Introduction to Programming and Computing for Scientists

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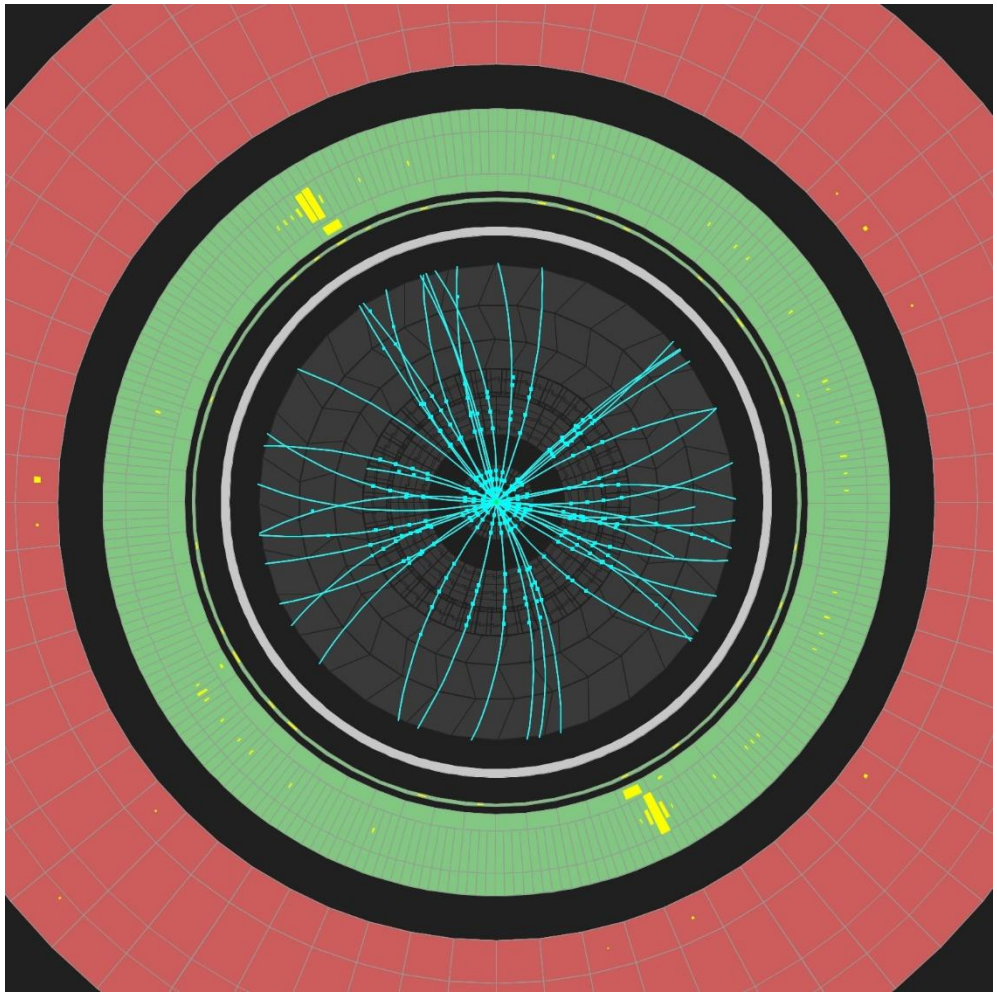
Lecture 5

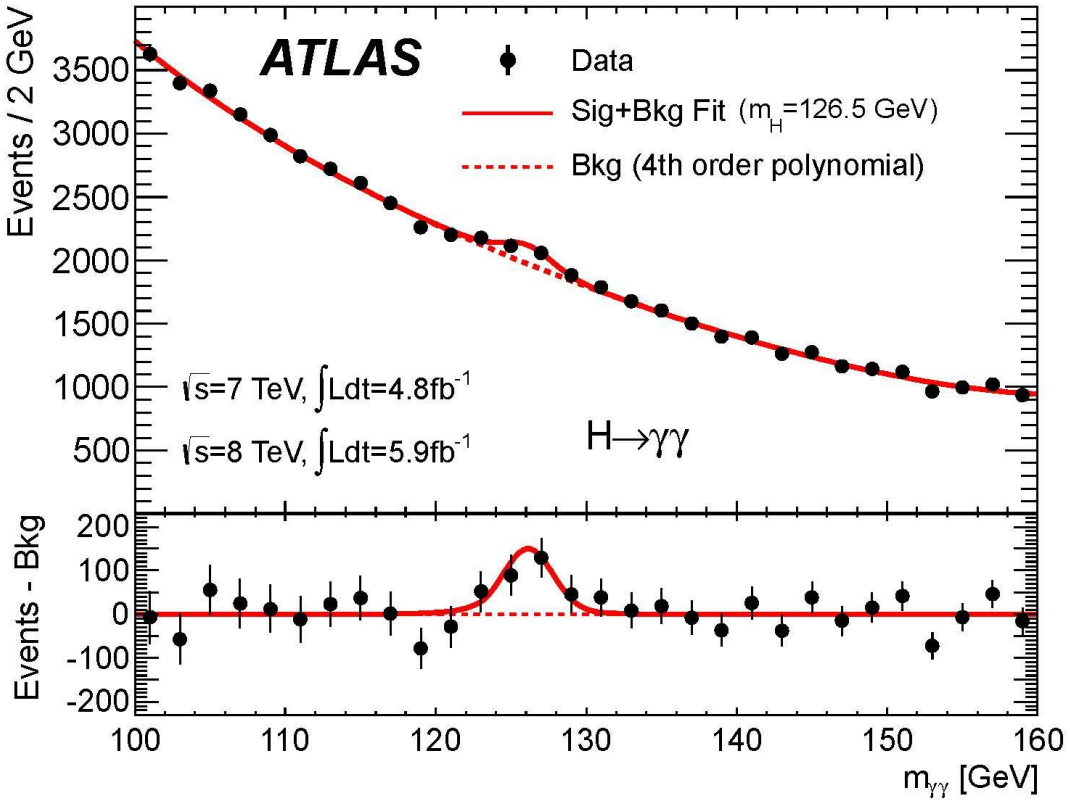
Data analysis

- Scientific research is always about **data analysis**
- Analysis is usually about finding patterns
  - Galaxies
  - Hurricanes
  - Particle tracks
  - Effects and phenomenae
- Example: Higgs boson decay into two photons
  - Patterns:
    - particle tracks (curved lines)
    - vertices (origin of tracks)
    - clusters of energy depositions



Statistical analysis

- When a pattern is found, its characteristics must be quantified
- Example: hundreds of Higgs to two photons decays
  - Most photon pairs are false positives – don't come from Higgs
    - Real signal must be extracted
  - Position of the peak (Higgs mass) must be measured



Statistical methods

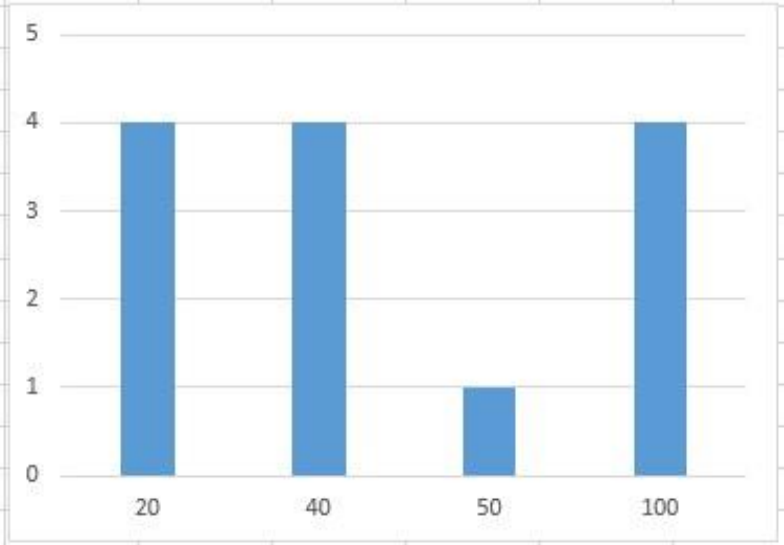
- Statistics is used to analyze data that have probabilistic nature and/or have random variations
  - Even several measurements of the same object with the same tool bring varying results, so statistics is needed to deduce the measured value and standard deviation
  - Statistic can be either *descriptive* (as in the example above), or *inferential* (hypothesis testing)
- Statistical methods are used to find patterns and to quantify the results
  - In the Higgs example, statistical analysis is used to, for example:
    - Identify location of the signals left by particles
    - Reconstruct track patterns from detected signals
    - Reconstruct vertices from tracks
    - Assign energy and momentum to tracks
    - Quantify position and width of the observed peak
    - Test hypothesis that the observed peak is consistent with the Higgs boson
- We need software tools to do all this analysis!

Histograms

- **Histograms** are an important tool of statistical data analysis
  - Much more than just a graphical representation of data
- Histograms record frequency of measurements in defined ranges (**bins**)
- Histograms are initially empty arrays, where a value of an element increments by 1 (or by an assigned weight) if the measurement belongs to a discrete bin associated with this element
  - Example: measurements of people's age is collected in a histogram with 100 bins, each bin is 1 year. If a person's age is 19, the 19^{th} bin is incremented by 1
  - Bins can be non-equidistant: e.g., one bin can accommodate ages 50-100
  - Histograms can be 2-dimensional: for example, weight versus height
    - More dimensions are impossible to visualise…
- When histogram filling is complete, each bin will contain a value, statistical error of which can be calculated from the number of entries in this bin and the weight of each entry (simply square root of number of entries if the weight is 1)
- A filled histogram with errors is practically identical to a graph

Example: a histogram in Excel

	A	B	C	D	E	F	G	H	I	J	K
1	Data (age)		*Bins*	*Frequency*							
2	15		0	0							
3	28		20	4							
4	64		40	4							
5	3		50	1							
6	85		100	4							
7	43		More	0							
8	11										
9	54										
10	35										
11	40										
12	22										
13	17										
14	74										
15											

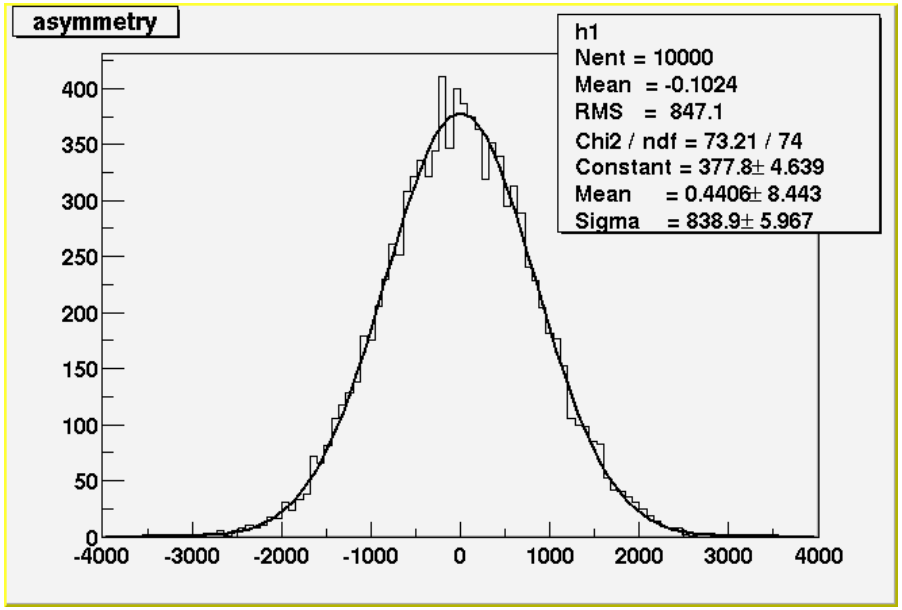


- Note 5 bin margins and 4 actual bins: one must specify both upper and lower margins
- Excel is not too good with non-equidistant bins – all appear with the same width
- Excel also doesn't show statistical errors automatically
- But of course, better analysis frameworks exist!

