Adapting C++ for Data Science

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What do we do with existing code written in C++?

rm --rf ‘em all?                 Keep expanding them randomly?

HEP has \( \sim O(20M) \) LoC written in C++

How often do you use Python relative to C/C++?

More Python

Half-and-half

More C++

Always C++

Neither

Always Python

PyHEP 2020, J. Pivarski
Tools

“Human brain has not evolved structurally a lot since 17th century however the development of mankind has, because we learned how to build better tools.”

The Printing Press

The Lightbulb

The Internet

(Image credit: Britannica Fine Art Images/Heritage Image/age fotostock)

(Image credit: Terren | Creative Commons)

(Image credit: Creative Commons | The Opte Project)
Language Design Principles

C++
- Efficiency
- Stability
- Backward compatibility

“Prioritizes Performance over Surprise which is sometimes surprising” T. Winters [Link]

Python
- Readability
- Simplicity
- Flexibility

“Special cases aren't special enough to break the rules” Zen of Python [Link]
Talking to a Dataset

Understanding the Language of a Dataset – a multistep, iterative, interactive, exploratory process:

- Interactivity = [human] productivity + *just enough* performance

“Interactive Supercomputing for Data Science“ W. Reus [Link]
Just Enough Performance

```python
def f(N = 100, M = 1000, L = 10000):
    for i in range(N):
        for j in range(M):
            for k in range(L):
                g(i, j, k)
```

Three desirata:
1. A language people already know
2. Covers the whole language, not a subset
3. Delivers bare-metal speed, not just a factor-of-several above X

Approaches:
- JIT compile using Numba – (1) & (3)
- Compile with Pypy – (1) & (2)
- Use a language such as Julia – (2) & (3)
- This talk offers a way to cover (1), (2) and (3)

“The inner loop principle“ J. Pivarski, private exchanges
What Is Python?

• Just enough performance when relying on bare-metal technologies

• NumPy is an enabler for an entire data science ecosystem

• NumPy is very good but sometimes far from bare metal, accelerators and across nodes (means to address the problem such as CuPy or Dask).

“This is why I love C++ and use Python for most of the work I do...”, a happy user on the internet
Brief, Incomplete & Inaccurate History of C++

“One of our main goals for GCC is to prevent any parts of it from being used together with non-free software. Thus, we have deliberately avoided many things that might possibly have the effect of facilitating such usage, even if that consequence wasn’t a certainty.” RMS

“LLVM Irrelevant”

“LLVM Just-In-Time Compiler”

“LLVM In-Time Compiler”

“One of our main goals for GCC is to prevent any parts of it from being used together with non-free software. Thus, we have deliberately avoided many things that might possibly have the effect of facilitating such usage, even if that consequence wasn’t a certainty.” RMS
Brief, Incomplete & Inaccurate History of C++

Relaxed constexpr, consteval, variable templates, mutexes, locking, nested namespaces, structured bindings, concepts, modules,

C++14-23

Tools supporting Data Science

Cling: The First C++11-compliant Interpreter

Lambdas, automatic type deduction, uniform initialization, nullptr, deleted and defaulted function, rvalue references, smart pointers, threading, new algorithms C++11

libc++, lld, lldb, clang-SA, clang-tidy, clang-format, llvm-jit, jitlink, address-, mem-, thread-, dataflow san bolt, ...

LLVM

2007

2011

2012

2017

2019

2022

Improvements in performance, usability without breaking existing code

C considers evolving faster!

Software engineer cost

HEP’s Contribution

LLVM Just-In-Time Compiler

28-Oct-2022

V.Vassilev – Adapting C++ for Data Science
My Pillars of Data Exploration

Recent C++ tool advancement is an enabling factor for:

• Interactive C/C++
• Automatic Language Interoperability
• Advanced bare-metal toolbox
Exploratory Programming With Interactive C++
Interactive C++. Key Insights

- Incremental Compilation
- Handling errors
  - Syntactic
  - Semantic
- Execution of statements
- Displaying execution results
- Entity redefinition

```cpp
#include <vector>
std::vector<int> v = {1,2,3,4,5};
std::sort(v.begin(), v.end()); // No semicolon
(std::vector<int> &){ 1, 2, 3, 4, 5 }
std::string v = "Hello World";
```
C++ in Notebooks

Xwidgets – User-defined controls

S. Corlay, Quantstack, Deep dive into the Xeus-based Cling kernel for Jupyter, May 2021, compiler-research.org
Interactive CUDA C++

S. Ehrig, HZDR, *Cling’s CUDA Backend: Interactive GPU development with CUDA C++*, Mar 2021, compiler-research.org
Interpreting C++. Cling

libClang

C/C++ Input

text

ast

transformations

LLVM JIT

MC (x86, NVPTX, ...)

