

PyROOT: Seamless Melting of C++ and Python

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ROOT

- ❖ “At the root of the experiments”, project started in 1995

- ❖ Open Source project (LGPL2)

 - ❖ mainly written in C++; 4 MLOC

- ❖ ROOT provides (amongst other things):

 - ❖ C++ interpreter, Python bindings

 - ❖ Efficient data storage mechanism

 - ❖ Advanced statistical analysis algorithms

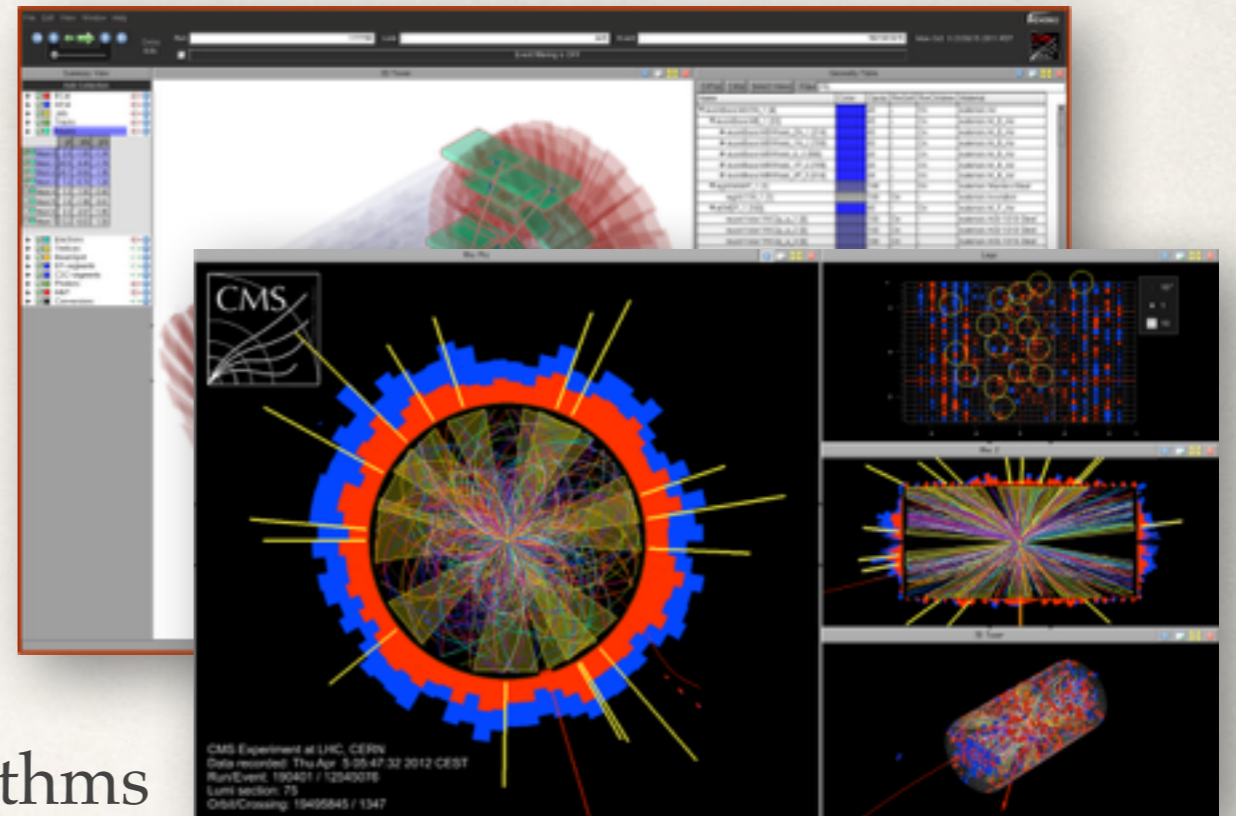
 - ❖ histogramming, fitting, minimization, statistical methods ...

