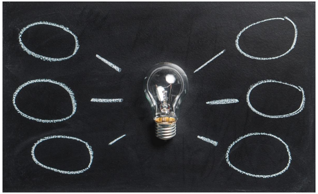
Julian Kunkel

High-Performance Data Analytics (HPDA)



Learning Outcomes

After the session, a participant should be able to:

- Name typical applications for high-performance data analytics
- Distinguish HPDA from D/P/S computing and how these topics blend
- Describe use-cases and challenges in the domain of D/P/S computing
- Describe how the scientific method relies on D/P/S computing
- Name big data challenges and the typical workflow
- Recite system characteristics for distributed/parallel/computational science
- Sketch generic D/P system architectures

Outline

High-Performance Data Analytics (HPDA)

Definition

*High-performance data analytics is the **process** of **quickly examining extremely large data sets** to find insights. This is done by using the **parallel processing** of high-performance computing to run powerful analytic software.*

Source: https://www.omnisci.com/technical-glossary/high-performance-data-analytics

Components to understand

- Understanding analysis processes
- Managing large scale data sets
- Applying parallel processing
- Characterizing performance factors of high-performance compute and storage

Distributed Computing

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

Definition

- Systems whose components[2] 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

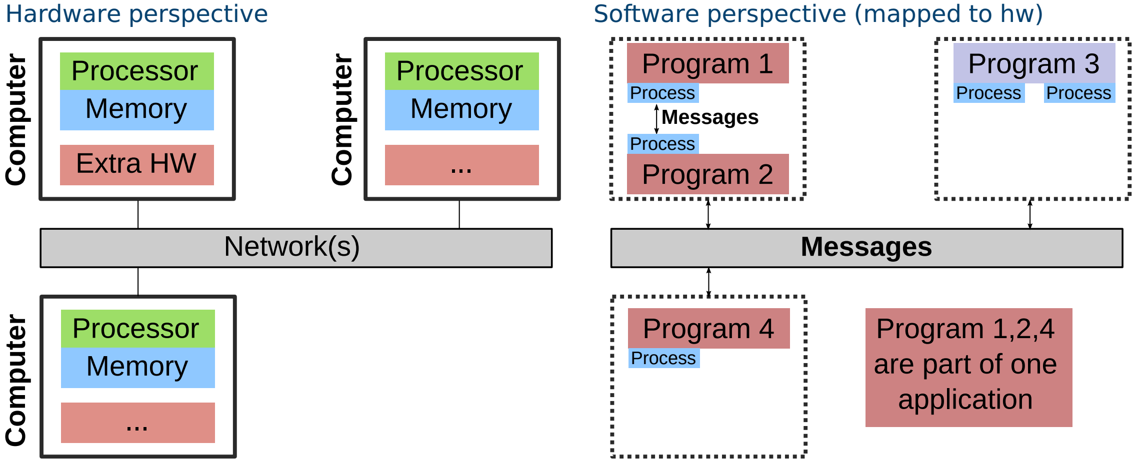
- Distributed memory: components have their own (private) memory
- Concurrency of components: different components compute at the same time
- Lack of a global clock: clocks may diverge
- Independent failure of components, e.g., due to power outage

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

2 In this context, means a component from 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



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”

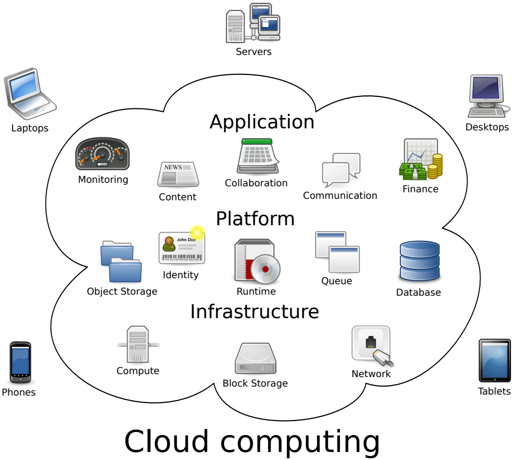
Algorithms (selection from real world examples)

- 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 energy[3]
  - 416 Terawatt = energy bill: 50 Billion £ (12 cents/kWh)
  - Estimate for 2025: 20% worldwide for all DCs?