Fitting histograms

- Most measured distributions can be described by a theoretical function with several parameters
  - Simplest: straight line, has 2 parameters: $F(x) = P_1 + P_2 x$
  - Gaussian is another example, has 3 parameters: $F(x) = P_1 e^{-(x-P_2)^2/2P_3^2}$
- Finding values of the parameters (and their errors) is the main goal of many analyses
- The process of finding parameters that describe the data best is called **fitting**
  - When parameters are good, the theory **fits** the data
- Several standard fitting algorithms exist. General approach is:
  - With initial parameters, calculate data to function "distance"
  - Change parameters step by step in order to minimize the "distance"
    - Algorithms of this minimization can be different
    - "Distance" depends on errors: with large errors, any function will fit
    - "Distance" can be estimated differently by different algorithms; most commonly used is the **chi-square** per **degree of freedom** test
      - Degrees of freedom depend on number of data points and free parameters: $ndf = N_{data} - N_{param}$

Example of a Gaussian fit

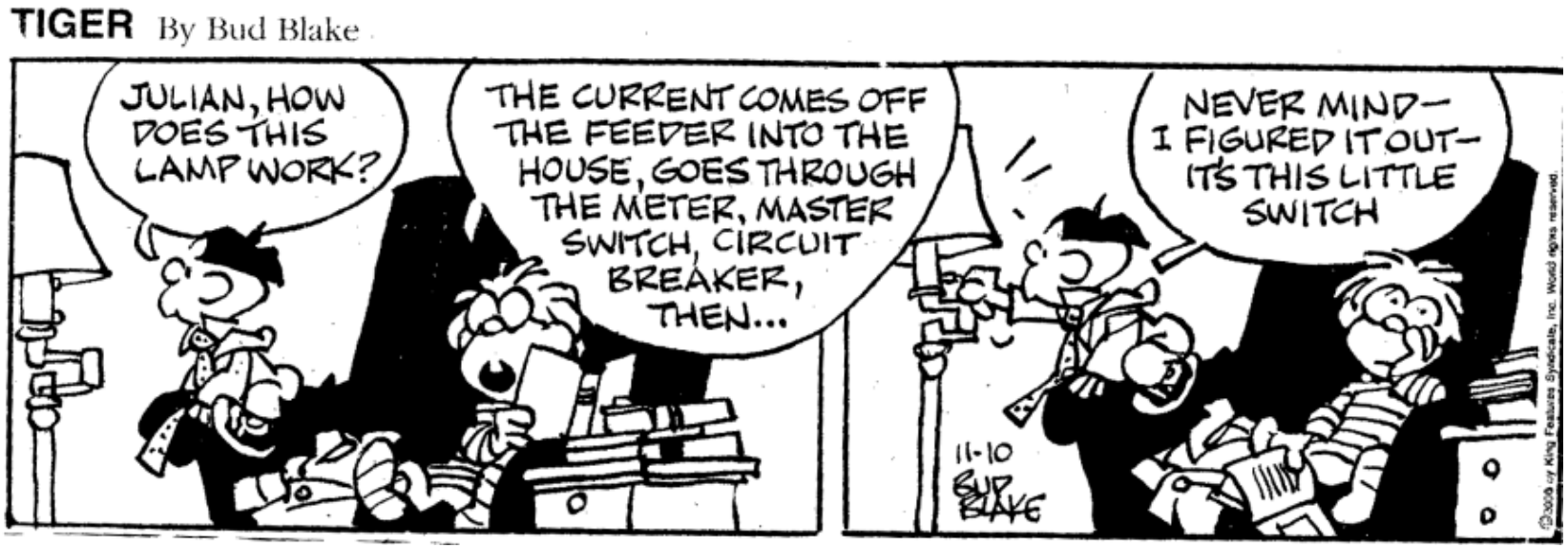


- The histogram has 10000 measurements – "entries"
  - Each bin has several entries
- The histogram is not normalized: the integral is not 1
- Gaussian function here has three parameters:
  - normalization constant
  - mean value
  - width (standard deviation, sigma)
- The value of chi-square per degree of freedom is close to 1 – a very good fit
- Each fit parameter has own errors

- Any good **analysis framework** can do fitting

Analysis frameworks and data formats

- **Frameworks** hide complex details, providing simple utilities, tools and services

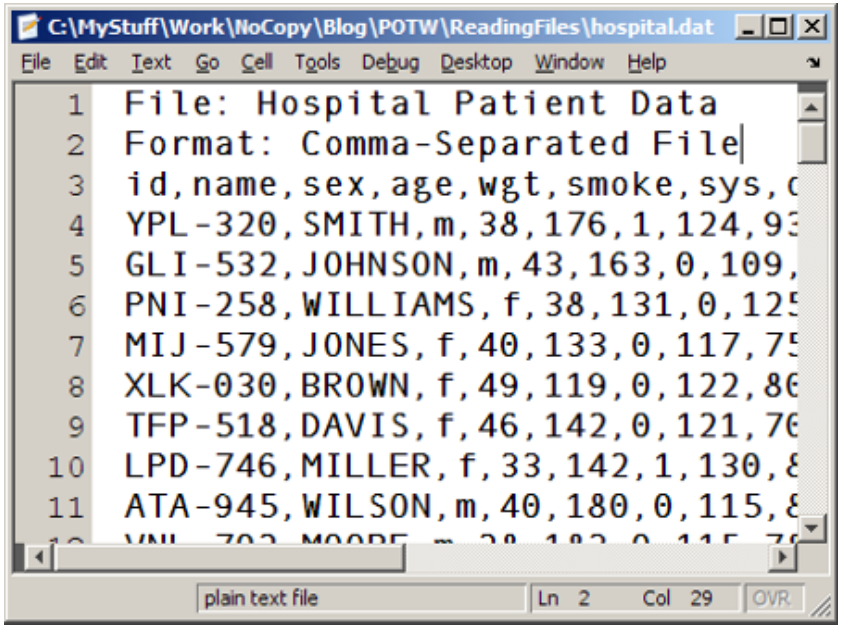


Strip borrowed from Suzanne Panacek slides

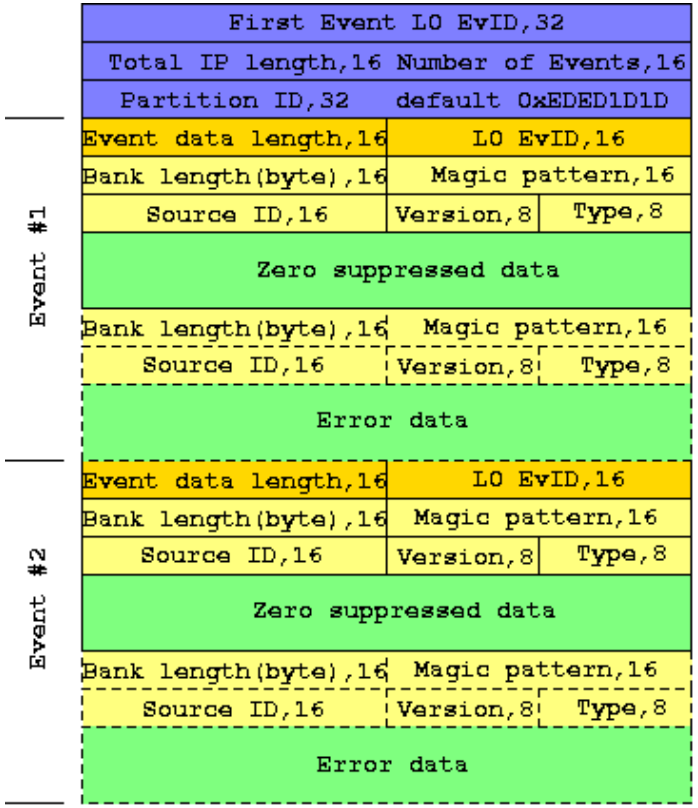
- Often the most complex detail to hide is the *data format*
- **Data format** in our context is a way of recording and organizing information
  - Binary or alphanumeric, possibly structured as tables, columns, raws or other record units, order of records, links between records etc etc etc
  - There are almost as many data formats as there are researchers
    - Some are even documented
- Different analysis frameworks are coupled to different data formats

Some data formats – examples

- Simple comma-separated alphanumeric file (CSV)
  - Common for small data sets
  - In this example, data file contains format description
  - Analysis framework: any, e.g. MS Excel



- Accelerator experiment data format
  - Blocks of specified bit-length
  - Information is compressed because of large data set size
  - Specialized analysis framework



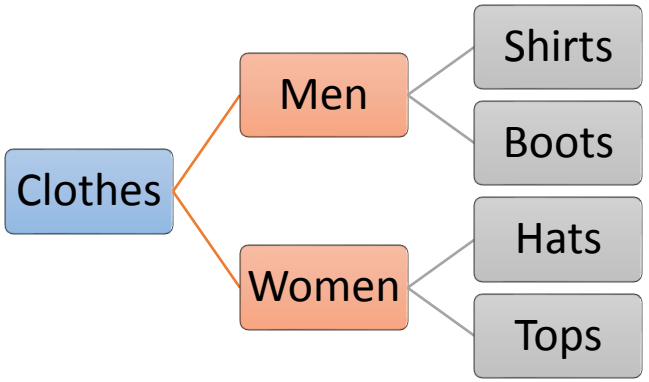
Organising data: hierarchies

- **Flat** data format example: individual entries

1	Men	Shirt	XL
2	Women	Top	M
3	Women	Hat	58
4	Men	Boots	46

- A CSV list on the previous slide is a typical flat data format
- Easy to understand, but difficult to handle when it grows very big
  - **Scalability** problem