GPGPU

CPU
Compiler (C++) As A Service

- Static Compiler
  - Abstract machine
  - Abstract user
  - Produced binary
  - Ahead of Time
  - Continuous Optimization (LLVM's OrcV2)
  - PGO

- In-Process Compiler As A Service
  - Binary started
  - Just-in-Time
  - Target machine
  - Concrete user(s)
  - Binary execution
  - Optimize
  - Deploy
  - Start
  - Execute

- Ahead of Time
- Just-in-Time
- Continuous Optimization

- Abstract user
- Concrete user(s)
- Deploy
- Start
- Execute
- Optimize
- Produced binary
- Binary started
- Binary execution
CaaS. Programming Model

```cpp
/// Call an interpreted function using its symbol address.
void callInterpretedFn(cling::Interpreter& interp) {
  // Declare a function to the interpreter. Make it extern "C"
  // to remove mangling from the game.
  interp.declare("#pragma cling optimize(1)

  extern "C" int cube(int x) { return x * x * x; }");

  void* addr = interp.getAddressOfGlobal("cube");

  using func_t = int(int);
  func_t* pFunc = cling::utils::VoidToFunctionPtr<func_t*>(addr);

  std::cout << "7 * 7 * 7 = " << pFunc(7) << 'n';
}
```

```cpp
// caas-demo.cpp
// g++ ... caas-demo.cpp; ./caas-demo
int main(int argc, const char* const* argv) {
    cling::Interpreter interp(argc, argv, LLVMDIR);

    callInterpretedFn(interp);

    return 0;
}
```

vvassilev@vv-nuc ~/.../builddir $ ./caas-demo
7 * 7 * 7 = 343
vvassilev@vv-nuc ~/.../builddir $
Automatic Language Interoperability
Automatic Language InterOp. Python

Performance Compared to Static Approaches

- No fundamental CPU performance difference

Note carefully that *everything* in Python is runtime: compile-time just means that the bindings *recipe* is compiled, not the actual bindings themselves!

- But heavy Cling/LLVM dependency:
  - ~25MB download cost; ~100MB memory overhead
  - Complex installation (and worse build)

Basic Performance Test: overload

<table>
<thead>
<tr>
<th>Tool</th>
<th>Execution time (ms/call)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>C++ (Cling w/ -O2; out-of-line)</td>
<td>1.8E-6</td>
</tr>
<tr>
<td>cppyy / ppy-c</td>
<td>0.50</td>
</tr>
<tr>
<td>cppyy / CPython</td>
<td>1.25</td>
</tr>
<tr>
<td>swig (builtin)</td>
<td>1.29</td>
</tr>
<tr>
<td>swig (default)</td>
<td>4.23</td>
</tr>
<tr>
<td>pybind11</td>
<td>6.97</td>
</tr>
</tbody>
</table>

⇒ C++ overload is resolved at compile time, not based on dynamic type
⇒ Largest overhead: Python instance type checking (avoidable, but clumsy)
⇒ There is no obvious benefit to “static” over runtime bindings

※ lower is better

W. Lavrijsen, LBL, cppyy, Sep 2021, compiler-research.org

The approach does not require the project maintainer to bother providing static bindings
Extending Data Scientist's Toolbox

Crossing the language barrier is expensive.

Our Compiler-As-A-Service Approach solves that.

In [1]: struct S { double val = 1.; };

In [2]: from libInterop import std
   python_vec = std.vector(S)(1)

In [3]: print(python_vec[0].val)
   
   1

In [4]: class Derived(S)
   def __init__(self):
      self.val = 0
   res = Derived()

In [5]: __global__ void sum_array(int n, double *x, double *sum) {
   for (int i = 0; i < n; i++) *sum += x[i];
 }

// Init N=1M and x[i] = 1.f. Run kernel on 1M elements on the GPU.
sum_array<<<1, 1>>>(N, x, &res.val);

compiler-research.org’s Compiler-As-A-Service Project Final Goal
Extending Data Scientist’s Toolbox. Results

Numba - PyROOT Example

```python
import numba
import math
import ROOT
import cppy.y.numba_ext  # Import the Numba extension
myfile=ROOT.TTree("vec_lv.root")
vector_of_lv=myfile.Get("vec_lv")
  # Vector of TLorentzVector

# Pure Python function
def calc_pt(lv):
    return math.sqrt(lv.Px() ** 2 + lv.Py() ** 2)

def calc_pt_vec(vec_lv):
    pt = []
    for i in range(vec_lv.size()):
        pt.append((calc_pt(vec_lv[i]),
                  vec_lv[i].Pt()))
    return pt

@numba.njit  # Numba decorator
def numba_calc_pt(lv):
    return math.sqrt(lv.Px() ** 2 + lv.Py() ** 2)

def numba_calc_pt_vec(vec_lv):
    pts = []
    for i in range(vec_lv.size()):
        pts.append((numba_calc_pt(vec_lv[i]),
                    vec_lv[i].Pt()))
    return pts

Pts = calc_pt(vec_lv)
Pts = numba_calc_pt_vec(vector_of_lv)
```