 - ❖ Multivariate analysis, machine learning methods

 - ❖ Scientific visualization: 2D/3D graphics, PDF, Latex

 - ❖ Geometrical modeler

 - ❖ PROOF parallel query engine

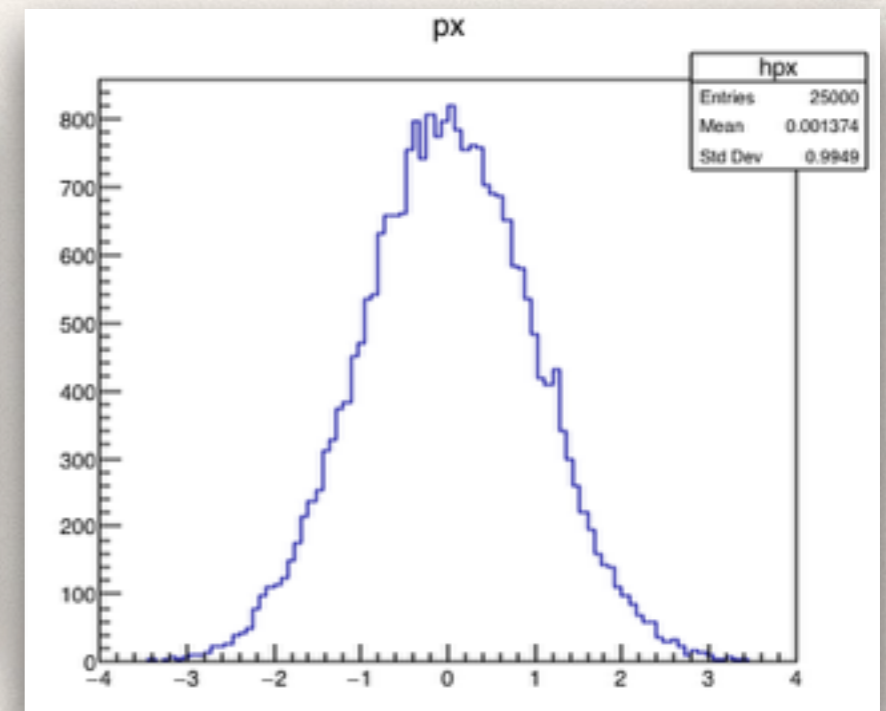


<http://root.cern.ch>

PyROOT

- ❖ The ROOT Python extension module (PyROOT) allows users to interact with any C++ class from Python
 - ❖ Generically, without the need to develop specific bindings
 - ❖ Mapping C++ constructs to Python equivalent
- ❖ Give access to the whole Python ecosystem