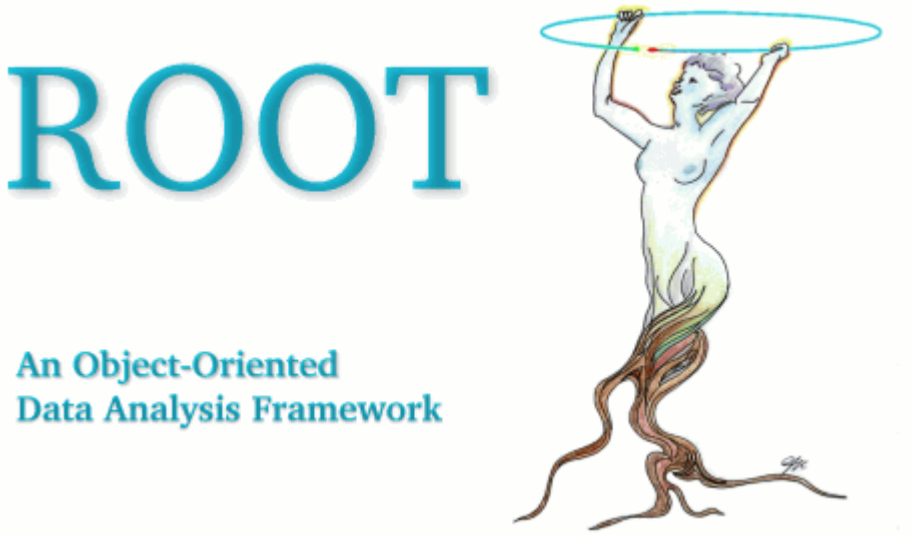
- **Hierarchical** data format: groups, objects



- Several hierarchical data formats exist
  - HDF5 – commonly used in natural sciences
  - ROOT – more powerful than HDF5, used mostly in particle physics

ROOT – an object-oriented analysis framework

- We will focus on **ROOT** – a specialized analysis framework developed at CERN
  - Free and available for almost all platforms
  - Relies on ROOT data format (a hierarchical database, actually)
  - Has built-in C++ interpreter – you can use C++ in ROOT , like Python



- A complete ROOT tutorial normally takes several days; many such tutorials can be found on-line
  - We will give a short introduction, re-using some official slides

What is ROOT?

- The ROOT system is an object-oriented (OO) framework for large scale data analysis (and even simulation)
  - Written in C++
  - Provides, among others,
    - An efficient hierarchical OO **database**
    - A C++ interpreter (**CINT**)
    - Advanced statistical **analysis** (multi-dimensional histogramming, fitting, minimization and cluster finding algorithms)
    - **Visualization** tools
    - And much, much more
  - The user interacts with ROOT via a graphical user interface, the command line or scripts
  - The command and scripting language is C++ (thanks to the embedded CINT C++ interpreter)
    - Large scripts can be compiled and dynamically loaded

How to get and set up ROOT

- ROOT is absolutely free and needs no licenses
- On Ubuntu, it is available from **`universe`** repositories
  - Install package **`root-system`**
- Otherwise, go to
  http://root.cern.ch
  and download what you need
  - Currently recommended version is **5.xx**
  - Installation from source is for brave people: will take some time and may produce odd error messages
- You can configure your ROOT preferences using **`~/.rootrc`** file
- There are also scripts **`rootlogon.C`**, **`rootlogoff.C`** (executed on logon and logoff) and **`rootalias.C`** (loaded on logon)
- History is saved in **`~/.root_hist`** file
- Read ROOT documentation for details (or Google “ROOT getting started”)

ROOT command line options

- Without options, typing **`root`** will start an interactive ROOT session
- Options are useful for non-interactive ROOT calls
  - Will come back to non-interactive batch processing later

```
> root -/?
    Usage: root [-l] [-b] [-n] [-q] [file1.C ... fileN.C]
    Options:
      -b : run in batch mode without graphics
      -n : do not execute logon and logoff macros as specified in .rootrc
      -q : exit after processing command line macro files
      -l : do not show splash screen
```

Several ways to work with ROOT

- Type **`root`** at the command line prompt
  - This starts a new "shell" from which you can work with data by using C++ instructions and scripts
  - One can also launch a ROOT GUI (see next slide)
  - To exit, type **`.q`**
  - To run a script (e.g. a tutorial), type **`.x <scriptname.C>`**
  - To load functions from a file, type **`.L <scriptname.C>`**
  - To execute a regular shell command, type **`.! <command>`**
- You can also link your code with the ROOT libraries and make the ROOT classes available in your own program
  - the libraries are designed and organized to minimize dependencies
- Other relevant commands:
  - **`rootcint`** – starts a utility to create a class dictionary for CINT. You will see how this utility is used is the section about adding your own class to ROOT.
  - **`cint`** – a C++ interpreter that can be used independently of ROOT

More ROOT tricks

- If you have a script (for example, myMacro.C), you can execute it non-interactively:

```
root -b -q 'myMacro.C("text")' > myMacro.log
```

  here **-b** stands for "batch" (non-interactive) and **-q** – for "quit after execution"

- CINT commands starting with dot (**.**)
  - See **.q .L .x** and **.!** above
  - Other useful commands:
    - **.?** (help)
    - **.U** (unload file loaded with .L)
    - **.files** (show all loaded files)
    - **.ls** (list objects, such as histograms)
- C++ instructions
  - **new Tbrowser** (starts a **graphical browser** for objects)
    - same as **TBrowser *b = new TBrowser()**

Built-in ROOT C and C++ interpreter: CINT

- Main goal: provide a framework for C and C++ "scripting" – somewhat like Python
- As a separate software, CINT code is available under an Open Source license
- It implements about 95% of ANSI C and 90% of ANSI C++
- It is robust and complete enough to interpret itself (90000 lines of C, 5000 lines of C++)
- Has good debugging facilities
- Has a byte code compiler
- In many cases it is faster than tcl, Perl and Python
  - Large scripts can still be compiled for optimal performance
- CINT is used in ROOT:
  - As command line interpreter
  - As script interpreter
  - To generate class dictionaries
  - To generate function/method calling stubs
- In ROOT, the command line, script and programming language become the same

Simple ROOT warm-up examples

```
root [] 35 + 89.3
(const double)1.2429999999999997e+02
root [] float x = 45.6
root [] float y = 56.2 + sqrt(x);
root [] float z = x+y;
root [] x
(float)4.5599998474121093e+01
root [] y
(float)6.2952777862548828e+01
root [] z
(float)1.0855278015136719e+02

root [] TF1 f1("Function drawing test","sin(x)/x",0,10);
root [] f1.Draw();
```

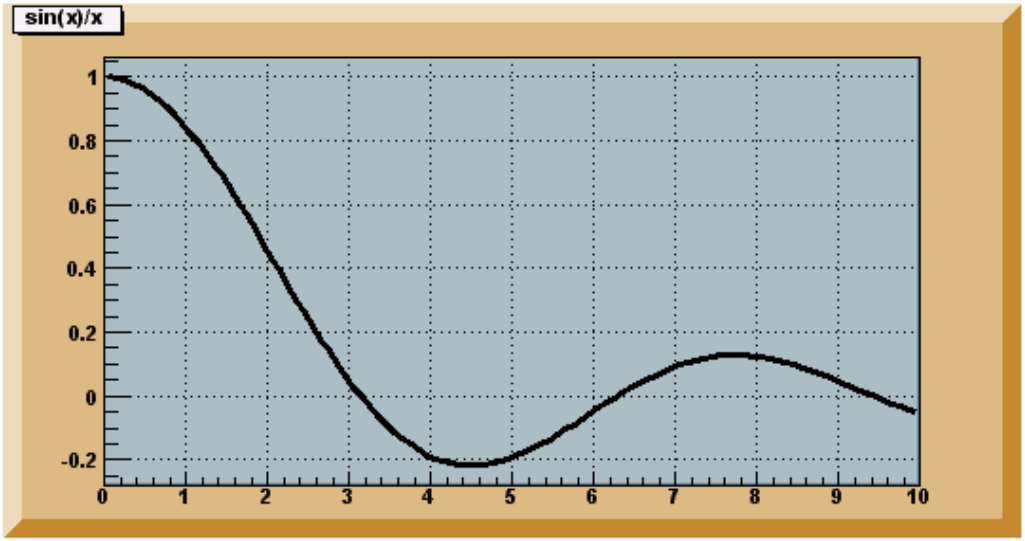
- Note that by default ROOT uses double precision
- TF1 is a ROOT class for functions of 1 variable (1-dimensional functions)
  - **`Draw`** is a method of the class
  - Use TAB to show all methods: **`root [] f1.<TAB>`**

Some ROOT conventions

- ROOT classes begin with **`T`** (like **`TF1`** above)
- Non-class types end with **`_t`** (for example, **`Int_t`**)
- Constants begin with **`k`** (for example, color red: **`kRed`**)
- ROOT uses machine-independent types, e.g.:
  - **`Bool_t`** – Boolean (0=false 1=true)
  - **`Char_t`** – signed character 1 byte
  - **`Int_t`** – Signed integer 4 bytes
  - **`Short_t`** – Signed short integer 2 bytes
  - **`Long64_t`** – Signed long integer 8 bytes
  - **`Float_t`** – Float 4 bytes
  - **`Double_t`** – Float 8 bytes (a.k.a. double precision)

Example of a ROOT session: CINT is used everywhere

```
Root > float x=5; float y=7;
Root > x*sqrt(y)
(double)1.322875655532e+01
Root > for (int i=2;i<7;i++) printf("sqrt(%d) = %f",i,sqrt(i));
sqrt(2) = 1.414214
sqrt(3) = 1.732051
sqrt(4) = 2.000000
sqrt(5) = 2.236068
sqrt(6) = 2.449490
Root > TF1 f1("f1","sin(x)/x",0,10)
Root > f1.Draw()
```



Scripts in ROOT

- Un-named Script: a simple short-cut (like a bash script)
  - Starts with { and ends with }
  - All variables are in the global scope
  - No class definitions
  - No function declarations
  - No parameters
- Named Script: essentially, a C++ program
  - C++ functions
  - Scope rules follow standard C++
  - Function with the same name as the file is executed with a *.x*
  - Parameters
  - Class definitions (derived from a compiled class at your own risk)

Examples of scripts

- "Macro" is a historical way of denoting scripts in ROOT
- **Un-named** Macro: `hello.C`

```
{
  cout << "Hello" << endl;
}
```

- **Named** Macro: `say.C`

```
void say(char * what = "Hello")
{
  cout << what << endl;
}
```

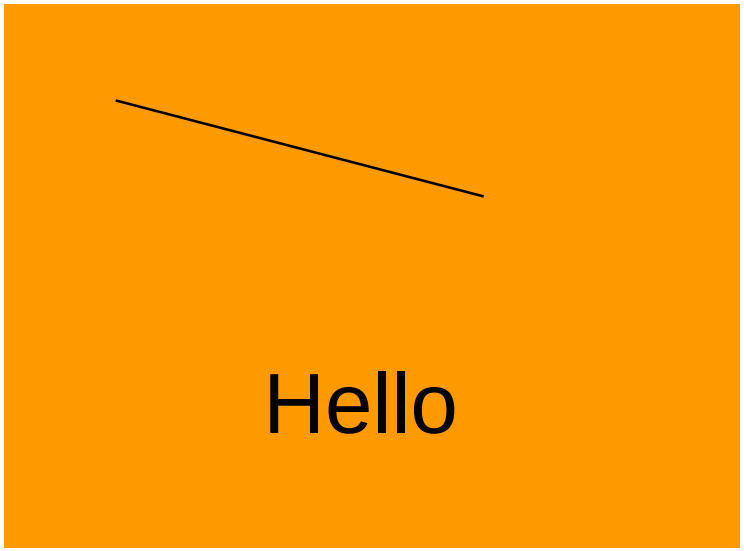
- Executing the Named Macro

```
root [3] .x say.C
Hello
root [4] .x say.C("Hi there")
Hi there
```