[3] For 2017: https://www.forbes.com/sites/forbestechcouncil/2017/12/15/why-energy-is-a-big-and-rapidly-
Estimate for 2019: https://www.cisco.com/c/en/us/solutions/collateral/service-provider/global-cloud-index-gci/white-paper-c11-738085.pdf

Challenges using Distributed Systems

- 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
- 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

Definition: Parallel Computing

Many calculations **or** the execution of processes are carried out simultaneously[4]

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)

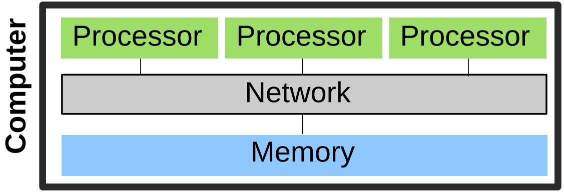
- Bit-level: process multiple bits concurrently (e.g., in an ALU)
- Instruction-level: process multiple instructions concurrently on a CPU
- Data: run the same computation on **different data**
- Task: run **different** computations concurrently

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

Parallel Architectures

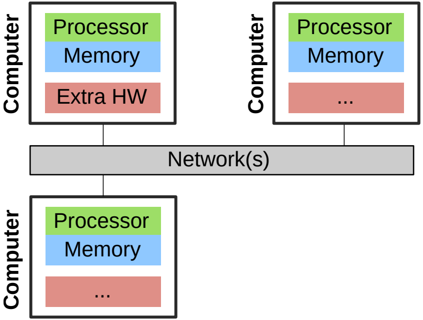
In practice, systems are a mix of two paradigms:

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!)

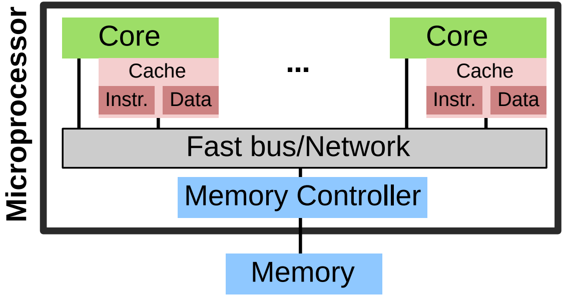


- Processor can only see own memory
- Performance of the network is key

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

Also see `https://en.wikipedia.org/wiki/Microarchitecture`

High-Performance Computing

Definitions

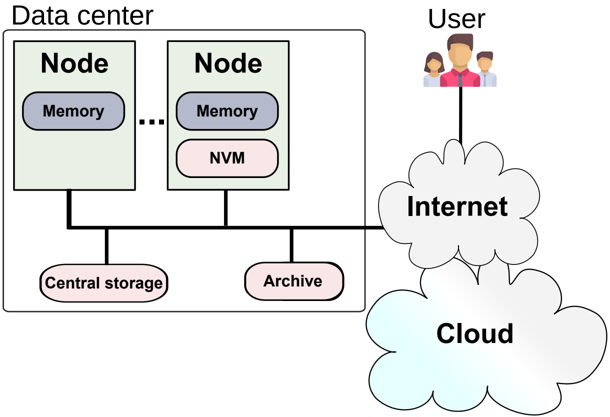
- HPC: Field providing massive compute resources for a computational task
  - ▶ Task needs too much memory or time for a normal computer
  - ⇒ Enabler of complex challenging simulations, e.g., weather, astronomy
- Supercomputer: aggregates power of many compute devices
  - ▶ Nowadays: 100-1,000s of servers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

Example: Summit (Rank 4 (June 2022) 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 powerful supercomputers

Supercomputers & Data Centers



Credits: STFC

JASMIN Cluster at RAL / STFC

Used for data analysis of the Centre for Environmental Data Analysis (CEDA)

HPC in Göttingen

GWDG: unversity data center and providing innovative technology solutions

- HPC systems for local scientists, German wide and for DLR
- Integrates research for HPC systems and services