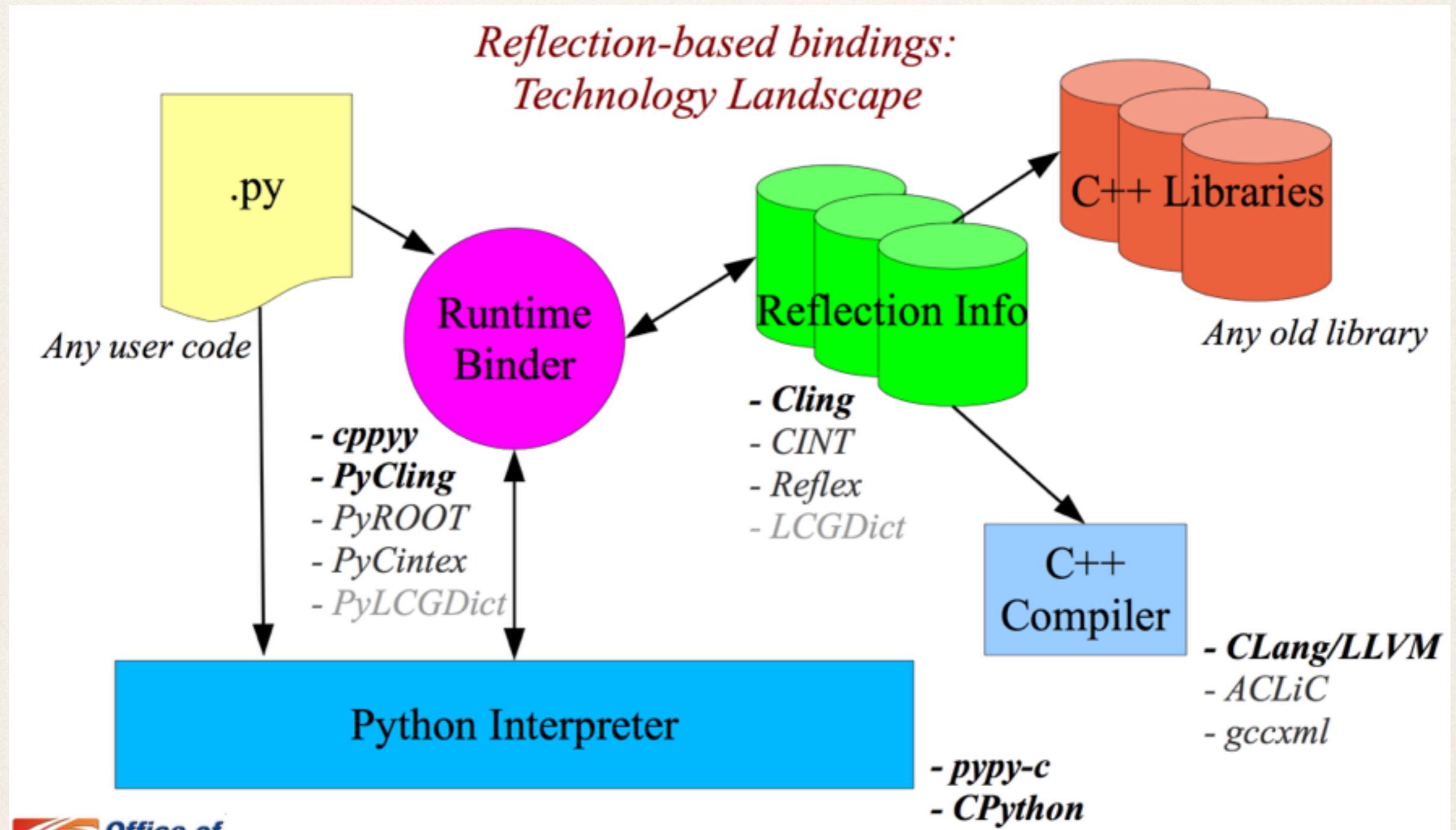
```
# Example: displaying a ROOT histogram from Python  
from ROOT import gRandom, TCanvas, TH1F  
c1 = TCanvas('c1', 'Example', 200, 10, 700, 500)  
hpx = TH1F('hpx', 'px', 100, -4, 4)  
for i in xrange(25000):  
    px = gRandom.Gaus()  
    i = hpx.Fill(px)  
hpx.Draw()
```



Why PyROOT is Special?

- ❖ Python bindings based on C++ reflexion information
 - ❖ Python classes are created dynamically when needed
 - ❖ C++ globals and functions appear automatically in Python
 - ❖ Much less work than using binding tools (e.g. boost, swig)
- ❖ Uniform mapping of C++ idioms to Python equivalent
 - ❖ Same behavior everywhere
 - ❖ Essential for managing large code bases
- ❖ Standard “Pythonizations” of C++ classes and constructs
- ❖ Two-way interaction
 - ❖ Calling Python from C++, and calling C++ from Python

Reflexion-Based Bindings



C++ to Python Mapping

C++	Python
basic_types: short, int, float, double, std::string, char*, ...	int, [long], float, str
basic_type*, C-array	array (module)
class, template class	class, class generator
STL classes	std.vector, std.list, std.shared_ptr,...
inheritance, dynamic_cast	inheritance, always final type
namespace	scope (dictionary)
pointer, reference	reference
exceptions	exceptions

Memory Management

- ❖ Python handles memory for the user by employing reference counting and a garbage collection. In C++ memory handling is done by hand or by a 'framework'
- ❖ Two global policies: *heuristics[default]* and *strict*
- ❖ For the *heuristic* policy the following rules are observed:
 - ❖ An object created on the python interpreter side is owned by python and will be deleted once the last python reference to it goes away
 - ❖ An object coming from a call is not owned. When the object goes out of scope on the C++ side, the python object will change type into an object that largely behaves like None
- ❖ Ownership can be set/relinquish for individual objects