Graphics in ROOT

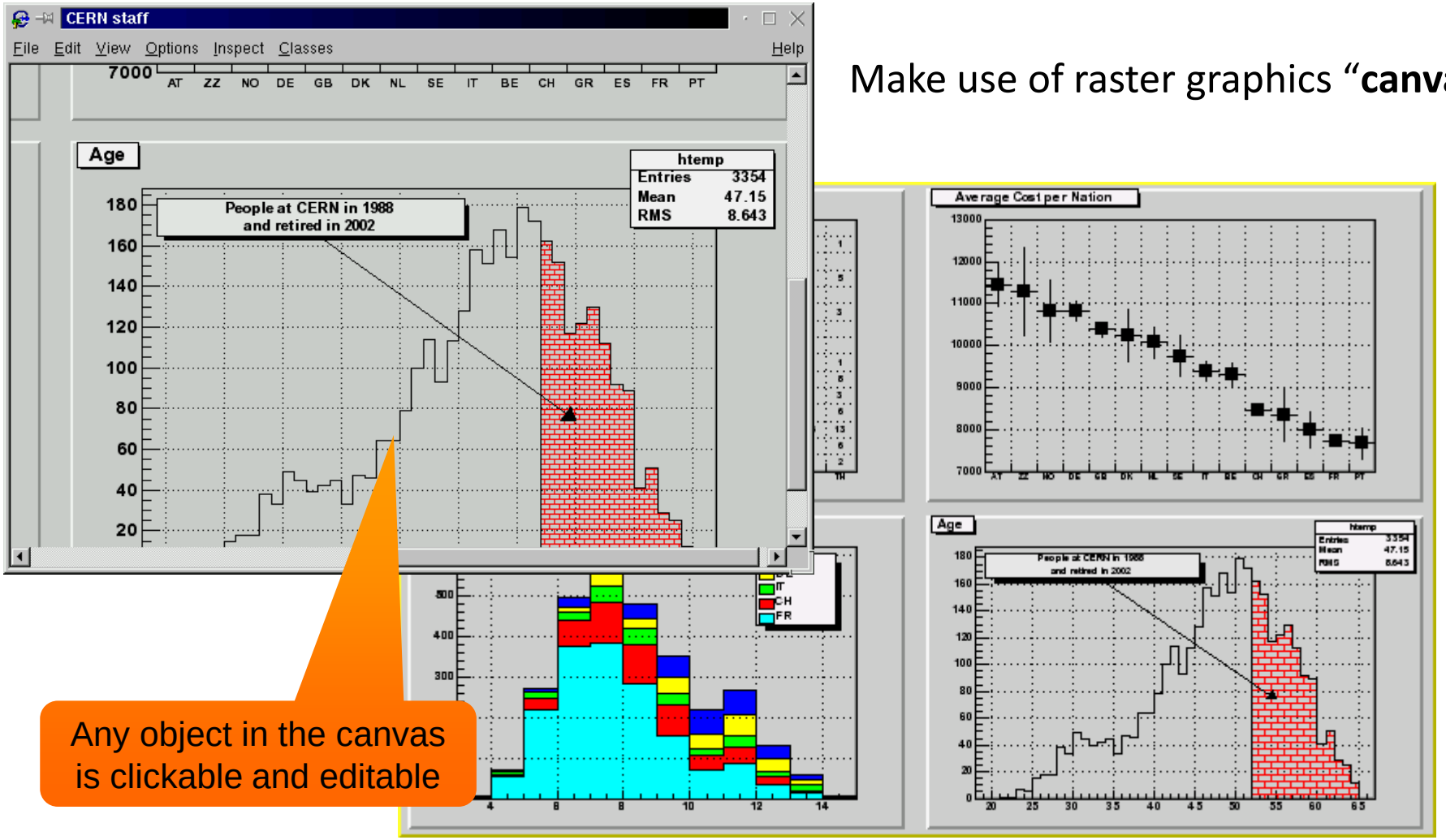
- ROOT is no Photoshop, and graphics is designed for scientific results representation

```
root [] TLine myline(.1,.9,.6,.6)
root [] myline.Draw()
root [] TText mytxt(.5,.2,"Hello")
root [] mytxt.Draw()
```



- The **`Draw`** function adds the object to the list of primitives of the current graphics "**pad**"
- If a pad does not exist, it is automatically created with a default range [0,1]
- When the pad needs to be drawn or redrawn, the **`Paint`** function is called

More advanced examples: histograms



Make use of raster graphics "**canvas**"

Plotting graphs

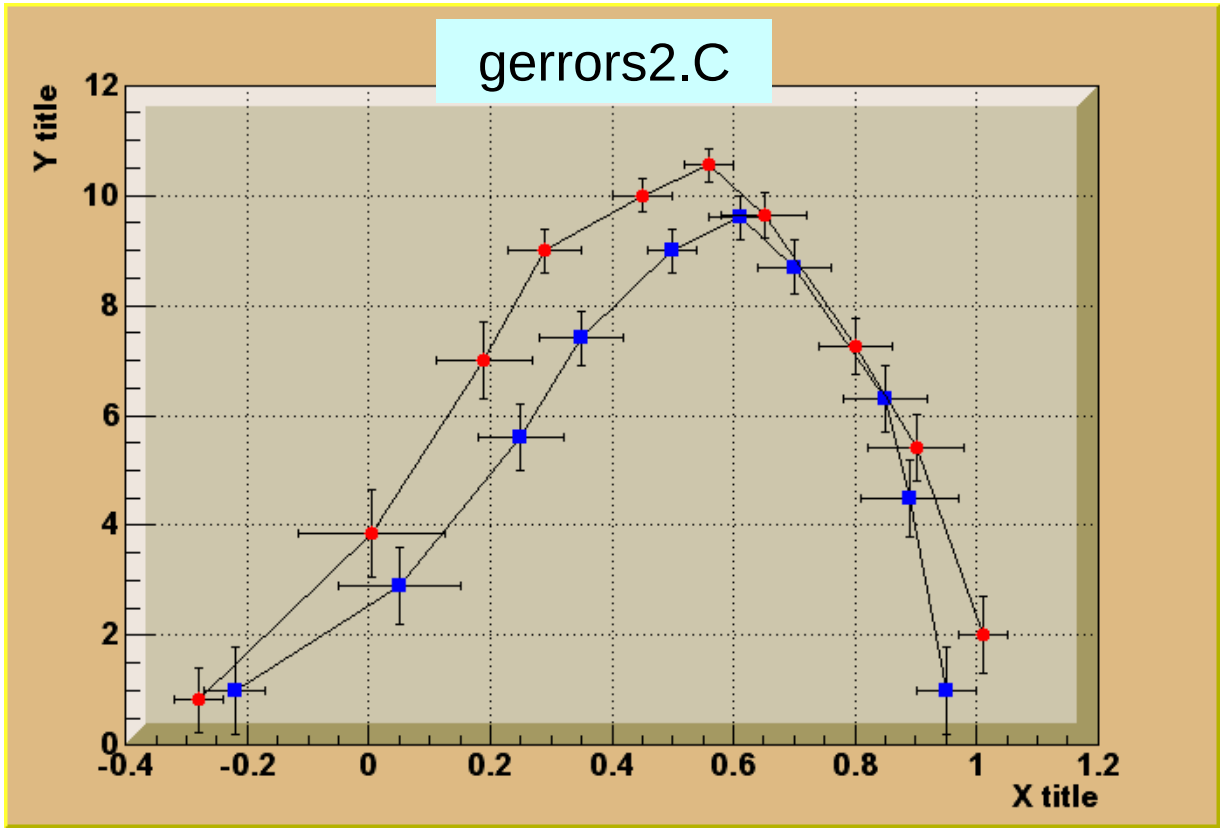
- Points to plot are specified by two vectors: **x** and **y** in this example, of length **n**
- Both symmetric and asymmetric errors can be plotted