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

Computational Science

Definitions

- Multidiciplinary 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

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

Scientific Method

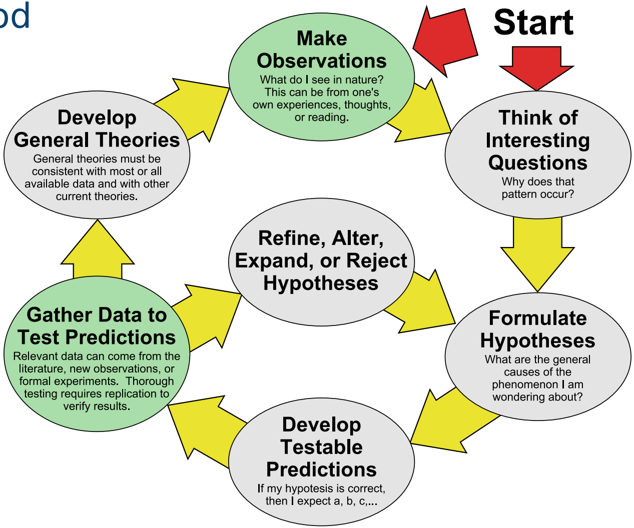
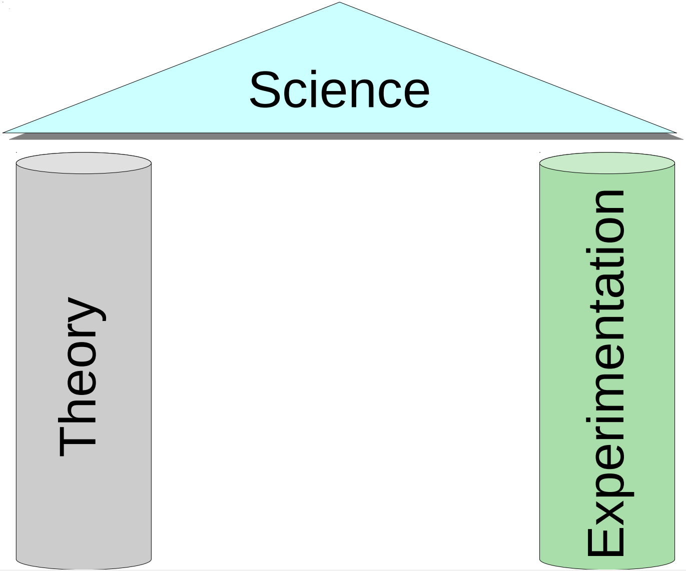
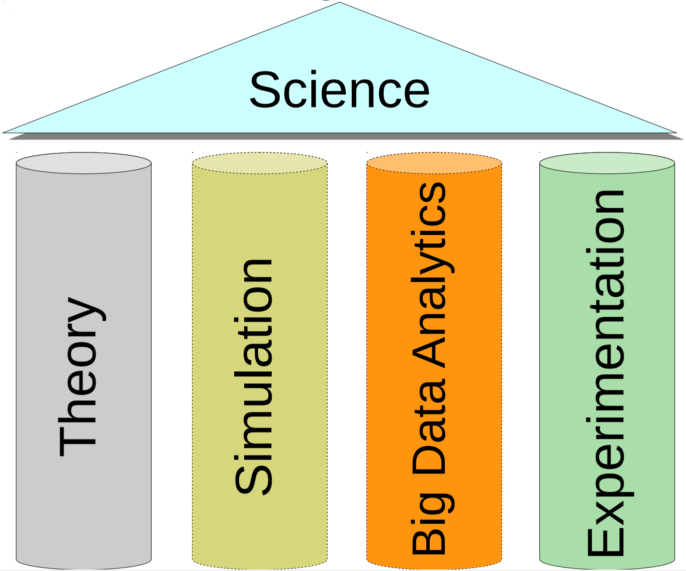


Figure: Based on "The Scientific Method as an Ongoing Process", ArchonMagnus `https://en.wikipedia.org/wiki/Scientific_method`

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 phenomena
- 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

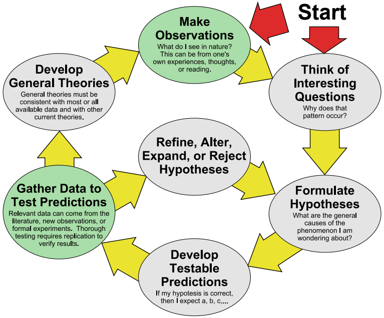
- Extracting insight from data to support decisions
  - Vast amounts of data are available
  - Many different/heterogeneous data sources that can be correlated
  - Raw data is of low value (fine grained)

