

Introduction to Programming and Computing for Scientists

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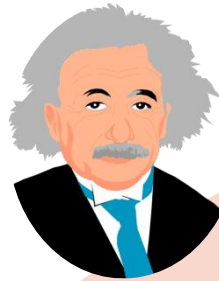
Lund University

Lecture 1

Evolution of science paradigms



- 1st paradigm:
Empirical science
- Descriptive



- 2nd paradigm:
Theoretical science
- Models



- 3rd paradigm:
Computational science
- Simulations



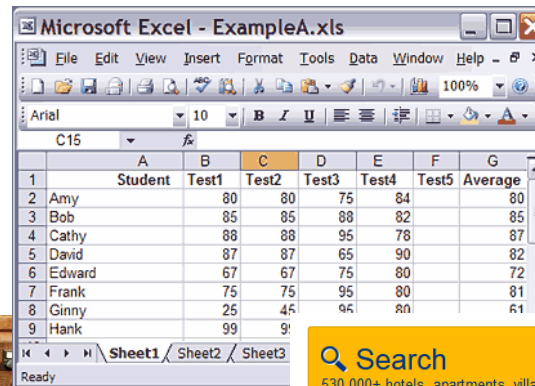
- 4th paradigm:
Data-intensive exploration
(e-Science)
- Unifies the rest
to explore
large data

after Jim Gray

It all starts with data

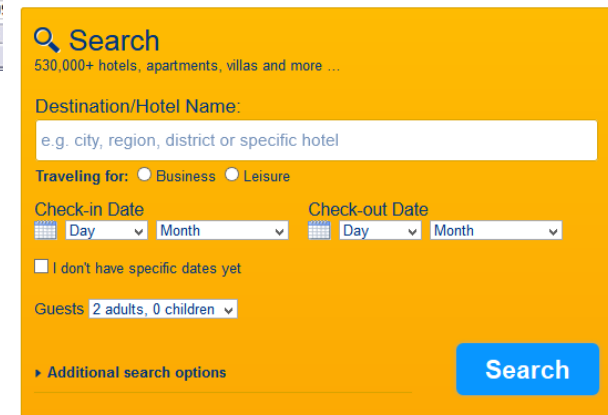
- The ultimate goal of science is to understand natural phenomenae
 - Understanding leads to anticipation, reproduction, prevention, utilization etc
- Information is key to understanding
 - **Data** is information organised in a structured manner
 - There are very many ways of structuring information

Date	Type of Machine	Number of Machine	Duration of Flight	Character of Flight
12	PBJ-1	35047	2.4	X
16	PBJ-1	35163	2.8	YX
16	PBJ-1	35164	2.8	YX
18	PBJ-1	35163	2.8	YX
19	PBJ-1	35047	3.1	YX
26	PBJ	35059	1.1	
28	PBJ	35053	1.0	



Microsoft Excel - ExampleA.xls

	A	B	C	D	E	F	G
1	Student	Test1	Test2	Test3	Test4	Test5	Average
2	Amy	80	80	75	84		80
3	Bob	85	85	88	82		85
4	Cathy	88	88	95	78		87
5	David	87	87	65	90		82
6	Edward	67	67	75	80		72
7	Frank	75	75	95	80		81
8	Ginny	25	45	95	80		61
9	Hank	99	99				



Search

530,000+ hotels, apartments, villas and more ...

Destination/Hotel Name:
e.g. city, region, district or specific hotel

Traveling for: Business Leisure

Check-in Date: Day Month Check-out Date: Day Month

I don't have specific dates yet

Guests: 2 adults, 0 children

Additional search options

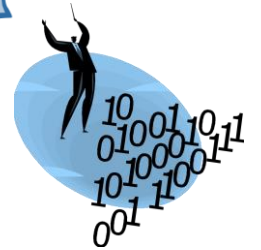
Search

All data today are digitized for computer processing

All scientific research needs **data**
(testing models, finding patterns)



All data and information are getting
digitized



Modern instruments can produce digital
data in **huge amounts**



Instruments and data are **accessible by**
all scientists on the planet



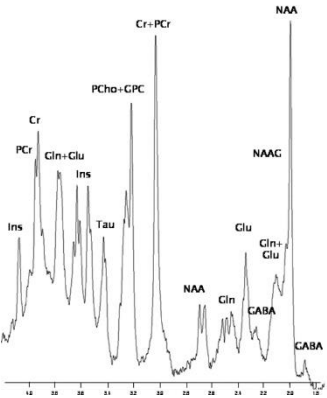
Different **data sets** are stored all over
the world



Scientific data: different scales

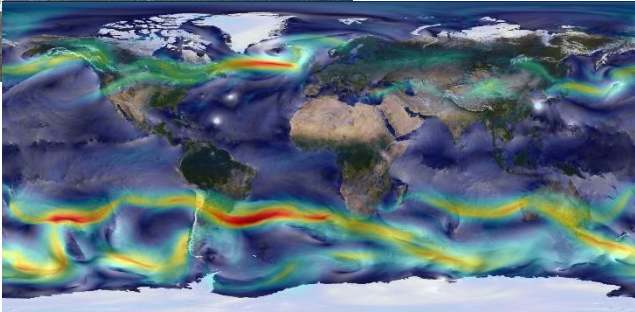
Small data

- Small devices
- Portable USB drives
- Personal computers

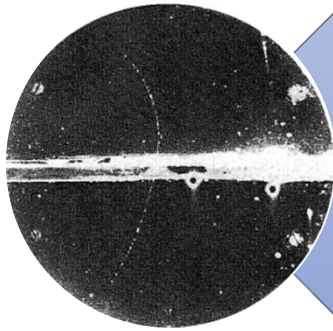


Large data

- Large devices
- Storage servers
- Supercomputers

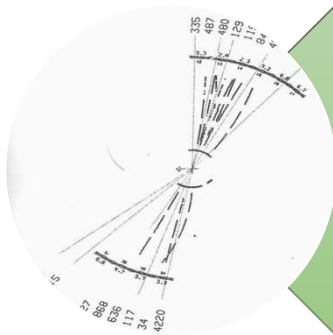


History: from small data to large data (particle physics case)



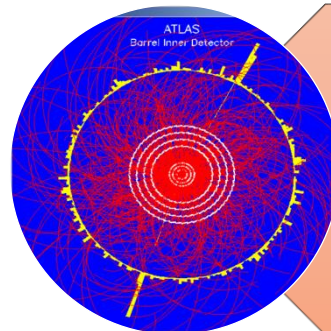
A discovery in 1930-ies

- **exclusive** measurements
- ~2 scientists in 1 country
- pen-and-paper



A discovery in 1970-ies

- more **inclusive** measurements
- ~200 scientists in ~10 countries
- supercomputers



