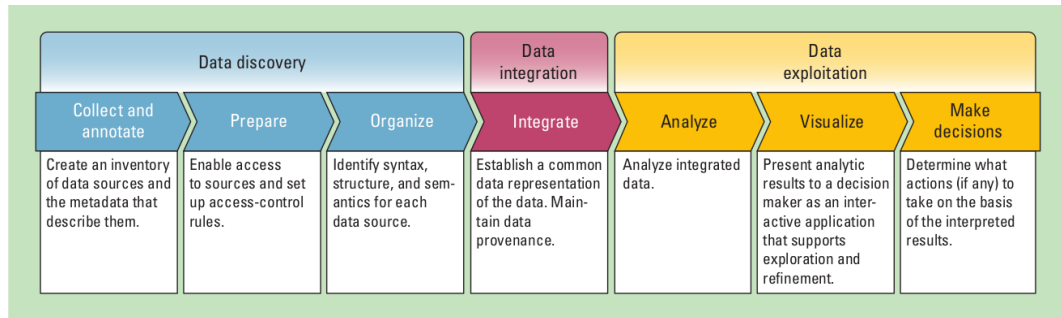


Figure: Source: Gilbert Miller, Peter Mork From Data to Decisions: A Value Chain for Big Data.

- Analysis tools: machine learning, statistics, interactive visualization
- Limitation: Interactivity by browsing through prepared results
- Indirect feedback between visualization and analysis

From Big Data to the Data Lake

- With cheap storage costs, people promote the concept of the data lake
- Combines data from many sources and of any type
- Allows for conducting future analysis and not miss any opportunity

Attributes of the data lake

- Collect everything: all time all data: raw sources and processed data
 - ▶ Decide during analysis which data is important, e.g., no “schema” until read
- Dive in anywhere: enable users across multiple business units to
 - ▶ Refine, explore and enrich data on their terms
- Flexible access: shared infrastructure supports various patterns
 - ▶ Batch, interactive, online, search

<http://hortonworks.com/blog/enterprise-hadoop-journey-data-lake/>

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Organization of the Module: Components



- Lecture (1h / week)
 - ▶ Delivers concepts and gives an overview
 - ▶ 4 lectures about distributed computing
 - ▶ 4 lectures about parallel computing
 - ▶ 1 invited talk (and this overview presentation)
- Practical (1h / week) – follows the schedule after the tutorial
 - ▶ Part 1: Students present their solution/questions to exercise tasks
 - ▶ Part 2: We discuss the new exercise such that everyone understands the questions
- Exercise (prescribed 3h / week)
 - ▶ Self-study to practice lecture content (feel free to team up!)
 - ▶ Each task comes with an estimated time for you to spend on it
 - ▶ Contains introductory and harder tasks
 - ▶ Store your work in a Git Repository – the portfolio of the course
- Group work: Some time of practical/tutorial may be used for group work

Role of Exercises and Group Work

Assessment

- Module: Assessment is 100% exam, however,
- Exercises and group work is formative assessment that prepares for the exam
- Feedback of the lecturer during practicals/tutorials
- Some quizzes are provided during lecture and for your self-study

Group work

- Discuss/Critique exercises of peers (groups of 2-4)
- Brainstorm/Design/Solve small tasks (groups of 2-4)
- The outcome should be stored in the Git portfolio

Proposed Learning Strategy/How to Achieve Good Marks



University of
Reading

- Understand learning outcomes (provided in each slide deck)
- Participate in exercises
 - ▶ To understand the topic, types of questions, and how to solve issues
 - ▶ To get feedback from the lecturer (e.g., if you present) and from peers
- Schedule time for the exercises, best to team up in learning groups
 - ▶ Try to do the 3h/week!
 - ▶ Always do the easy tasks, if you are busy you may miss some harder tasks
 - ▶ Partial solutions are better than no attempt
- Do the quizzes
- Do further reading of topics you are interested in
- Team up again to prepare for the exam
- Ask questions to colleagues and to us
- We will support your learning journey but **YOU** are responsible for it

Communication

- Blackboard provides
 - ▶ Slides for lectures/practical, exercise sheets
 - ▶ Most important announcements
 - ▶ Reading lists for topics
- Teams channel for communication/tutorial
 - ▶ We use it for any announcement
 - ▶ Please use it for any purpose around the topic!
 - ▶ To solve exercises, to share an interesting link, to ask a question
 - ▶ To find peers to work with

Summary



- Simulation and Big data analytics is a pillar of science
 - ▶ Supports building of hypothesis and experimentation
- Challenges: 5 Vs – Volume, velocity, variety, veracity, value

Characteristics and Differences of DC/PC

	Distributed computing	Parallel computing
Motivation	Decentrality/low costs	Performance/feasability
Enables	business/cloud/big data analytics	interactivity/computational science
Communication	message passing	may use shared resources
Fault-tolerance	tolerate errors	needs reliable hardware
Application	Weakly-coupled Multiple programs/vendors	Tightly-coupled Single application/vendor