Analytics

- Analyzing data ⇒ 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

Group Work

- What question(s) you'd like to solve using the scientific method?
- Define the question, hypotheses, how could this be tested? What data is needed?
- Time: 5 min
- Organization: breakout groups - please use your mic or chat



Example Predictive Models

Similarity is a (very) simplistic model and predictor for the world

- Humans use this approach in their cognitive process
- Uses the advantage of BigData

Weather prediction

- You may develop and rely on complex models of physics
- Or use a simple model for a particular day; e.g., expect it to be similar to the weather of the typical day over the last X years
  - Used by humans: rule of thumb for farmers

Preferences of Humans

- Identify a set of people which liked items you like
- Predict you like also the items those people like but haven't rated

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

Outline

BigData Challenges & Characteristics

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

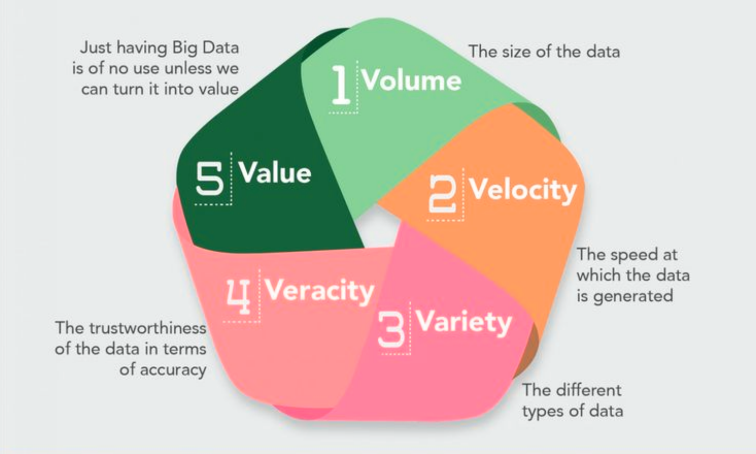


Figure: Source: MarianVesper (Forrester Big Data Webinar. Holger Kisker, Martha Bennet. Big Data: Gold Rush Or Illusion?)

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. 50 Gigawebpages[5]
- YouTube per year 76 PByte (2012[6])

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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 Kilometer Array 700 TB/s (in 2018) [8]
- 100k Google searches per second [9]
- Facebook 30 Billion content pieces shared per month [10]

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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

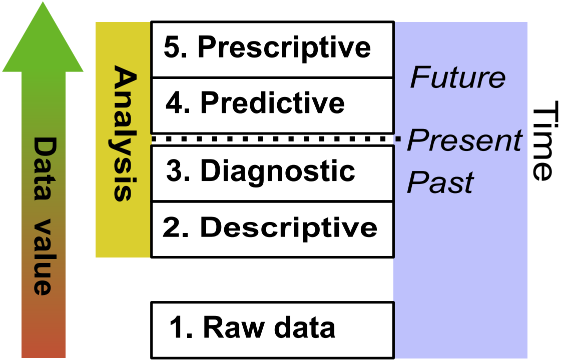
- Raw data of Big Data is of low value
  - For example, single observations of the weather, a bill
- The output of a large scale climate simulation that cost 10k to run
  - It still needs to be analyzed to come to conclusions!

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 analytics[11]
   - "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