`TGraphErrors(n,x,y,ex,ey)`

`TGraph(n,x,y)`

`TCutG(n,x,y)`

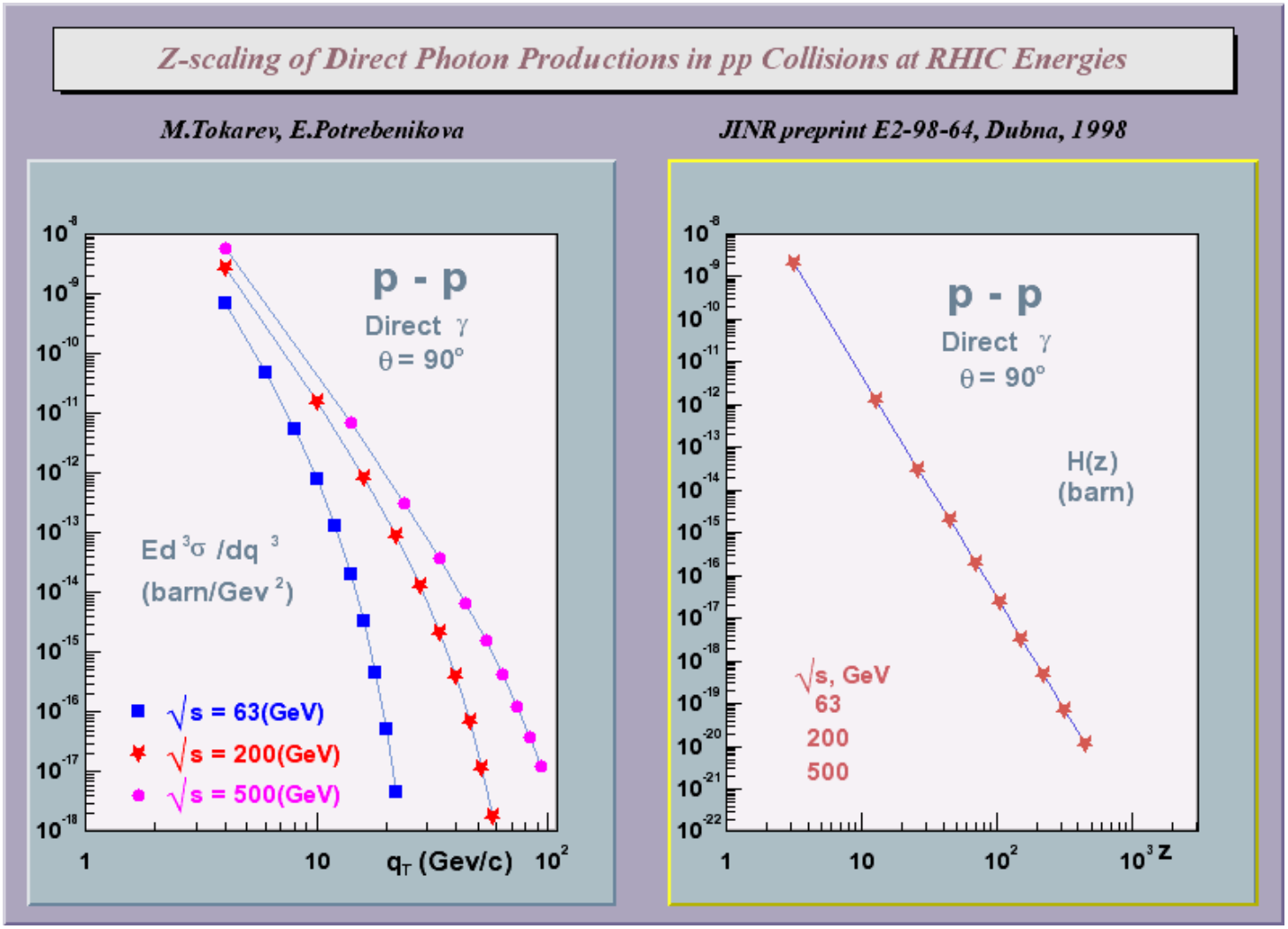
`TMultiGraph`



`TGraphAsymmErrors(n,x,y,exl,exh,eyl,eyh)`

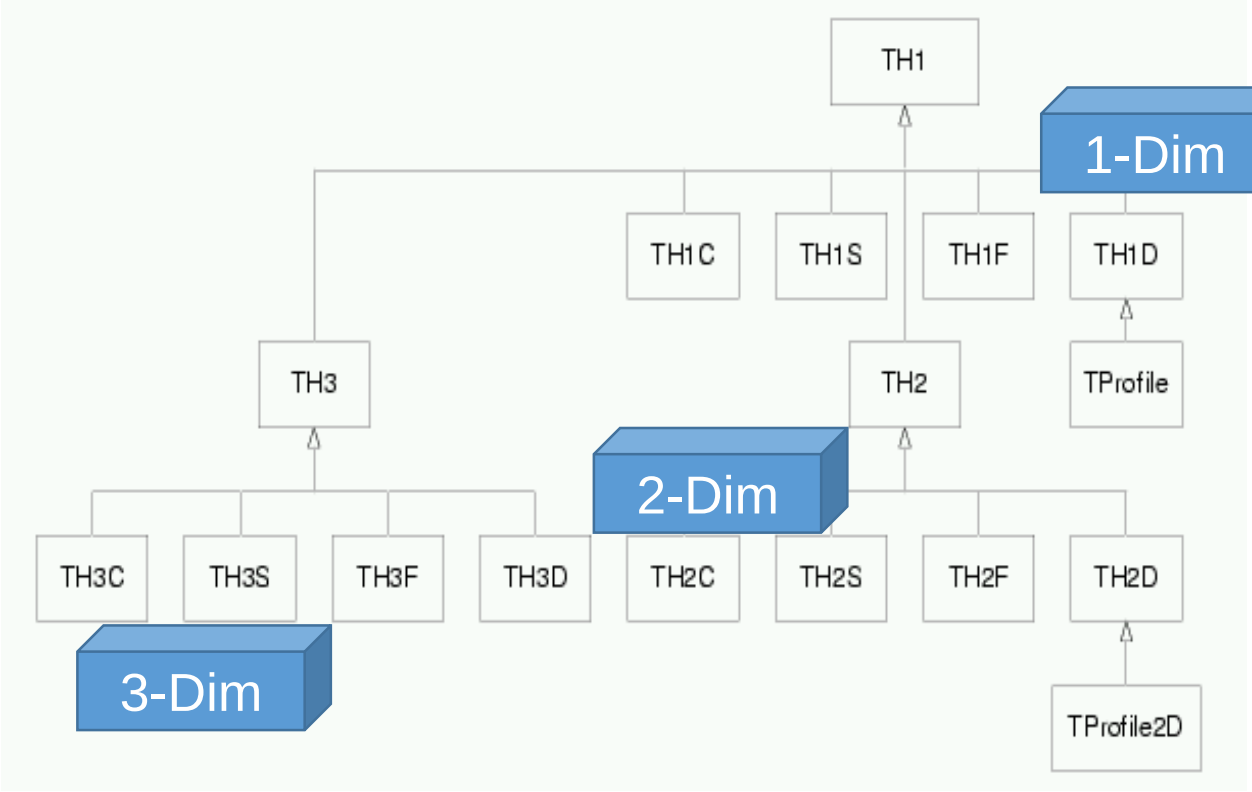
More graphs: legend, annotations

zdemo.C

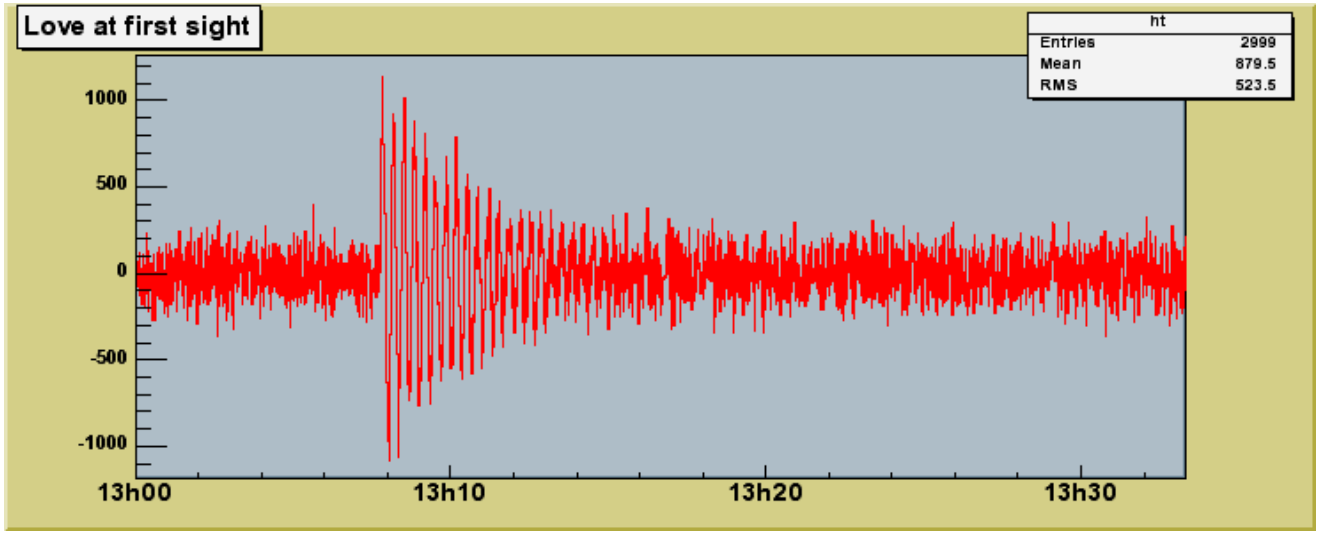


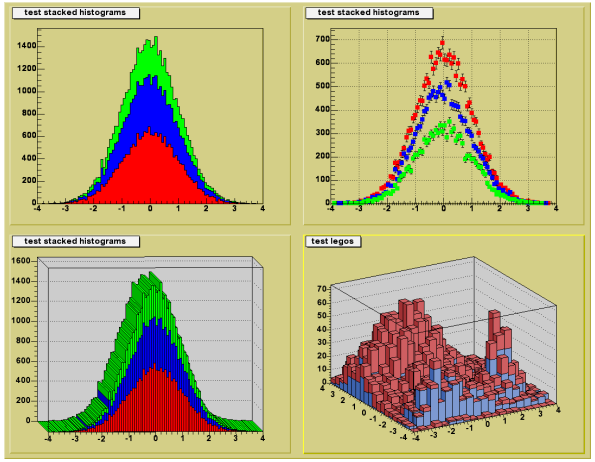
Histogram classes in ROOT

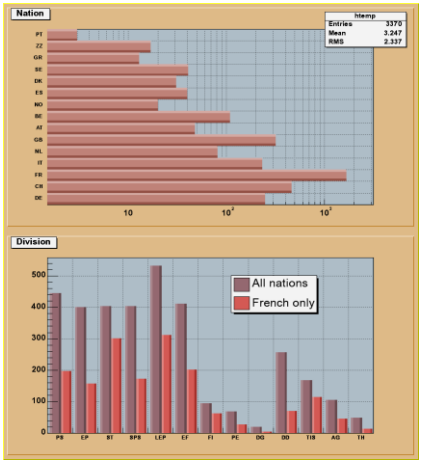
- 1- and 2-dimensional histograms are most common
  - **C**, **S**, **F** and **D** stand for the content type: **D** is double
- Profile histograms are 2-dim histograms "compressed" into 1-dim by calculating mean values
- 3-dimensional histograms are essentially graphs