Function Overloading

- ❖ A single Python function acts as a proxy to the set of overloaded C++ functions

```
void func(int) { cout << "func(int) called" << endl;}
void func(double) { cout << "func(double) called" << endl;}
void func(int, double) { cout << "func(int, double) called" << endl;}
```

```
from ROOT import func
func(10)
func(9.9)
func(1,2.)
```

```
func(int) called
func(double) called
func(int, double) called
```

```
func('a')
```

```
-----
TypeError                                 Traceback (most recent call last)
<ipython-input-6-fa56e76b52e2> in <module>()
----> 1 func('a')

TypeError: none of the 3 overloaded methods succeeded. Full details:
void ::func(int) =>
    could not convert argument 1 (int/long conversion expects an integer object)
void ::func(double) =>
    could not convert argument 1 (a float is required)
void ::func(int, double) =>
    takes at least 2 arguments (1 given)
```


Running Python from ROOT

- * ROOT user can run any Python command and eventually switch to the python prompt from the ROOT prompt
- * The interpreter state will be preserved in between calls

```
root [0] TPython::Exec( "print 1 + 1" )
2
root [1] b = TPython::Eval( "TBrowser()" )
(class TObject*)0x8d1daa0
root [2] TPython::Prompt()
>>> i = 2; ^D
root [3] TPython::Prompt()
>>> print i
2
```

Python Callbacks

```
from ROOT import TF1, TH1F, TCanvas

class Linear:
    def __call__( self, x, par ):
        return par[0] + x[0]*par[1]

# create a linear function for fitting
f = TF1( 'pyf3', Linear(), -1., 1., 2 )

# create and fill a histogram
h = TH1F( 'h', 'test', 100, -1., 1. )
f2 = TF1( 'cf2', '6.+x*4.5', -1., 1. )
h.FillRandom( 'cf2', 10000 )

# fit the histo with the python 'linear' function
h.Fit( f )

# print results
par = f.GetParameters()
print 'fit results: const =', par[0], ', pitch =', par[1]
```

E.g. Fit
function in
Python

```
FCN=115.87 FROM MIGRAD      STATUS=CONVERGED      29 CALLS      30 TOTAL
                        EDM=1.68681e-15  STRATEGY= 1      ERROR MATRIX ACCURATE
EXT PARAMETER
NO.   NAME      VALUE      ERROR      STEP      FIRST
      NAME      VALUE      ERROR      SIZE      DERIVATIVE
  1   p0      9.88413e+01  9.94190e-01  4.56265e-03  6.71977e-08
  2   p1      7.55552e+01  1.53812e+00  7.05889e-03 -2.14706e-08
fit results: const = 98.8412955492 , pitch = 75.5551735795
```

Python inheriting from C++ class

```
class Base {  
    ...  
    virtual void Foo() { cout << "base::Foo" << endl; }  
    void CallFoo() { this->Foo(); }  
};  
  
class PyBase : public Base { ... };
```

C++

Adaptor
class

```
class PyDerived(ROOT.PyBase):  
    def __init__(self): ROOT.PyBase.__init__(self, self)  
    def Foo(self): print 'Python::Foo'
```

Python

```
d = PyDerived()  
d.CallFoo()  
o = ROOT.Base()  
o.CallFoo()
```

```
Python::Foo  
base::Foo
```

CLING

- * Replaces CINT: a radical change at the core of ROOT
- * Based on LLVM and CLANG libraries.
 - * Piggy back on a production quality compiler rather than using an old C parser
 - * Future-safe - CLANG is an active C++ compiler
 - * Full support for C++11 / 14 with carefully selected extensions
 - * Script's syntax is much stricter (proper C++)
 - * Use a **C++ just in time compiler (JIT)**
 - * A C++11 package (e.g. needs at least gcc 4.8 to build)
- * Support for more architectures (ARM64, PowerPC64)