11 Descriptive and diagnostic analysis are like forensics

Analytics Abstraction Level

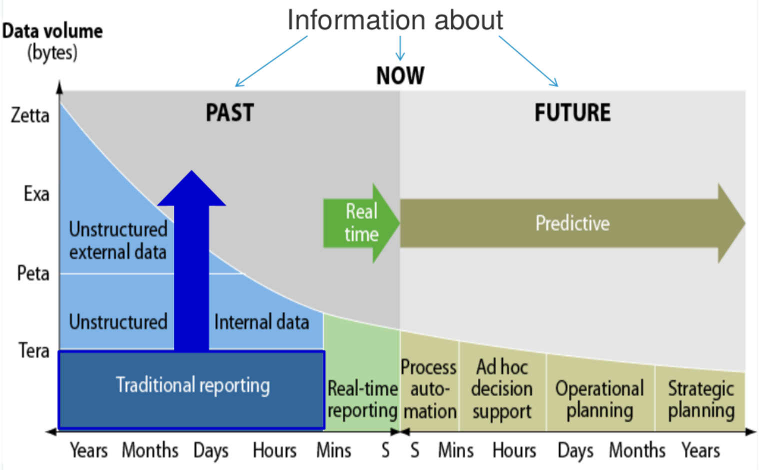
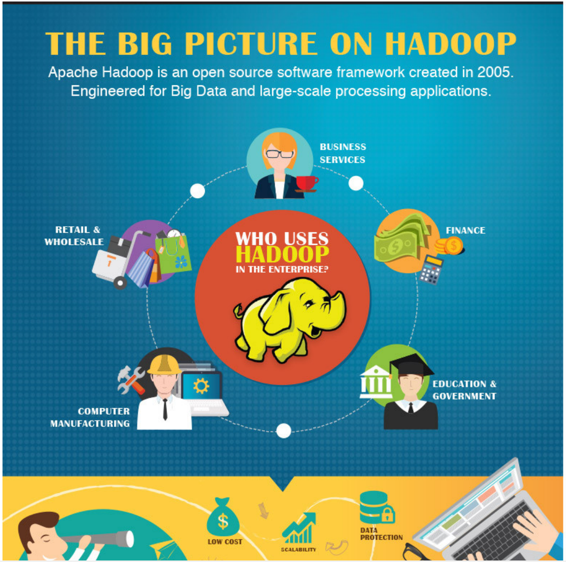
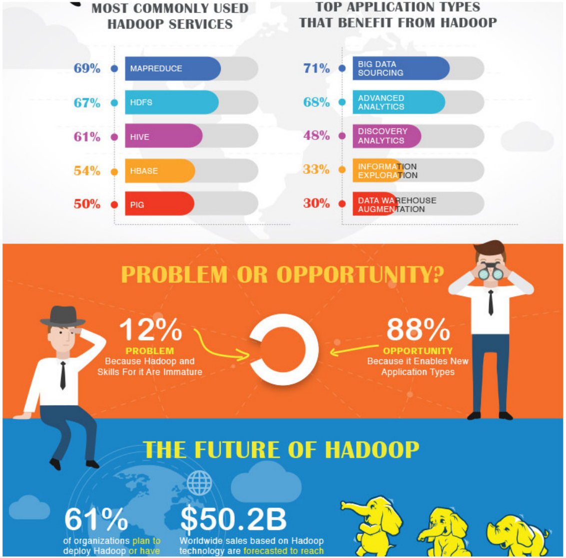


Figure: Source: Forrester report. Understanding The Business Intelligence Growth Opportunity. 20-08-2011

Outline

Advertisement for a Big Data Platform





Use Cases for BigData Analytics

Increase efficiency of processes and systems

- Advertisement: Optimize for target audience
- Product: Acceptance (like/dislike) of buyer, dynamic pricing
- Decrease financial risks: fraud detection, account takeover
- Insurance policies: Modeling of catastrophes
- Recommendation engine: Stimulate purchase/consume
- Systems: Fault prediction and anomaly detection
- Monetization: Extract money from gamers [27]

Science

- Epidemiology research: Google searches indicate Flu spread
- Personalized Healthcare: Recommend good treatment
- Physics: Finding the Higgs-boson, analyze telescope data
- Enabler for social sciences: Analyze people's mood
- Automatize classification

Example Use Case: Deutschland Card [2]

Goals

- Customer bonus card which tracks purchases
- Increase scalability and flexibility
- Previous solution based on OLAP

Big Data Characteristics

- Volume: O(10) TB
- Variety: mostly structured data, schemes are extended steadily
- Velocity: data growth rate O(100) GB / month

Results

- Much better scalability of the solution
- From dashboards to ad-hoc analysis within minutes

Example Use Case: DM [2]

Goals

- Predict required number of employees per day and store
- Prevent staff changes on short-notice