Examples of histograms



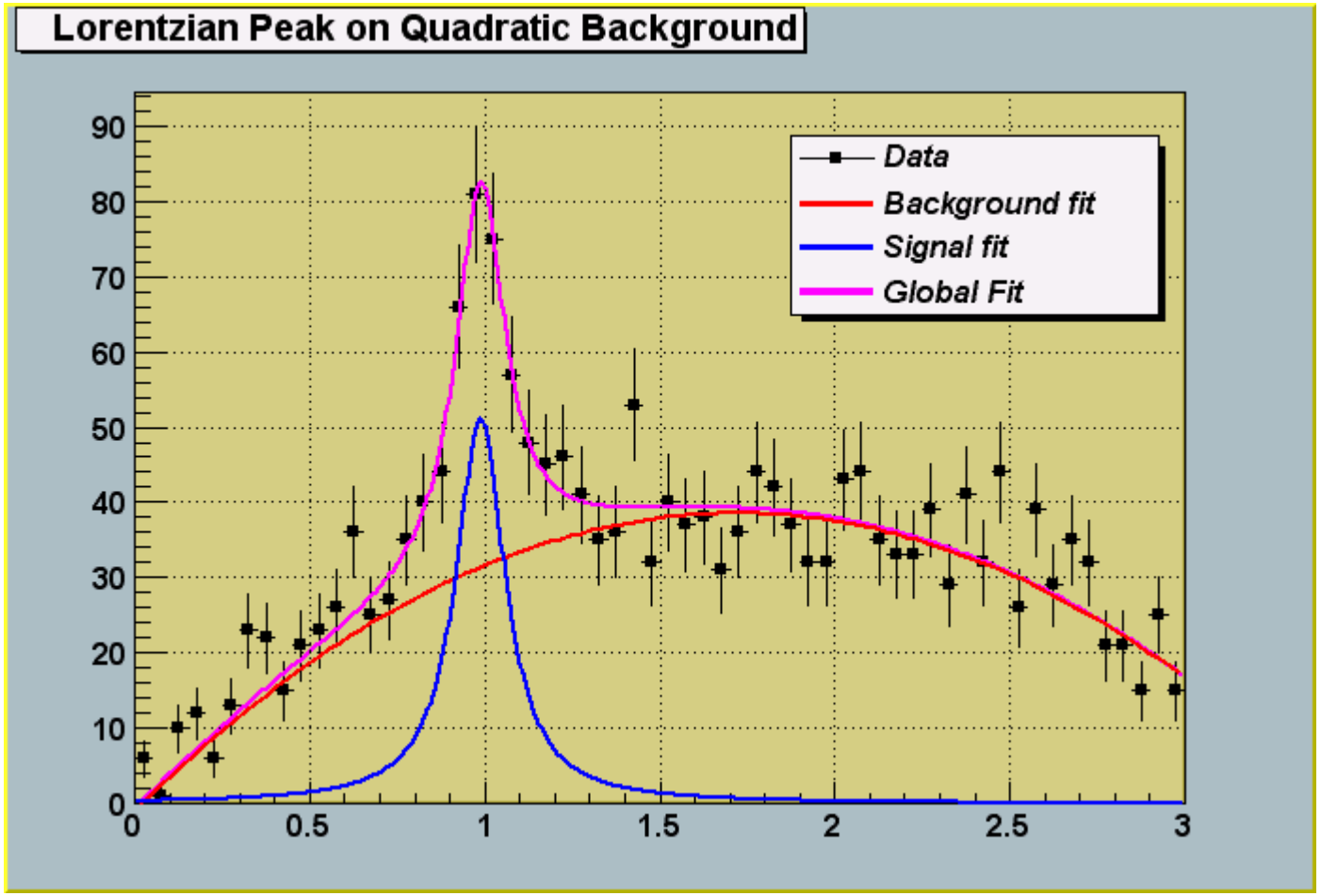




Fitting in ROOT

- Histograms can be fitted with any function via **`TH1::Fit`**. Two fitting algorithms are supported: **Chi-square** method and **Log Likelihood**
- The user functions may be of the following types:
  - standard functions: **`gaus`**, **`landau`**, **`expo`**, **`poln`**
  - combination of standard functions; **`poln + gaus`**
  - A C++ interpreted function or a C++ precompiled function
- An option is provided to compute the integral of the function bin by bin instead of simply compute the function value at the center of the bin.
- When an histogram is fitted, the resulting function with its parameters is added to the list of functions of this histogram. If the histogram is made persistent (saved as a file), the list of associated functions is also persistent.
- One can retrieve the function/fit parameters with calls such as:
  - `Double_t chi2 = myfunc->GetChisquare();`
  - `Double_t par0 = myfunc->GetParameter(0);` //value of 1st parameter
  - `Double_t err0 = myfunc->GetParError(0);` //error on first parameter

Fitting example



Random numbers and histograms

- **`TH1::FillRandom`** can be used to randomly fill an histogram using either of:
  - the contents of an existing **`TF1`** analytic function
  - another histogram

- Example: the following two statements create and fill an histogram 10000 times with a default Gaussian distribution of mean 0 and sigma 1:

```
TH1F h1("h1","histo from a gaussian",100,-3,3);
h1.FillRandom("gaus",10000);
```

- **`TH1::GetRandom`** can be used to return a random number distributed according the contents of an histogram

ROOT data format

- ROOT uses an own data format to store data (called **root**)
- A root-file has a tree-like structure, much like a directory:
  - Has sub-directories, can have many levels
  - Instead of files, it has objects – e.g. histograms
- A root-file is stored in a machine-independent format, so can be used on Linux or Windows without conversion
- File structure:
  - Each file has a header, containing information about the file and records in it
  - Header is followed by the top directory description (name, timestamp etc)
  - It is followed by histogram records
    - Each such record also has a header
  - Next comes Class Description List
    - ROOT stores data and classes in the same file!
  - Last three entries are the list of keys, list of free segments, and the address where the data end

ROOT I/O: reading and writing data

- **`Tfile`** creates a new file or opens an existing file
  - By default, an existing file is opened read-only

Program Writing

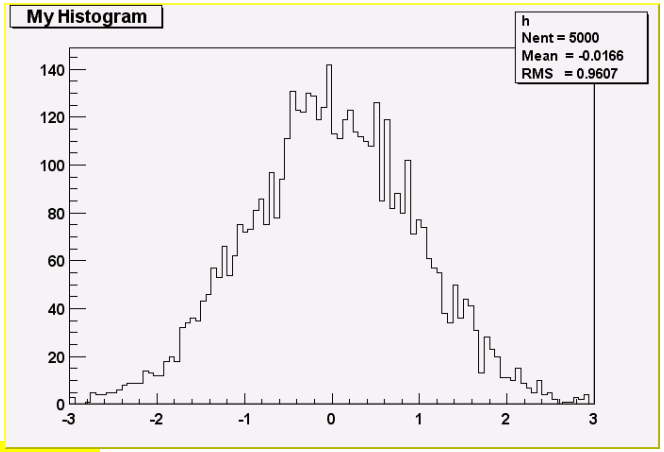
demoh.C

```
TFile f("example.root","new");
TH1F h("h","My histogram",100,-3,3);
h.FillRandom("gaus",5000);
h.Write();
```

Program Reading

demohr.C

```
TFile f("example.root");
TH1F *h = (TH1F*)f.Get("h");
h->Draw();
f.Map();
```

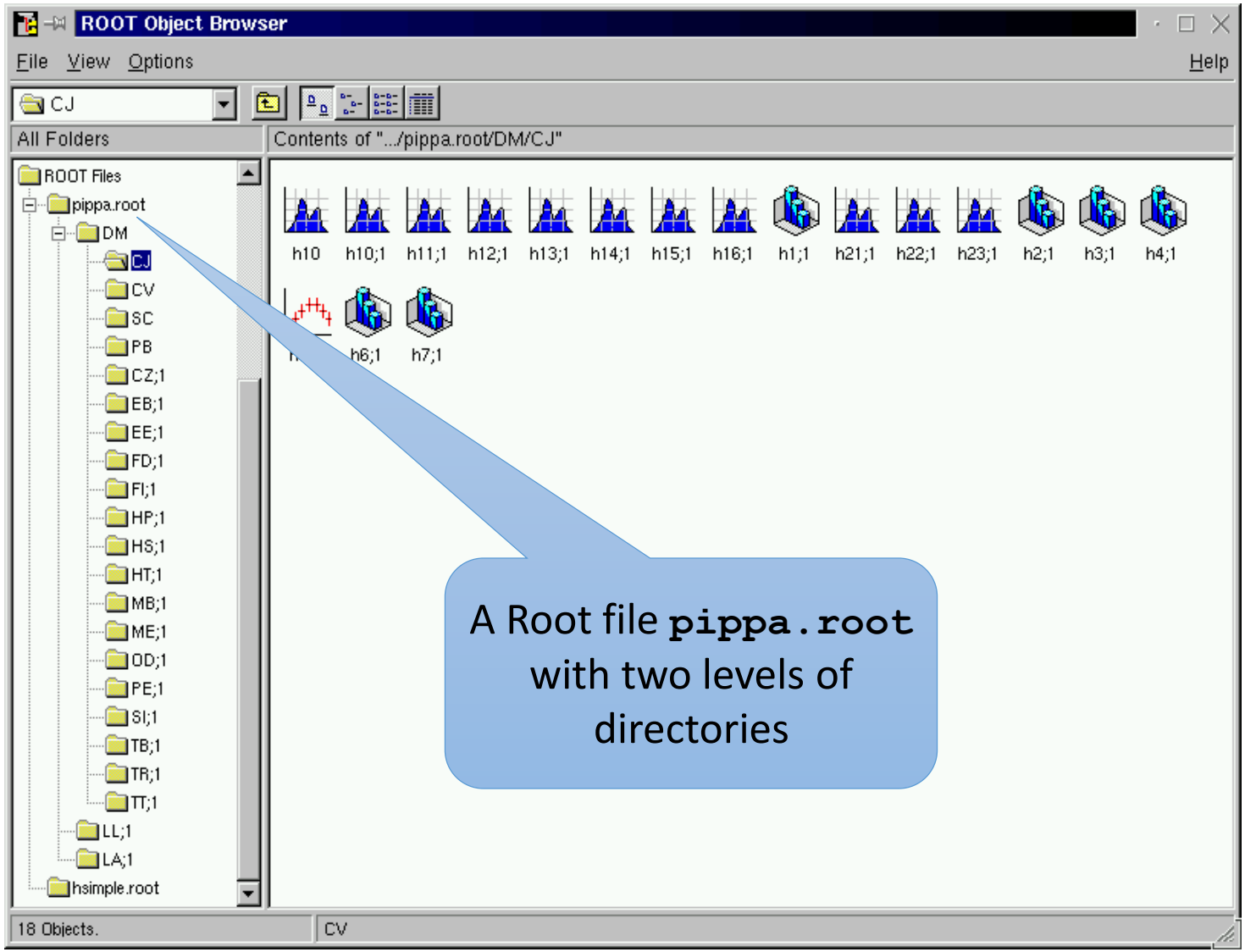



```
20010831/171903  At:64     N=90     TFile
20010831/171941  At:154    N=453    TH1F          CX =  2.09
20010831/171946  At:607    N=2364   StreamerInfo  CX =  3.25
20010831/171946  At:2971   N=96     KeysList
20010831/171946  At:3067   N=56     FreeSegments
20010831/171946  At:3123   N=1      END
```

`Map()` prints timestamp, address of the record start, nr. of bytes in the record, its class name and compression factor

ROOT file browser

- Objects in a file (e.g. histograms) can be browsed and manipulated using a GUI



ROOT can open files remotely

```
• TFile *f1 = TFile::Open("local.root")

• TFile *f2 = TFile::Open("root://cdfsga.fnal.gov/bigfile.root")

• TFile *f3 = TFile::Open("rfio:/castor.cern.ch/alice/aap.root")

• TFile *f4 = TFile::Open("dcache://main.desy.de/h1/run2001.root")

• TFile *f5 = TFile::Open("chirp://hep.wisc.edu/data1.root")

• TFile *f5 = TFile::Open("http://root.cern.ch/geom/atlas.root")
```