A discovery today

- mostly inclusive measurements
- ~2000 scientists in ~100 countries
- hundreds of Linux servers, supercomputers, Clouds etc

Exclusive and inclusive measurements

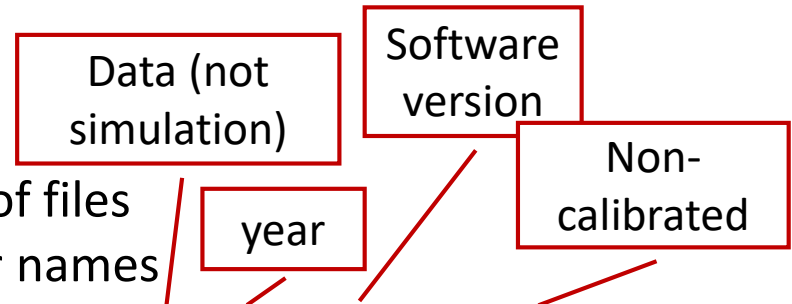
- **Exclusive** measurement: focussed on one particular object, process or phenomenon, excluding all others
 - Example: measure all particles emitted at a particular angle
 - Simpler experimental setup
 - Little data, simple analysis
- **Inclusive** measurement: registers all the processes, objects etc
 - Example: digital sky survey (could produce 1 Exabyte a day, 1 EB = 10^9 GB)
 - More complex experimental setup
 - Lots of data, complicated analysis (“needle in a haystack” problem)
- Inclusive measurements can be “filtered” to exclude unwanted information
 - **Threshold**: minimal value of the measurement to be recorded
 - **Trigger**: a set of conditions that must be satisfied in order to record measurements
 - A trigger may consist of a number of thresholds on different observables, or other requirements (simultaneous occurrences, absence of other effects etc)

Raw data, derived data, metadata, data sets

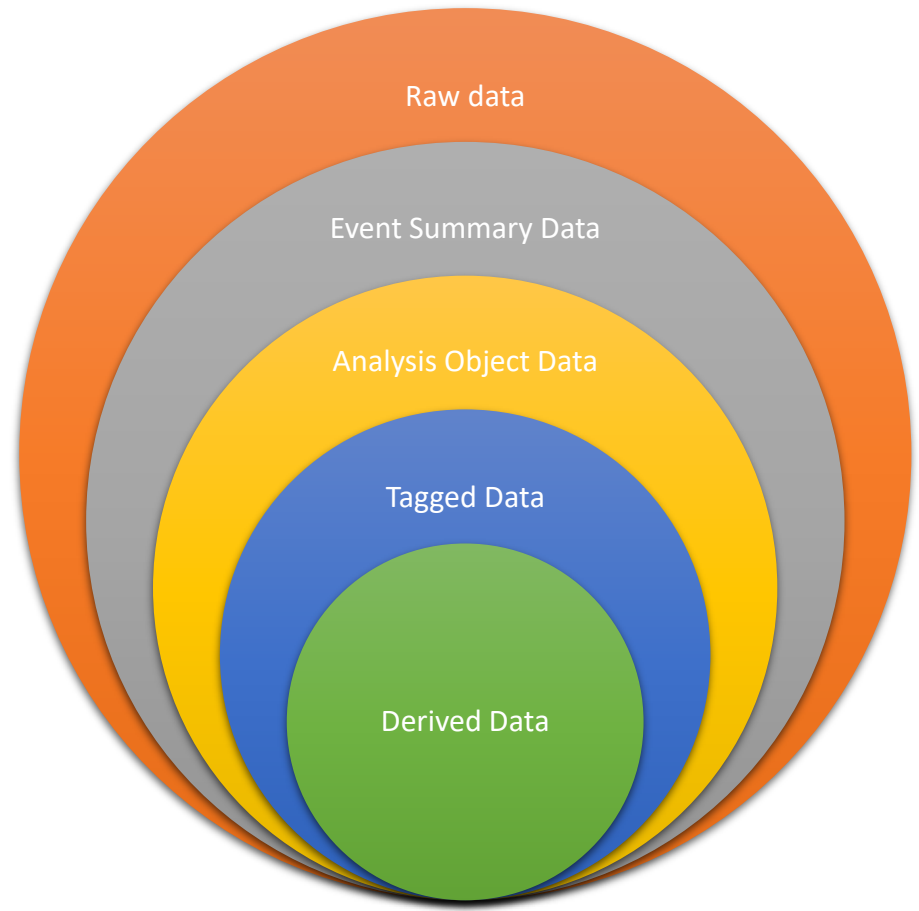
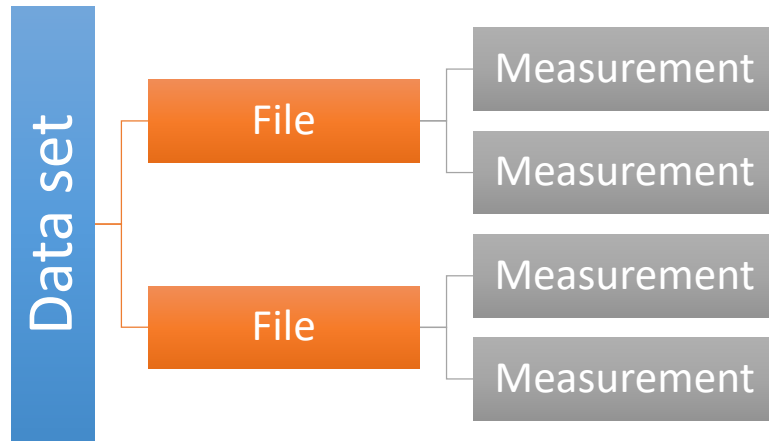
- **Raw data**: data as acquired by an experimental device or method
 - Examples: filled questionnaires, unprocessed satellite images, electronic hits in a detector
 - Raw data often contain unnecessary or excessive information, have large volume, and are recorded in different method-specific ways
- **Derived data**: data derived from raw data by applying various algorithms: filtering, compression, enhancement etc
 - There can be a chain of derived data
 - Derived data usually contain less information, but can also contain additional information as a result of processing
- **Metadata**: data about data, such as time stamps, data ownership, quick summary etc
 - Metadata often are stored together with data
- **Data set**: a set of data characterised by common data taking conditions
 - Examples: same year, same object, same device settings etc
 - Data and data sets can be mutable (can be changed) or immutable (never change once recorded)

Where are the data?