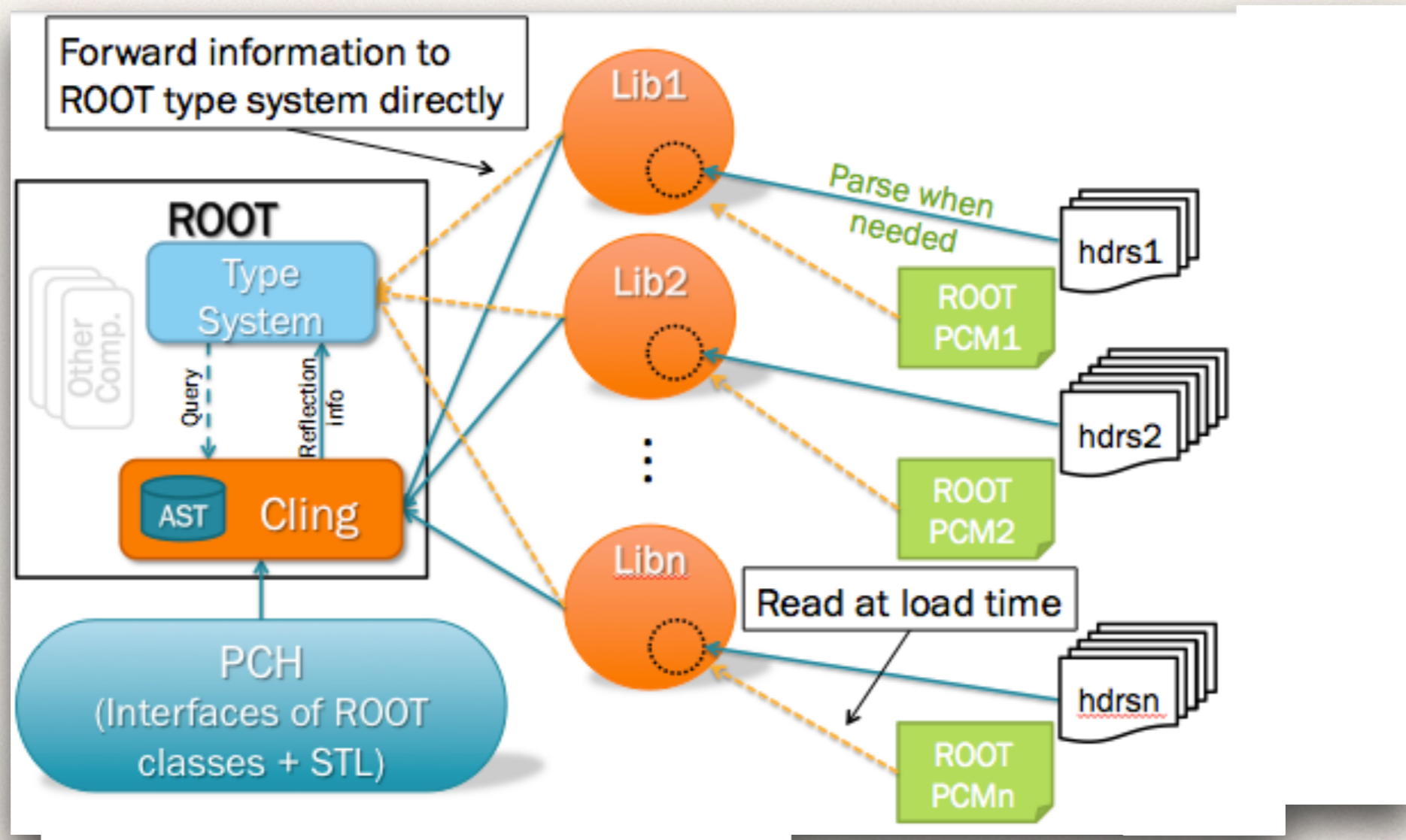


Clang, the AST and ROOT

- * C++ entities in Clang: **Abstract Syntax Tree (AST)**
 - * Classes, functions, templates, statements ...
 - * Exists in memory and can be persisted on disk in two forms:
 - * 1) **Pre-Compiled Header**: can load only one, file granularity
 - * 2) **Pre-Compiled Modules**: can load many, AST node granularity
 - * Both queried lazily by the compiler
- * Original ROOT6 design: AST source of information for
 - * ROOT Dictionaries: a thin layer around portions of AST
 - * Reflection and I/O
 - * Interactive function calls

Evolution Reflex/CINT -> CLING

- ❖ With ROOT 6 CLING replaces CINT
- ❖ PyROOT has been adapted to the new way to obtain reflection information



Python with JIT Reflection

```
#include <iostream>
class A {
public:
    A(const char* n) : m_name(n){}
    void printName() {std::cout<< m_name
                        << std::endl;}

private:
    const std::string m_name;
};
int dummy() {return 42;}
```