Big Data Characteristics

- Input data: Opening hours, incoming goods, empl. preferences, holidays, weather
- Model: NeuroBayes (Bayes + neuronal networks)
- Predictions: Sales, employee planning
- 450.000 predictions per week

Results

- Daily updated sales per store
- Reliable predictions for staff planning
- Customer and employee satisfaction

Example Use Case: OTTO [2]

Goals

Optimize inventory and prevent out-of-stock situations

Big Data Characteristics

- Input data: product characteristics, advertisement
- Volume/Velocity: 135 GB/week, 300 million records
- Model: NeuroBayes (Bayes + neuronal networks)
- 1 billion predictions per year

Results

- Better prognostics of product sales (up to 40%)
- Real time data analytics

Example Use Case: Smarter Cities (by KTH) [2]

Goals

- Improve traffic management in Stockholm
- Prediction of alternative routes

Big Data Characteristics

- Input data: Traffic videos/sensors, weather, GPS
- Volume/Velocity: 250k GPS-data/s + other data sources

Results

- 20% less traffic
- 50% reduction in travel time
- 20% less emissions

Example Facebook Studies

“Insight” from [11] by exploring posts

- Young narcissists tweet more likely.
  Middle-aged narcissists update their status
- US students post more problematic information than German students
- US Government checks tweets/facebook messages for several reasons
- Human communication graph has an average diameter of 4.74

Manipulation of news feeds [13]

- News feeds have been changed to analysis people’s behavior in subsequent posts
- Paper: “Experimental evidence of massive-scale emotional contagion through social networks”

Learning Behavior

Games

- DeepMind playing Atari games [29]
- AlphaGo wins vs. humans in playing Go [26]
- AI beating world's best gamer in Dota 2 [28]

Motion

- Learning hand motion by human training [30]
- Robots learning to pick up items [31]

Systems: Fault Prediction and Anomaly Detection

Smart buildings [24]

- Predicting faults of heating and ventilation of an hospital
- Predicted 76 of 124 real faults and 41 of 44 exceptional temperatures
- May consider weather to control systems automatically

Google DeepMind AI [25]

- Controlling 120 variables in the data center (fans, ...)
- Saves 15% energy of the overall bill

Automatize Classification

Analysis of multimedia

- Voice, face, biometric recognition
- Speech recognition
- Counting (animal) species on pictures / videos
- Finding patterns on satellite images (e.g., dam, thunderstorms)
- Anomalies in behavior (depressed people)
- Anomalies in structures (operational condition)

Outline

Learning Objectives of the Lecture

- Assign big data challenges to a given use-case
- Outline use-case examples for high-performance data analytics
- Estimate performance and runtime for a given workload and system
- Create a suitable hardware configuration to execute a given workload within a deadline
- Construct suitable data models for a given use-case and discuss their pro/cons
- Discuss the rationales behind the design decisions for the tools
- Describe the concept of visual analytics and its potential in scientific workflows
- Compare the features and architectures of NoSQL solutions to the abstract concept of a parallel file system
- Appraise the requirements for designing system architectures for systems storing and processing data
- Apply distributed algorithms and data structures to a given problem instance and illustrate their processing steps
  - in pseudocode
- Explain the importance of hardware characteristics when executing a given workload

Organization of the Module: Components

- Lecture (2h / week)
  - Delivers concepts and gives an overview
  - 1 invited talk (and this overview presentation)
- Practical for discussion of the exercise (2h / week)
  - Follows the schedule of the lecture, **optional**
  - 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 4h / 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
  - Recommend to store your work in a Git Repository – a portfolio of the course
- Group work: Some time of practical 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 for your exercises
- Some questions are provided during lecture/exercises and for your self-study

Group work

- Discuss/Criticize 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

- 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 4h/week!
  - Always do the easy tasks, if you are busy you may miss some harder tasks
  - Partial solutions are better than no attempt
- (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

- Webpage: https://hps.vi4io.org/teaching/autumn_term_2023/hpda
- Webpage provides
  - Slides for lectures/practical
  - Exercise sheets
  - Reading lists for topics
- StudIP for communication
  - We use it for announcements
  - 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

- HPDA: process of quickly examining large data sets
- 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/feasibility
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

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