- Scientific data are often stored as files
- A data set may consist of a large number of files
 - Such files would typically have similar names
 - File names often contain metadata, e.g. `data14ver8nocalib.dat`
- There are many different ways of writing data to a file
 - Alphanumeric text files: strings or arrays of data and keywords, readable by any document processing utility
 - Binary files: packaged information to be read by a dedicated software
 - Examples: JPEG pictures, Excel spreadsheets, ROOT files
- Data can also be stored in databases
 - A database is a structured file (or set of files), interpreted by a specialized software
 - Data from a database are read directly, from files – sequentially
 - Databases can establish relations between data objects
 - Databases are needed to enable quick access to large amounts of data
 - Typically, databases are hosted by specialised servers, and are accessed (*queried*) remotely, using special *query languages*
 - Files are easy to copy and transfer, databases are not

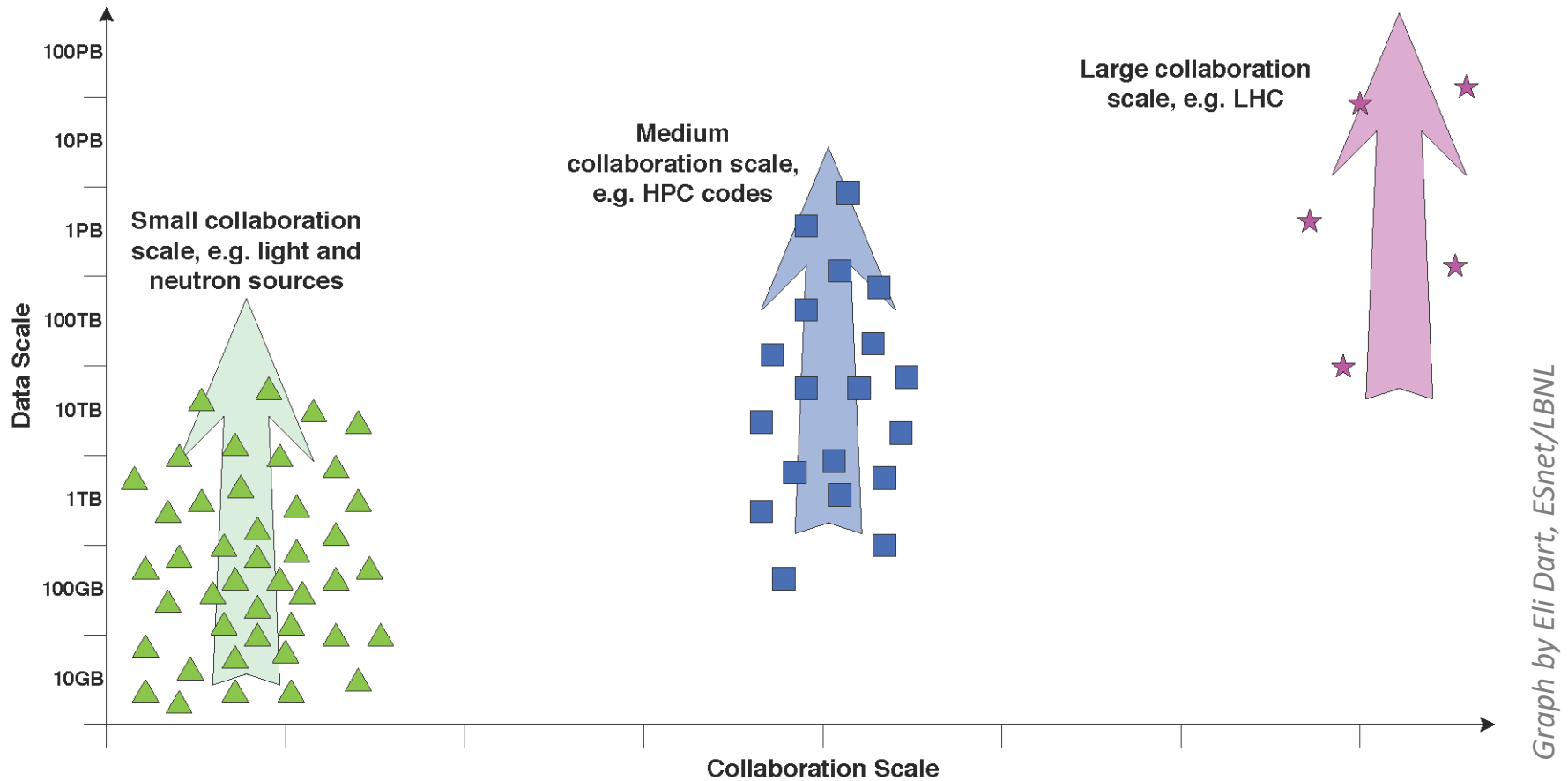


Example of data hierarchy: particle physics



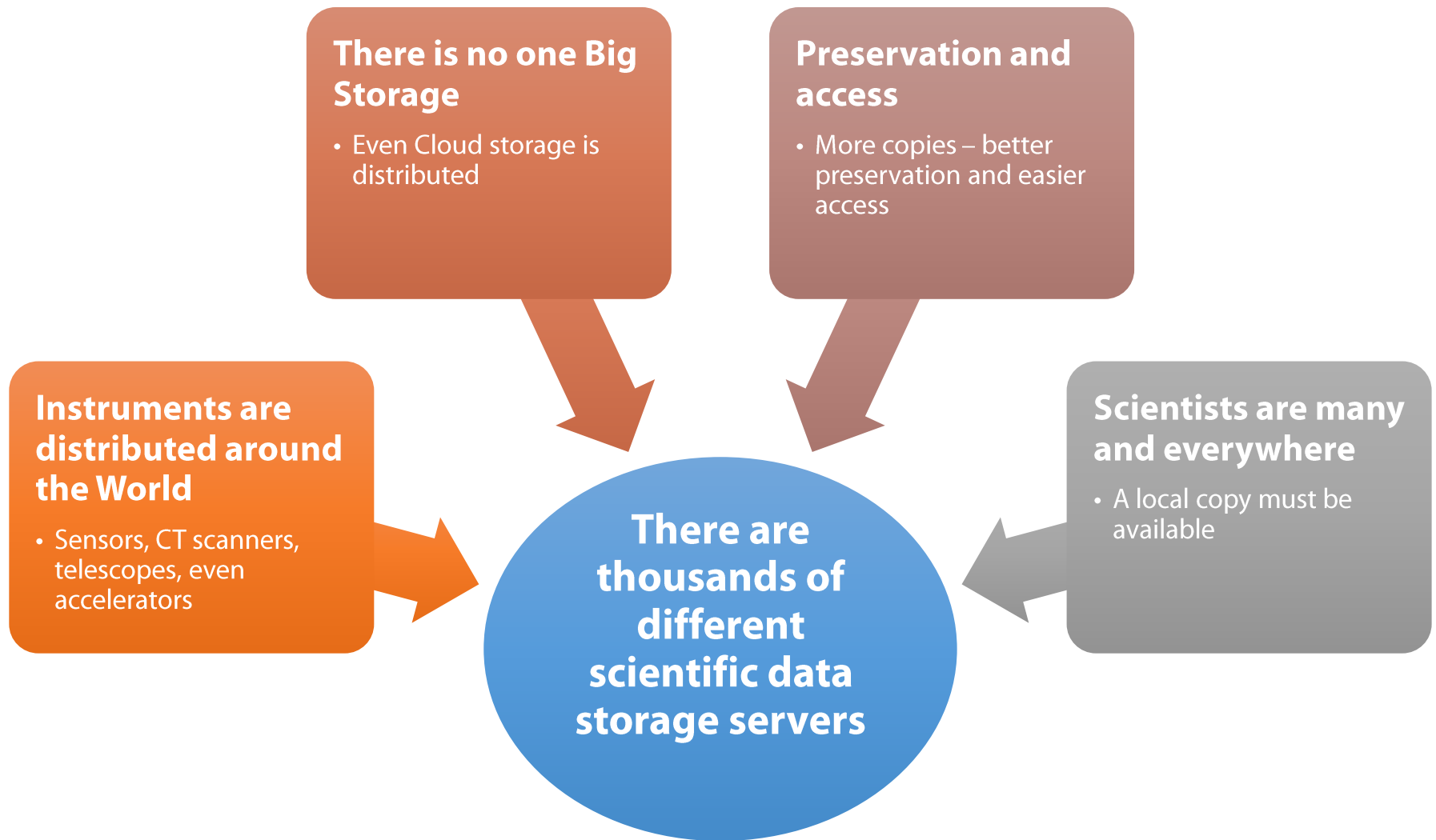
- Different sciences use different data models
- Data are often recorded in structured files
- Each file contains many measurements
- Many files recorded in identical conditions constitute a data set
- Data sets are derived from each other: from raw data to analysis objects

Sizes of scientific data sets and scientists teams



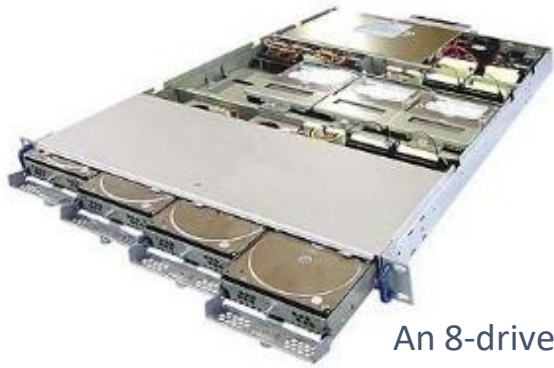
- Larger is data set, more scientists work on collecting and analyzing it
 - Need to follow common rules, have common software etc
- Petabytes and Exabytes of data are a reality today

Data are stored all over the World



What do storage servers look like

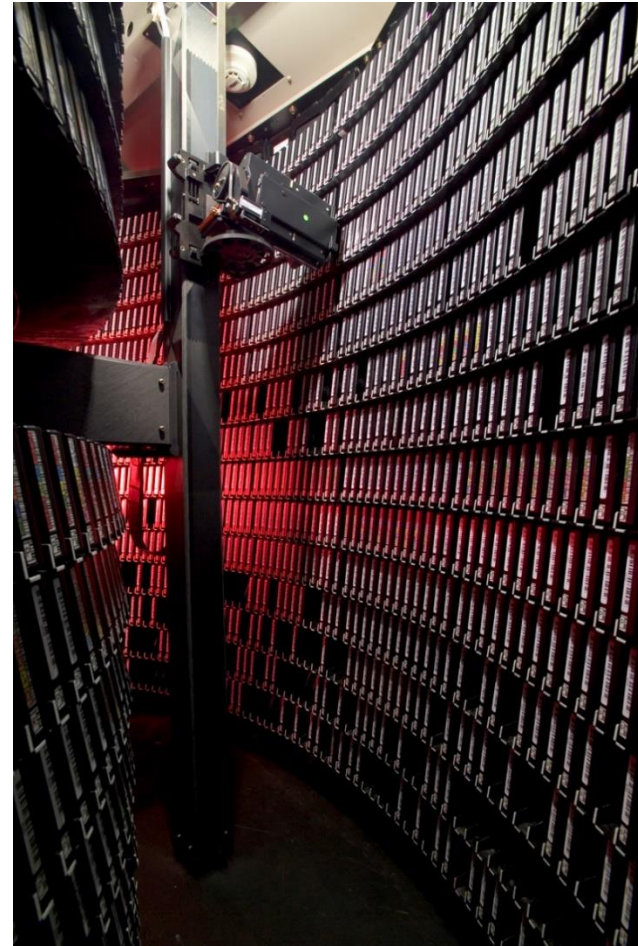
From Computer Desktop Encyclopedia
©2004 The Computer Language Co., Inc.