A.h

No need for dictionaries!!

```
import ROOT
ROOT.gInterpreter.ProcessLine('#include "A.h"')
a = ROOT.A('my name')
a.printName()
ROOT.dummy()
```

python

Great potential for 3rd party libraries

42

my name

C++11

many C++11 keywords
and concepts

C++

```
constexpr int data_size() { return 5; }  
auto N = data_size();  
  
template<class L, class R> struct MyMath {  
    static auto add(L l, R r) -> decltype(l+r) { return l+r; }  
};  
  
template class MyMath<int, int>;
```

```
print 'N =', ROOT.N  
print '1+1 =', ROOT.MyMath(int, int).add(1,1)
```

Python

```
N = 5  
1+1 = 2
```


Recent Features

- ❖ Multiple virtual inheritance fully supported
 - ❖ Uses clang AST to get the relative offsets
- ❖ New C++11 declarations (resolve to simpler terms)
 - ❖ E.g. auto \rightarrow real type after the compiler is done with it
- ❖ C++11 implementations not visible to bindings
 - ❖ \Rightarrow automatically okay
- ❖ Python3 support
 - ❖ Almost completed the support for recent versions of Python
 - ❖ LHC experiments using Python 2.x

Pythonizations

- ❖ PyROOT is mostly about automatic bindings
 - ❖ Sine qua non: unwieldy and unmaintainable otherwise
- ❖ Dictionaries (incl. for experiment data) widely available
 - ❖ and maintained for I/O and CLING in experiment releases
- ❖ Automatic bindings often feel too much like C++
 - ❖ Some C++ idiosyncrasies still visible
 - ❖ Memory management is not 100% solved
- ❖ Some limited, still generic, **Pythonizations** exist
 - ❖ E.g. TFn, TTree, looping over `std::vector`, etc.
- ❖ Other packages such as *rootpy* provides a more pythonic ROOT

Pythonization Examples

```
from ROOT import vector
v = vector(str)()
v.push_back('a')
v.push_back('b')
v.push_back('c')
for c in v:
    print c
```

```
a
b
c
```

iterators

```
from ROOT import std, TH1, TH1F
p = std.shared_ptr<TH1>()
if not p : p = TH1F()
p
```

```
<ROOT.TH1F object at 0x10130a810>
```

shared
pointers

Pythonization Examples

```
mymap = ROOT.map(str,int)()
mymap['a'] = 1
mymap['b'] = 2
```

operator []

```
print mymap
for label, value in mymap:
    print label,value
```

iterators
std<pair> to tuple

```
<ROOT.map<string,int> object at 0x11c9a9790>
a 1
b 2
```

```
print len(mymap)
```

```
2
```

std::map::size()

Performance

```
for i in xrange(100): # make it measurable
    sumAge = 0
    for entry in tree:
        sumAge += entry.Age
print sumAge
```

Python

```
158151
CPU times: user 1.64 s, sys: 181 ms, total: 1.82 s
Wall time: 1.74 s
```

```
int sumAge;
for( int i = 0; i < 100; i++) { // make it measurable
    TTreeReader reader(tree);
    TTreeReaderValue<int> age(reader, "Age");
    sumAge = 0;
    while (reader.Next()) {
        sumAge += *age;
    }
}
cout << sumAge << endl;
```

C++

```
158151
CPU times: user 51.9 ms, sys: 2.74 ms, total: 54.6 ms
Wall time: 54.8 ms
```

example reading a TTree
(cernstaff.root)

No surprise, C++ is
much faster!!