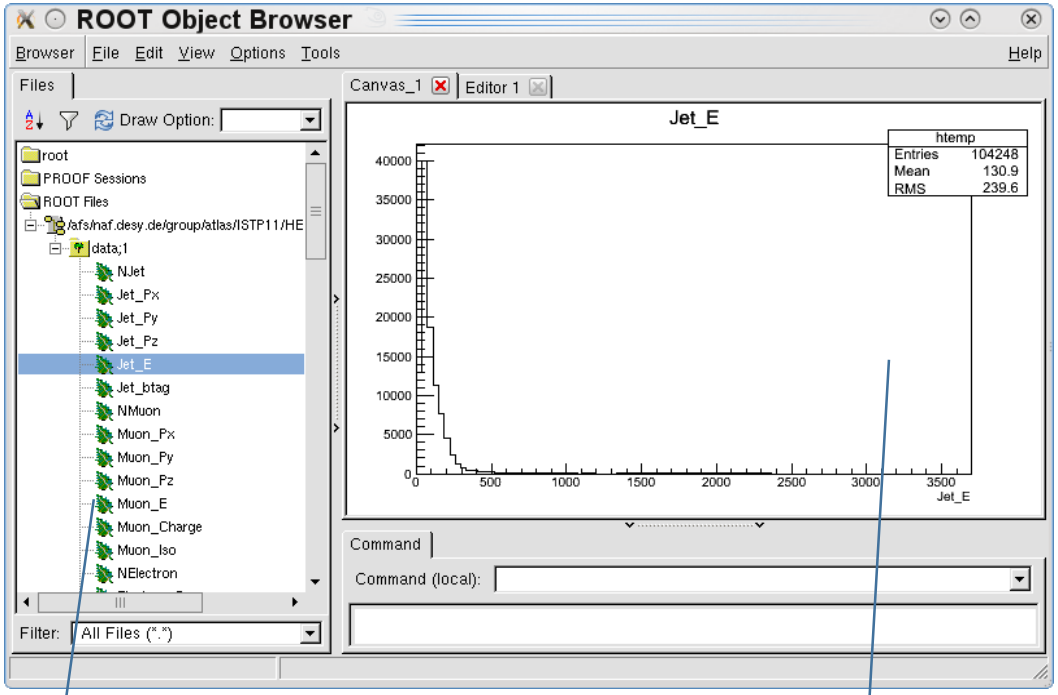
Saving your pictures

- A pad/canvas may be saved in many formats using either the GUI menu or via **`TPad::SaveAs`** function. Possible formats are:
  - **`canvas.C`** : a C++ script is automatically generated. The canvas may be generated again via **`.x canvas.C`** – good for re-producing your figures
  - **`canvas.ps(eps)`** Postscript or Encapsulated PS
  - **`canvas.svg`** : Scalable Vector Graphics
  - **`canvas.gif`**
  - **`canvas.root`**: keep objects in the ROOT format

But how does ROOT store data?

- Histograms and function plots are not actually data
- Data are stored in complex “tables”
  - Each entry can be a complex structure: a combination of numbers, strings, vectors etc
  - Such “tables” can have structure themselves, like a directory tree
- Simplest data structure in ROOT: **Ntuple**
  - Similar to a spreadsheet or a CSV list
  - Each “row” is one entry, and each column corresponds to a variable
    - Each variable belongs to a separate **branch**
    - Restricted to `float` variables, and maximum of 12 variables
- If the data are complex, and many variables need to be recorded, ROOT **Tree** must be used
  - Ntuple on steroids
  - Unlimited amount of branches
  - Any variable type
  - Many other advanced features, outside the scope of this lecture

Example of a ROOT tree in the browser



Variables (leaves on branches)

Simply click on a variable to plot its values across entire tree

More ROOT goodies

latex3.C

Full LateX support on screen and postscript

Formula or diagrams can be edited with the mouse

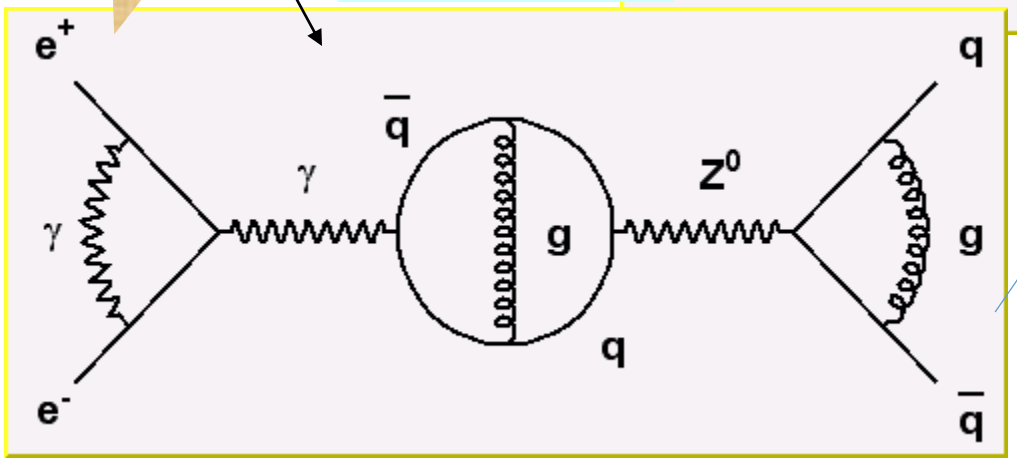
Born equation

$$\frac{2s}{\pi\alpha^2}\frac{d\sigma}{d\cos\theta}(e^+e^- \to f\bar{f}) = \left|\frac{1}{1-\Delta\alpha}\right|^2 (1+\cos^2\theta)$$

$$+ 4\,\mathrm{Re}\left\{\frac{2}{1-\Delta\alpha}\chi(s)\left[\tilde{g}_v^{e}\tilde{g}_v^{f}(1+\cos^2\theta) + 2\,\tilde{g}_a^{e}\tilde{g}_a^{f}\cos\theta\right]\right\}$$

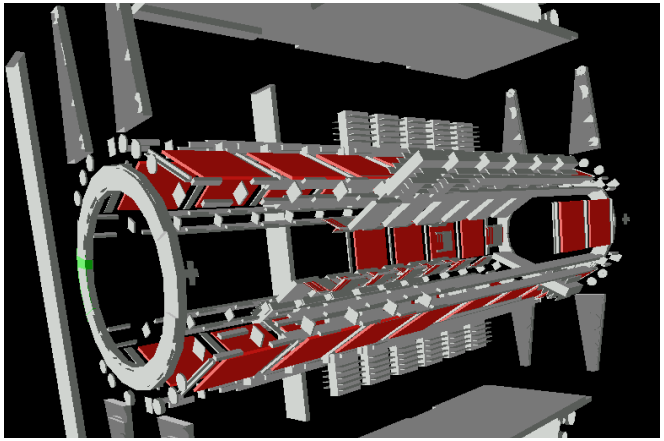
$$+ 16\left|\chi(s)\right|^2\left[(\tilde{g}_a^{e2} + \tilde{g}_v^{e2})(\tilde{g}_a^{f2} + \tilde{g}_v^{f2})(1+\cos^2\theta) + 8\,\tilde{g}_a^{e}\tilde{g}_a^{f}\tilde{g}_v^{e}\tilde{g}_v^{f}\cos\theta\right]$$

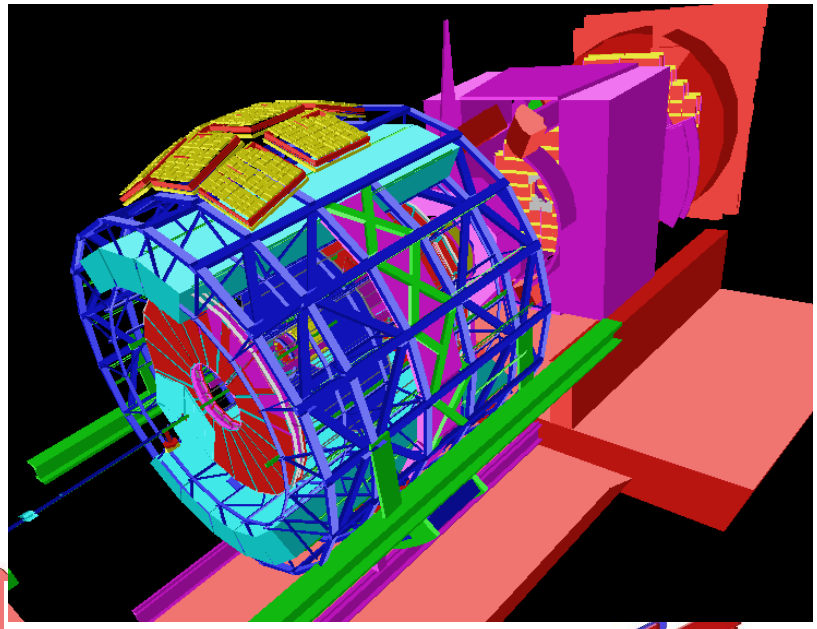
Feynman.C

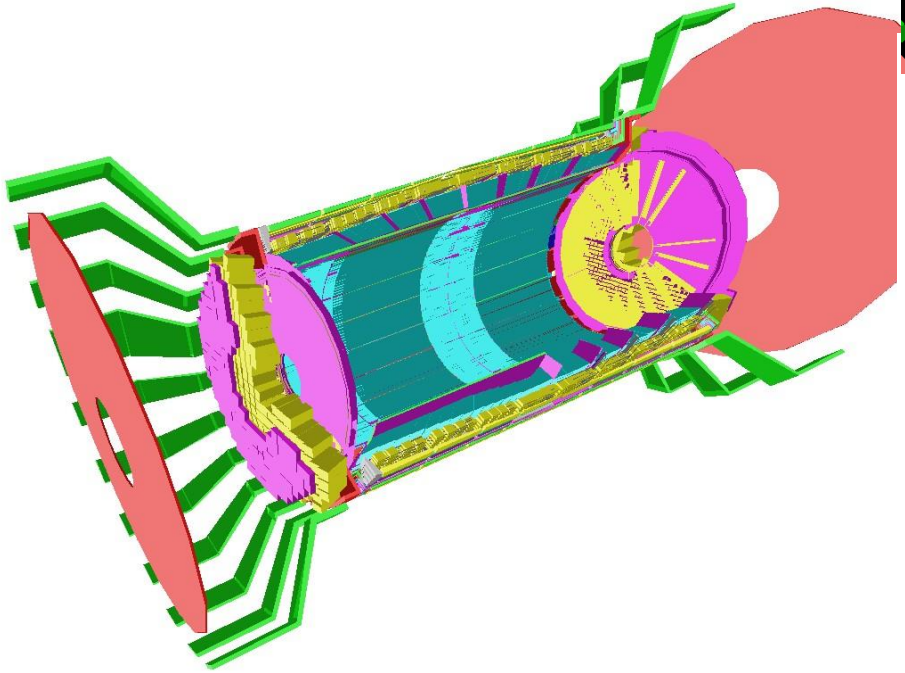


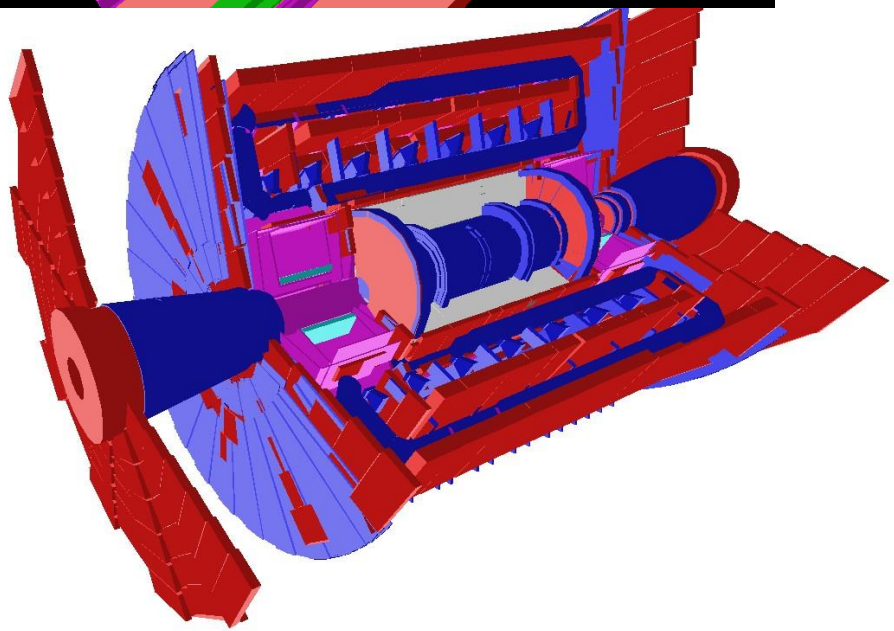
TCurlyArc
TCurlyLine
TWavyLine
and other building blocks for Feynman diagrams