An 8-drive rack unit



A disk storage rack fragment

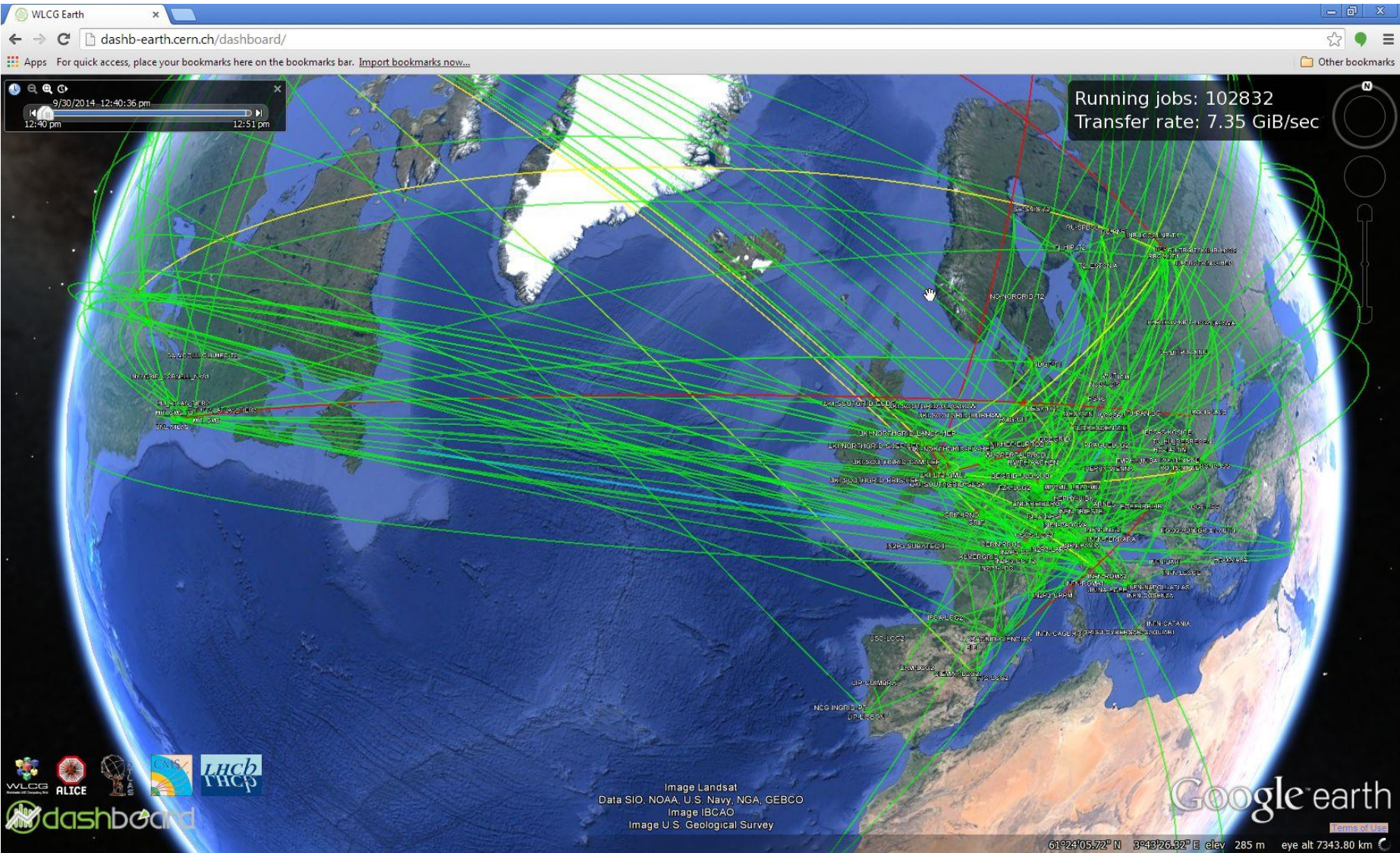


Tape robot at Fermi National Accelerator Laboratory (USA)

How to find my data?

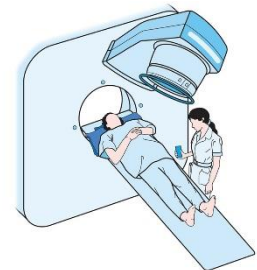
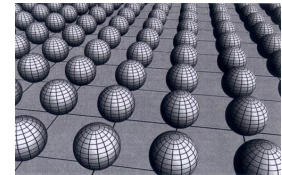
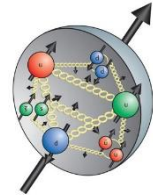
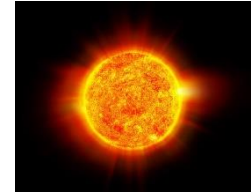
- Step #1: Ask your supervisor!
- Hint: Master-copies are usually preserved and catalogued by the scientists who collect the data
 - There's no catalogue of catalogues though (Google is still your friend)
- Small data sets are simply copied to office computers and USB memory sticks
 - Memory sticks capacity increases, but data volumes increase, too
 - Office computers become more powerful and can process more data
- Large data sets can be too large for your office computer!
 - Petabytes (1 PB = 1 million GB) are stored in specialized storage centers of research labs
 - Approach #1: get login/password for the computer that has access to the data set
 - Usually, a large High Performance Computer in a research lab
 - Approach #2: send your analysis program to a distributed computing system (*Grid*), which will find the best place for it to work
 - This is not available yet to all sciences, but is used in particle physics

CERN data: distributed across the World



Information can also be computer-generated

- Some data are difficult to measure experimentally
 - Inaccessible location
 - Lack of adequate experimental tools
 - Very rare or hypothetical processes
 - Ethical issues
- If a scientific model exists for a process, such data can be computer-generated – **simulated**
 - Nuclear explosions
 - Effects of drugs
 - Planet formation
 - Aerodynamic characteristics
 - Quantum effects
 - Weather forecasts
 - Etc etc etc...
- Simulation of probabilistic processes (common in e.g. subatomic physics) relies on random number generators – hence called **Monte Carlo**



Why do we need simulation in physics?

- To design new experiments and plan for new searches
 - Any new theory can be coded and plugged into a simulation program
- To identify unexpected experimental signals
 - When simulation prediction does not correspond to experimental data, it might mean that we see an unexplained phenomenon (or there is a bug in the program)
- To correct for experiment imperfections
 - Our devices are never 100% efficient, and sometimes produce fake signals