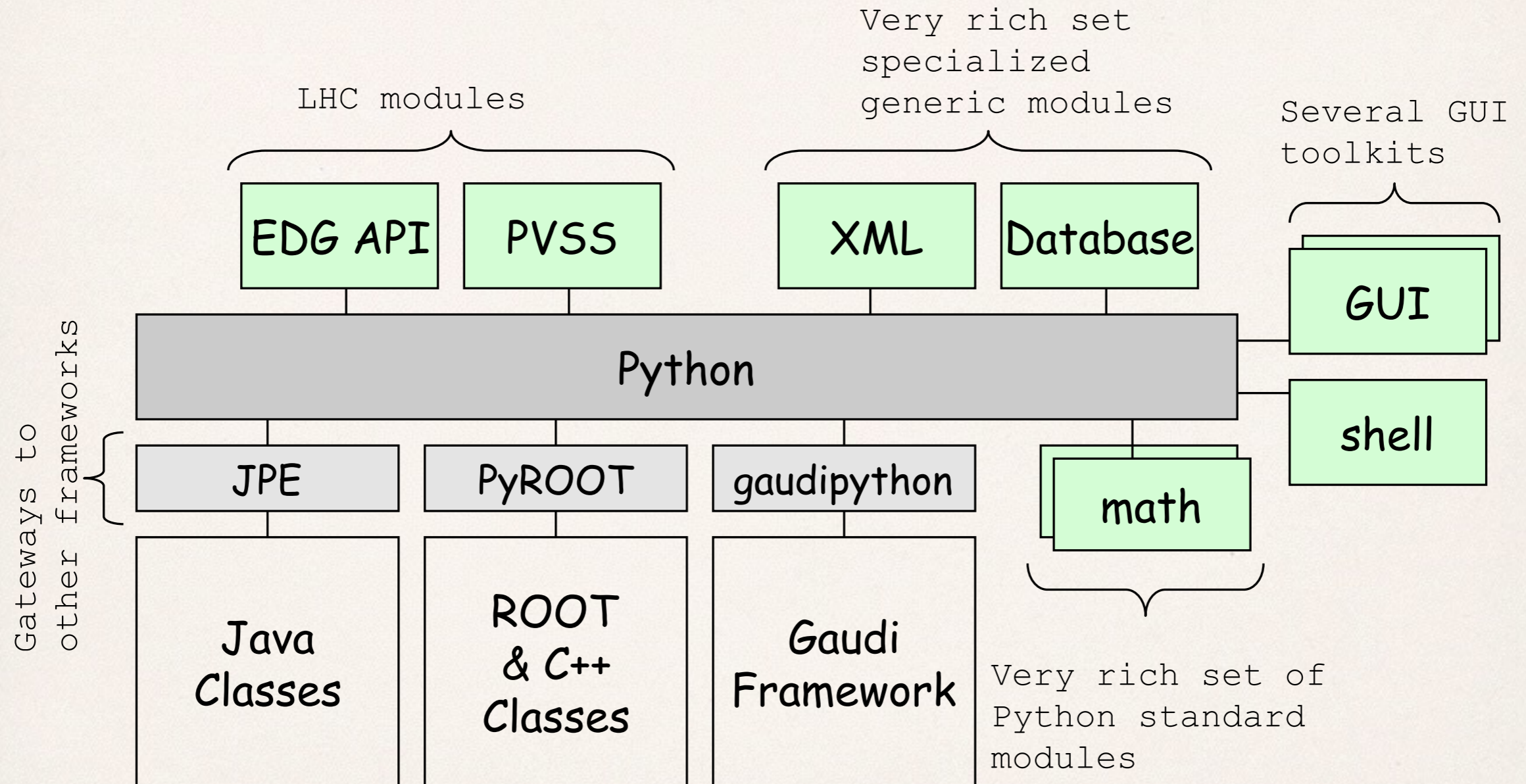
Functional Chains

- * Prototyping some ideas of 'declarative / functional' chains of basic concepts such as map, filter, reduce, accumulate, etc.
 - * Inspired from data analytic tools such as Spark
- * The user specifies the **What** and system chooses **How**
 - * Actions are only triggered at the end of the chain
 - * Great opportunity for optimizations (partitioning, caching, re-ordering, etc.)

```
hist = ttree.filter(lambda event: event.Emiss > 40)
          .flatMap(lambda event: event.tracks)
          .map(lambda track: sqrt(px**2 + py**2))
          .histo(100, 0, 20)
```

The chain is only executed when is completed

Python as a Software Bus



Conclusions

- ❖ PyROOT provides a very complete and generic binding between C++ and Python (not limited to ROOT classes)
 - ❖ See next two talks for applications of PyROOT in different domains
- ❖ PyROOT has been delivering good service to many physicists that prefer to use Python for interacting with ROOT
 - ❖ Difficult to assess the adoption level
 - ❖ From last survey, ~52% of ROOT users use the Python interface
- ❖ The JIT compilation coming with ROOT 6 provides even a more flexible and dynamic interface
 - ❖ JIT can help to recover the bad performance of interpreted Python by generating code for the “loops” and “number crunching”