Volume graphics in ROOT

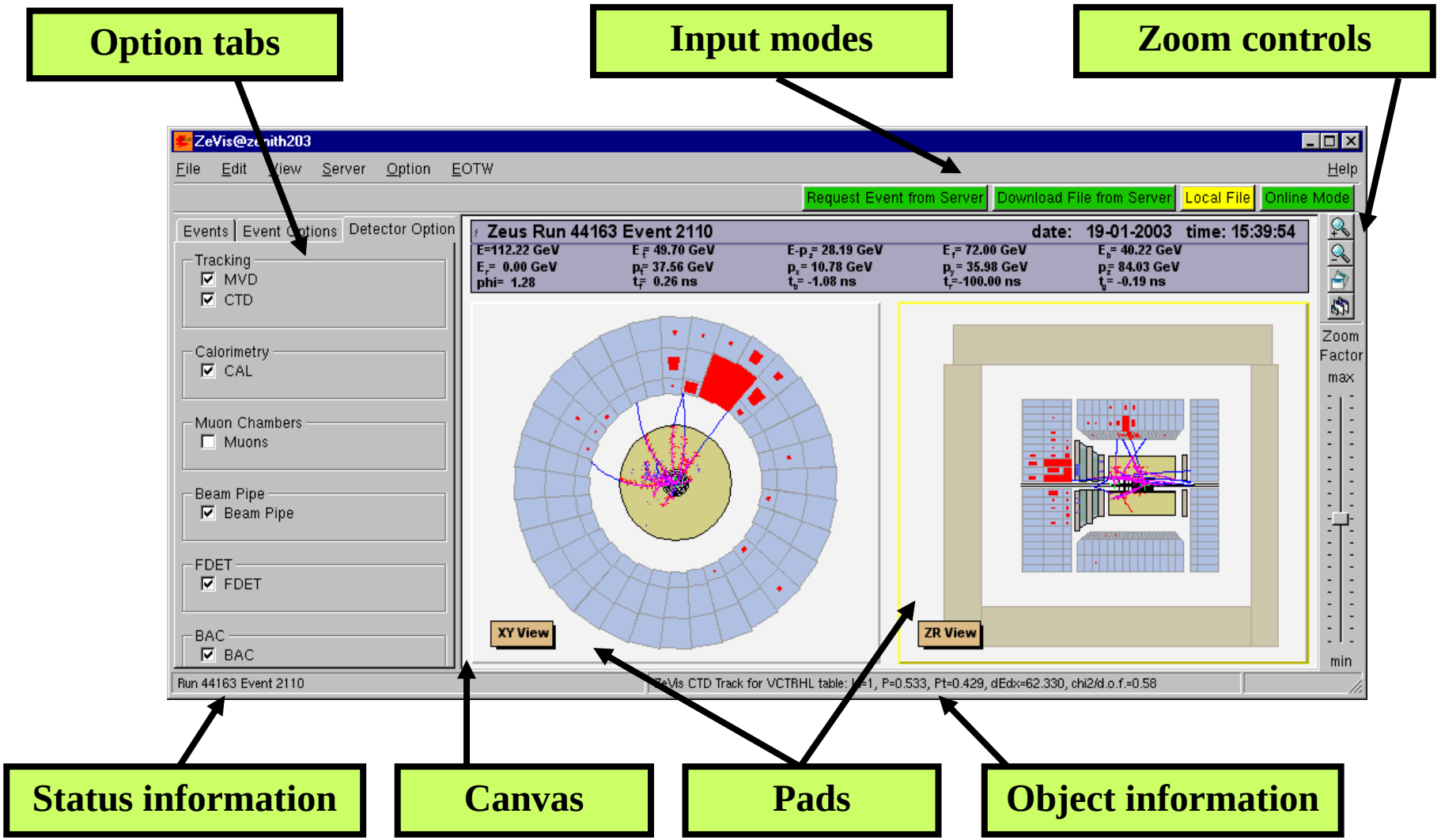








Event display tool written in ROOT



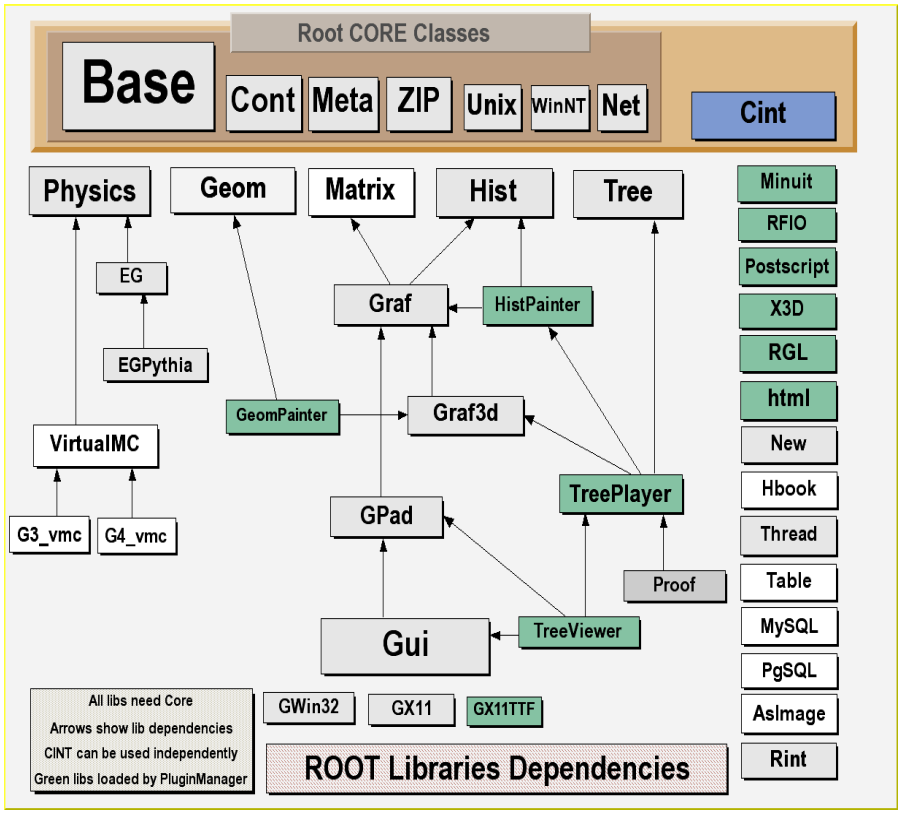
Summary of ROOT services and utilities

- Histogramming and Fitting
- Graphics (2D, 3D)
- Input/Output to file or socket: specialized for histograms, **Ntuples** (Trees)
- Collection Classes and Run Time Type Identification
- User Interface
  - GUI: Browsers, Panels, Tree Viewer
  - Command Line interface: C++ interpreter **CINT**
  - Script Processor (C++ compiled $\leftrightarrow$ C++ interpreted

A little bit extra: ROOT library structure

- ROOT libraries are a layered structure
- The CORE classes are always required (support for RTTI, basic I/O and interpreter)
- The optional libraries (you load only what you use) Separation between data objects and the high level classes acting on these objects. Example, a batch job uses only the histogram library, no need to link histogram painter library.
- Shared libraries reduce the application link time
- Shared libraries reduce the application size
- ROOT shared libraries can be used with other class libraries

The libraries

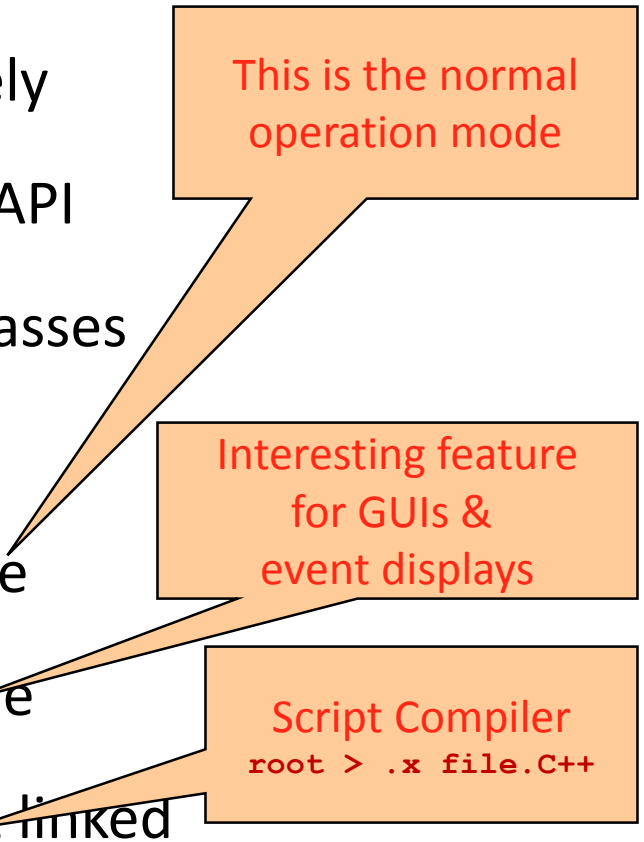


- Over 700 classes

- 950,000 lines of code
- CORE (10 Mbytes)
- CINT (3 Mbytes)
- Green libraries linked on demand via plug-in manager (only a subset shown)

ROOT: a Framework and a Library

- User classes
  - User can define new classes interactively
  - Either using calling API or sub-classing API
  - These classes can inherit from ROOT classes
- Dynamic linking
  - Interpreted code can call compiled code
  - Compiled code can call interpreted code
  - Macros can be dynamically compiled & linked



Dynamic linking in ROOT

A Shared Library can be linked dynamically to a running executable module

- either via explicit loading,
- or automatically via plug-in manager

A Shared Library facilitates the development and maintenance phases

Dynamic linking from Shared libraries

The "standard" ROOT executable module can dynamically load user's specific code from shared libraries.

```
Root >  gSystem->Load("libNA49")
Root >  gSystem->Load("libUser")
Root >  T49Event event
Root >  event.xxxxxxx
```