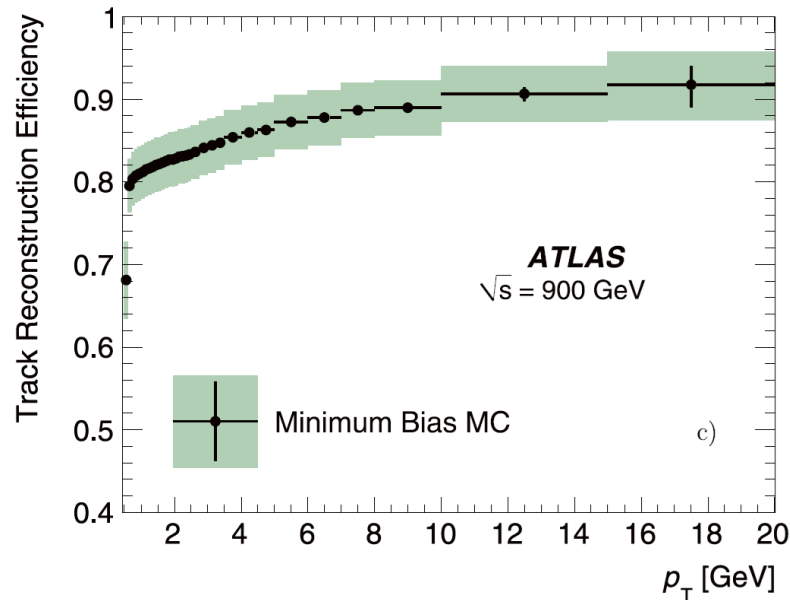
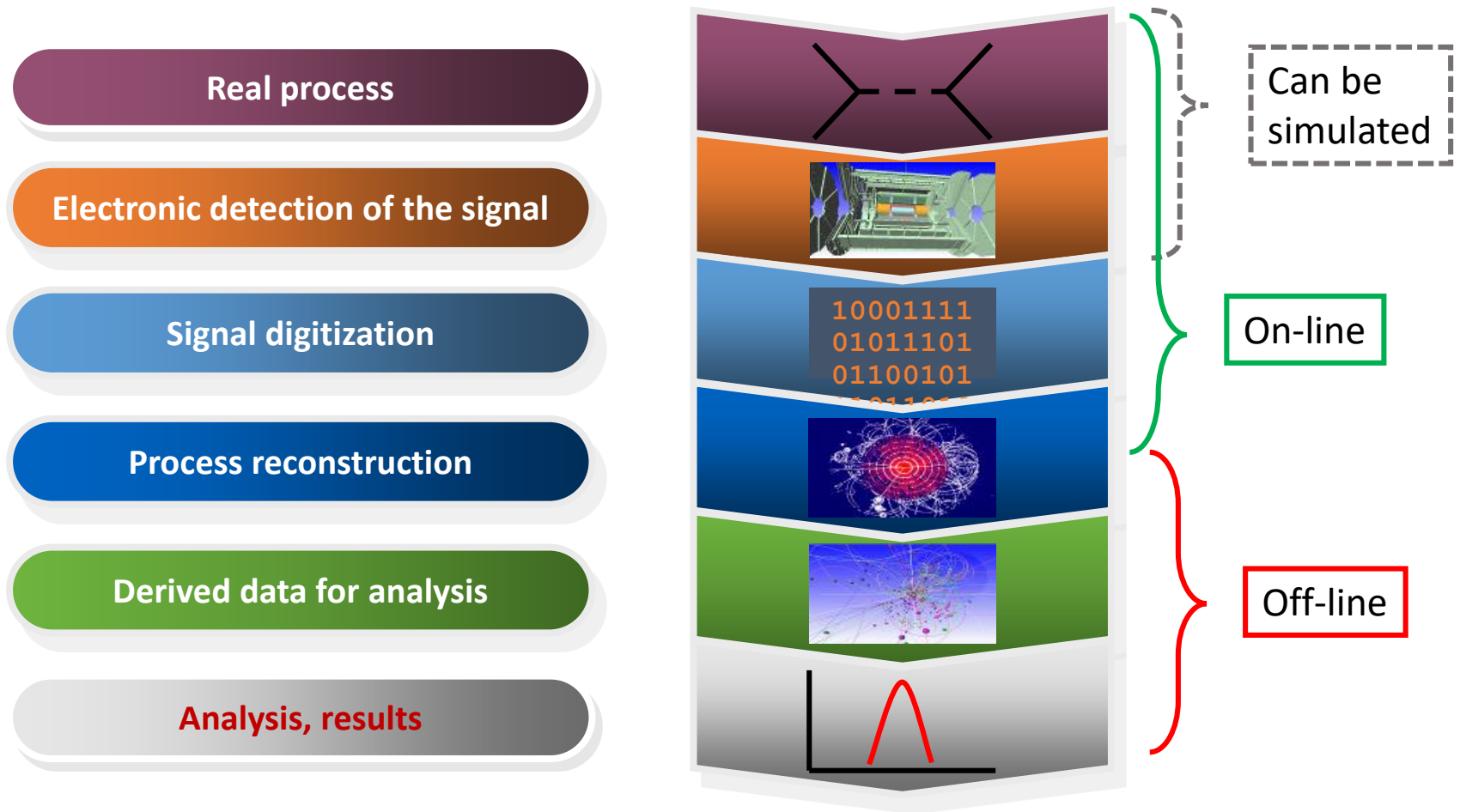


Figure from Phys. Lett. B 688 (2010) 21–42

Data acquisition and processing: particle physics case



- Every such step requires computing
 - Even the tiniest detectors are driven by programmable microchips
- **Software is a scientific tool**

On-line vs off-line

- Refers to the time and manner in which data are being processed
 - **On-line**: data are processed real-time while being taken, usually at a specialized computer embedded within the experimental device
 - **Off-line**: data are processed after the experiment finishes, normally by other computers elsewhere
- On-line processing has to be fast, so not very complex
 - Produces raw data and some derived data (using triggers and fast filters)
- Off-line processing can be as complex as necessary
 - Produces derived data and simulation
- Terminology actually comes from computer science, where it describes different algorithms

Special data need special software

- Many scientific data sets are small enough to be processed by generic software tools, for example:
 - Spreadsheets: good for social sciences and simple processing
 - MATLAB, Origin etc: offer specialized languages for complex processing and modelling, as well as advanced visualization
- There are reasons why not everybody uses such commercial tools:
 - **Data volumes:** when data are very big and/or very complex, commercial tools are not suitable (too generic, or too rigid, or too expensive)
 - **Data formats:** custom-built instruments produce data in customized formats
 - Particle physics detectors, telescopes, satellites etc
 - Customized formats often appear due to the necessity to compress raw data
 - **Simulation:** advanced complex models are beyond the scope of commercial tools
- What do we do when MATLAB doesn't help? **We develop our own software!**

What kind of software do scientists develop?

- Some examples:
 - Device programming
 - “firmware” that makes custom-made experimental devices working, executed on-line
 - On-line pattern recognition
 - fast software that can be used for triggering or raw data filtering
 - Device calibration, alignment etc
 - higher-level software needed to correct for technical imperfections, can be executed on-line or off-line at a generic computer
 - Raw data pre-processing, production of derived data
 - more complex software, takes large computing resources and longer time; executed both on-line and off-line

What kind of software do scientists develop?

- More examples:
 - Device performance simulation, process modelling
 - complex and demanding software implementing various interaction models and simulation of physics processes; executed off-line
 - Data analysis
 - algorithms for statistical analysis, pattern recognition, data mining etc etc; off-line
- System software
 - tools and services to support data storage, management and processing across different computers
- Data presentation and publication
 - software for visualisation of results, preparation of plots, typesetting – nowadays mostly professional tools are used

Software is a tool that you can make yourself

- In many scientific disciplines, experimental devices and tools are manufactured on industrial scale
 - Even unique accelerators and telescopes are made from industry-produced components and assembled by professional engineers
 - In areas like particle physics or radioastronomy, students rarely have a chance to make an own scientific tool – unless it is a prototype of some new technology
- Inclusive measurements produce data that can not be used without heavy computer processing and comparison with models (simulation)
- **Software is a scientific tool**, as important as any other instrument
- There are infinite possibilities to improve software or develop a better one
 - Inadequate software means that it may take months or even years to analyze data, and the results may not be accurate enough...
 - ...or even wrong, if there are bugs
- Many research projects require development of new analysis or modelling algorithms – you will have to make your tool yourself

Specifics of scientific software

- While other scientific instruments are made mostly by professionals, scientific software is made mostly by amateurs
 - Algorithms require knowledge of the research object, which professional software engineers don't have
 - Still, some scientists are good programmers

Good programmers know what to write.
Great ones know what to rewrite (and reuse).
Eric S. Raymond

- Scientific software is often rather simplistic, poorly documented, and is not easy to install outside the computer where it was developed
- On the bright side, scientific software is usually freely available to be used, modified and customized

We will start with software useful for students

- Admittedly biased towards tools used in particle physics
 - Basic principles are the same everywhere
- Most typical programming tasks of a student:
 - Modelling and simulation – needs no data even
 - Data analysis and presentation of results

Example of simulation software: Pythia

- Pythia was known as the Oracle of Delfi, possessed immense predictive powers (until year 393)
- In 21st century, Pythia is arguably the most successful particle physics Monte Carlo generator
- Pythia highlights:
 - Software to simulate particle collisions (particularly in accelerators)
 - Can simulate hard processes: Standard Model and beyond, resonance decays etc
 - Showers: initial- and final-state radiation, transverse momentum ordered
 - Underlying event: multiple interactions, colour-connected beam remnants
 - Hadronisation: Lund model, particle decays, Bose-Einstein effects
 - Various auxiliary utilities



Adapted from T. Sjöstrand, LU

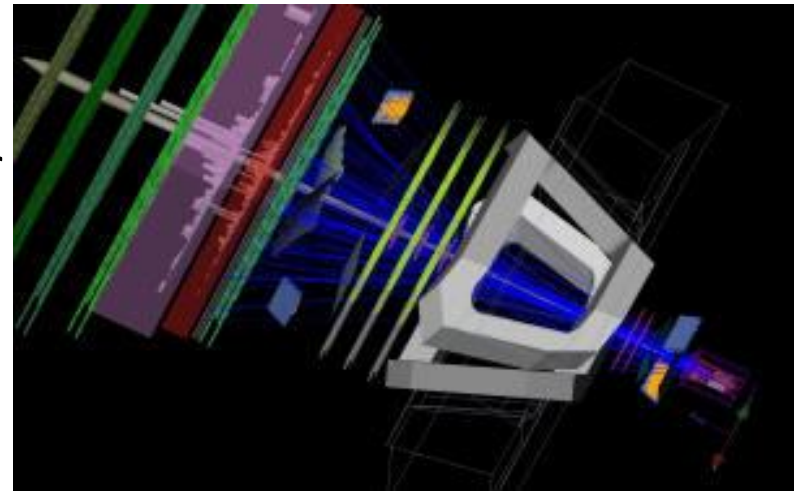
Simplest code using Pythia 8 (C++)

```
// File: main01.cc. The charged multiplicity distribution at the LHC.
#include "Pythia.h"
using namespace Pythia8;
int main() {
    // Generator. Process selection. LHC initialization. Histogram.
    Pythia pythia;
    pythia.readString("HardQCD:all = on");
    pythia.readString("PhaseSpace:pTHatMin = 20.");
    pythia.init( 2212, 2212, 14000.);
    Hist mult("charged multiplicity", 100, -0.5, 799.5);
    // Begin event loop. Generate event. Skip if error. List first one.
    for (int iEvent = 0; iEvent < 100; ++iEvent) {
        if (!pythia.next()) continue;
        if (iEvent < 1) {pythia.info.list(); pythia.event.list();}
        // Find number of all final charged particles and fill histogram.
        int nCharged = 0;
        for (int i = 0; i < pythia.event.size(); ++i)
            if (pythia.event[i].isFinal() && pythia.event[i].isCharged())
                ++nCharged;
        mult.fill( nCharged );
    }
    // End of event loop. Statistics. Histogram. Done.
    pythia.statistics();
    cout << mult;
    return 0;
}
```

Adapted from T. Sjöstrand, LU

Example of simulation software: GEANT

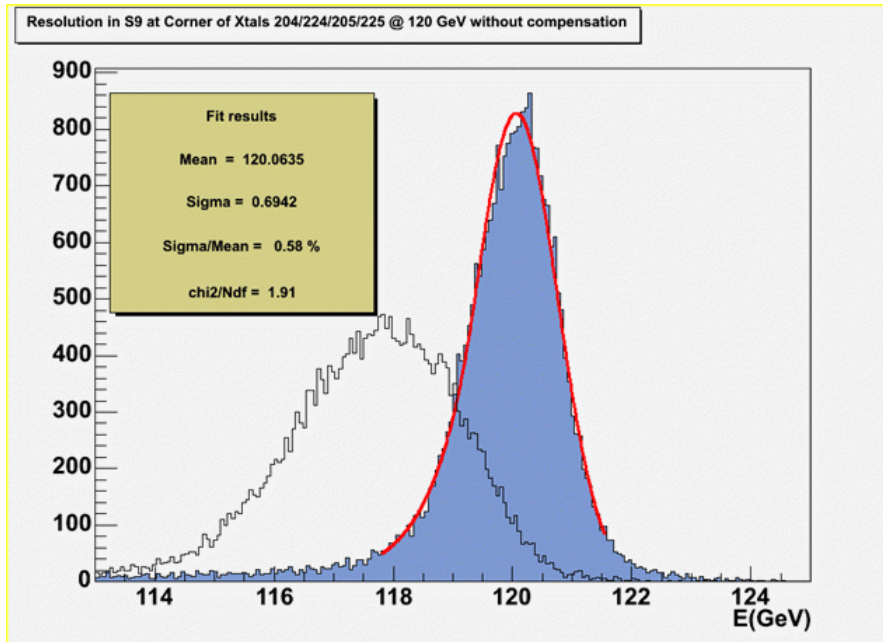
- Our experimental devices are never perfect!
- But we know how they work
 - In particle physics, we know how particles interact with materials
 - This is also relevant for radiation therapy
- Every detector (and even a human body) can be simulated by software
 - Making use of knowledge of particle interactions with matter
 - Needs precise knowledge of detector geometry, magnetic field, gas status etc
 - Although largely deterministic, has some probabilistic effects as well



- Most complete detector simulation software: GEANT (version 4 is the latest)
 - Pythia (or other good Monte Carlo) and GEANT are absolutely necessary to calculate corrections for detector inefficiencies

Figure taken from geant.cern.ch

Final analysis: ROOT



Plot taken from root.cern.ch

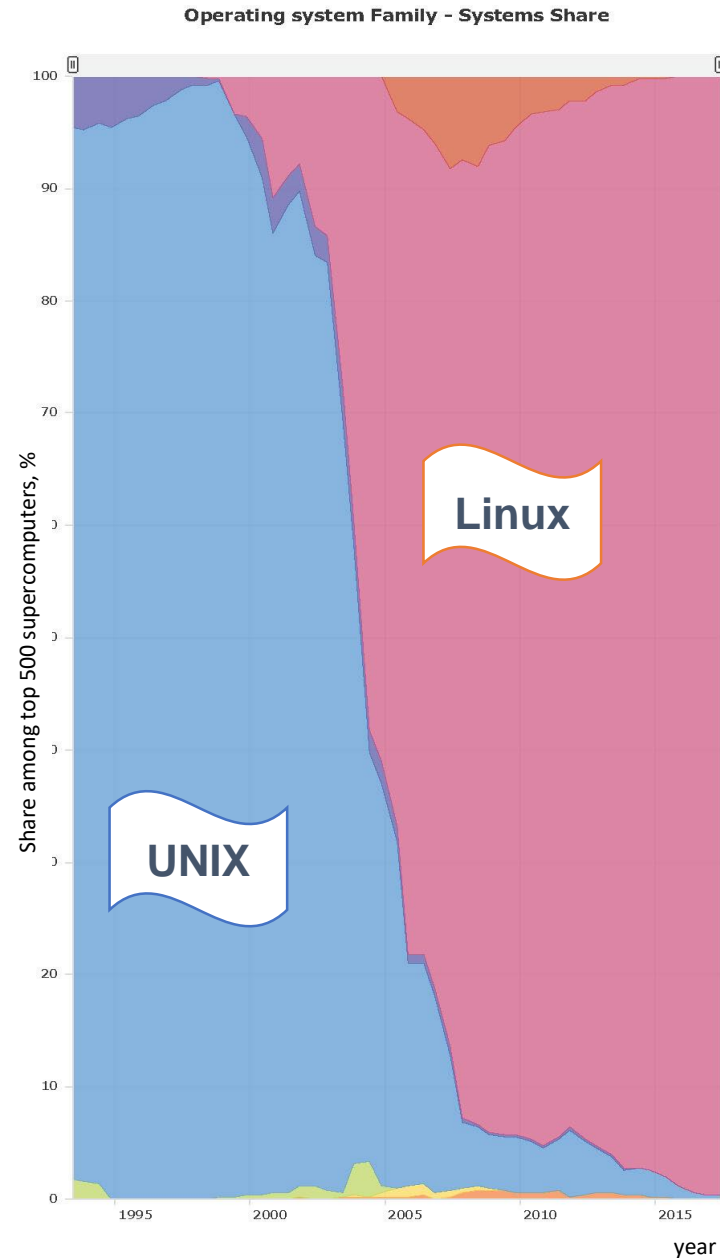
- ROOT is a C++ based tool and framework (program and library) for data analysis
 - C++ as script language with interpreter
 - Graphical interface for interactive visualization
 - Input/Output and analysis of large amounts of data
 - Histogramming, plotting, fitting
 - Physics and mathematics
 - Object organisation
 - Parallel analysis via network

Big data need big computers

- Even the most advanced desktop workstation will take years to process Petabytes of data
 - And will require a dedicated network connection to transfer all that
- Similarly, simulation of a statistically significant sample on a workstation will take years
- But we need our Nobel prize tomorrow!
 - It took ~2 weeks of massive data processing to find a hint of the Higgs boson – the fastest discovery of this kind
- Solution: use supercomputers or large computer clusters, with large attached storage and very fast network
 - 10 Gbps now, 1 Tbps in the near future
- There is a catch: big computers need special operating systems

Operating systems (OS)

- An operating system is software that makes computers work, orchestrating different components – hardware and software
- Microsoft Windows, Mac OS X or Android OSs were designed for personal computers
- On servers, computer clusters and supercomputers, **Linux** is by far dominant
 - Comes in many flavors – *distributions*
 - Often – *RedHat Linux* or its derivatives
 - Most Linux distributions are actually free and their code is open for everybody to tweak



How do Linux clusters look like

A very old traditional Linux cluster



The newest *Aurora* Linux cluster in Lund

We use Linux!

- Linux is a UNIX-like OS designed to be flexible and portable to about any hardware
 - UNIX was designed as an OS for multiuser environments (as opposed to personal computing), capable of handling many simultaneous tasks
- Linux is not really meant for desktop PCs, but it gives the user real control of the system
 - It is also more difficult to infect by viruses, since every Linux machine is different
 - It still has vulnerabilities, but they are quickly rectified by the worldwide community of volunteer developers
- Linux comes in many distributions: *RedHat*, *Debian*, *SuSE*, their derivatives, etc
 - Differ in software packaging, organization of directories, policies etc
 - Software that works on one Linux system may not work on another
- Scientific Linux is a derivative of RedHat; the future of Scientific Linux is bleak, and it will probably give way to another RedHat derivative, CentOS
- For personal use, Ubuntu (a derivative of Debian) is the best, as it was designed to be user-friendly
 - Actually, Android is also Linux, but stripped of many characteristic components

Some peculiarities of working with Linux

- **Command-line interface (CLI)**

- Most stages of scientific computing do not require graphical interfaces
 - Many scientific softwares do not even have graphical interfaces
- Scientific software tools have many options and parameters that are difficult to accommodate in graphical tools
 - CLIs support basic programming, scripting
- When connecting to a remote computer, graphics slows down the work – and can even be a security threat when intercepted
- For these reasons, we communicate with computers by typing instructions

```
# echo $[2+2]  
4
```

- **Non-interactive and batch processing**

- Analysis of large data sets, or a complex simulation, can take hours and even days
- You may need to execute several analyses or simulations at the same time
- On Linux, such tasks can be executed in a non-interactive mode, in “background”
- For batches of many such tasks, special softwares exist to take care of processing
 - Called “batch systems”, many different kinds exist

Short summary

- Experimental sciences work with increasingly large data sets, and theoretical sciences use increasingly complex models
- The largest experimental data sets are produced by complex and unique instruments, and require unique software
- To analyze such data, or to simulate various phenomena on a large scale, massive computing power is needed
- Linux clusters are the main working horse of scientific computing
- Knowledge of Linux and programming is essential for many scientists

Home assignment (see [Live@Lund page for MNXB01](#)):

- Please fill the short programming background questionnaire by tomorrow