When the Pure Python pipeline is compared against the Numba pipeline in the above example we get a 17x speedup. [link]

100x should be within reach

B. Kundu, Princeton, *Efficient and Accurate Automatic Python Bindings with Cppy & Cling*, Tue, ACAT22
Advanced Bare-Metal Toolbox
For Data Science
Domain-Specific Tools For Data Science

Opening up the toolchain allows us to build domain-specific extensions better adapted for our field. We also can extract dataset-specific knowledge:

- Reasoning about algorithm precision and numerical stability
- Providing exact and fast gradients using automatic differentiation techniques
- Enabling sensitivity analysis across HEP components using differentiable pipelines
CaaS. Domain-Specific Data Science Tools

```cpp
#include <...>

// Derivatives as a service.

void gimme_pow2dx(cling::Interpreter &interp) {
  // Definitions of declarations injected also into cling.
  interp.declare("double pow2(double x) { return x*x; }");
  interp.declare("#include <clad/Differentiator/Differentiator.h>");
  interp.declare("#pragma cling optimize(2)")
  interp.declare("auto dfdx = clad::differentiate(pow2, 0);

  cling::Value res; // Will hold the evaluation result.
  interp.process("dfdx.getFunctionPtr()", &res);
  ...
}
```

Can generate computationally efficient gradients for codes with differentiable properties.

```sh
vvassilev@vv-nuc ~/.../builddir $ ./caas-demo
dfdx at 1 = 2.000000
dfdx code: double pow2_darg0(double x) {
  double _d_x = 1;
  return _d_x * x + x * _d_x;
}
```

28-Oct-2022
CaaS. Precision Tuning With Clad

Taylor-based Estimation Floating Point Errors for a dataset using AD:

\[ S_{x_i} \equiv \left| \frac{\partial f}{\partial x_i} \cdot x_i \right| \]

AD enables sensitivity analyses we could not do before.

Case Study: Simpson’s Rule

<table>
<thead>
<tr>
<th>Precision configurations</th>
<th>Absolute Error</th>
<th>Clad’s Estimated Upperbound</th>
<th>Variables in lower precision (out of 11)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10-byte extended precision</td>
<td></td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>(long double)</td>
<td></td>
<td></td>
<td>6</td>
</tr>
<tr>
<td>Clad’s mixed precision</td>
<td></td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>IEEE double-precision</td>
<td></td>
<td></td>
<td>-</td>
</tr>
<tr>
<td>(double)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IEEE single-precision</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(float)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

“Demoting” low-sensitivity variables to lower precision improves performance by ~10% in this example.

Clad’s estimate also agrees that there is no significant change in the final error. This can be useful in the cases where an accurate ground-truth comparison is not available.

G. Singh, Princeton, *Floating Point Error Estimation Using AD*, SIAM UQ22
CaaS. Exact and Fast Gradients With Clad

Automatic Differentiation in RooFit
A different approach: Translating models to code

What that we want to differentiate

Some way to expose differentiable properties of the graph as code.

C++ code the AD tool can understand

C++ code the AD tool can understand

The AD tool

Derivative code of the model!


While speeding up RooFit, after completion of the project we will be able to ask:

*How sensitive is an output with respect to a given input parameter?*
Sensitivity Analysis At Scale

Adapting our hypothesis to the data is an optimization problem.

Differential programming is a programming paradigm in which software is susceptible to automatic differentiation.

The “Analysis” steps have started moving forward including ROOT. The “Simulation” steps follow. G4 is the biggest challenge.

Progress in the area will be discussed at Differentiable and Probabilistic Programming for Fundamental Physics, in June 2023 in TUM.
Impact of Interactive C++ in Physics

Scientific breakthroughs such as the discovery of the big void in the Khufu’s Pyramid, the gravitational waves and the Higgs boson heavily rely on the ROOT software package which uses interactive C++ and Cling.

Conclusion

• C++ tools can bring us bare metal performance

• Existing tools can be reorganized and/or generalized with minimal efforts to enable new opportunities

• We should maintain them and grow them focusing on what they are good for

• Our community has unique multi-language expertise that can allow us doing more science with the same budget
Thank You!

Selected References

• [https://blog.llvm.org/posts/2020-12-21-interactive-cpp-for-data-science/](https://blog.llvm.org/posts/2020-12-21-interactive-cpp-for-data-science/)
• [https://blog.llvm.org/posts/2021-03-25-cling-beyond-just-interpreting-cpp/](https://blog.llvm.org/posts/2021-03-25-cling-beyond-just-interpreting-cpp/)
• [https://Compiler-Research.org](https://Compiler-Research.org)
• [https://root.cern](https://root.cern)
• [Interactive C++ for Data science, CppCon21](https://www.linkedin.com/in/vgvassilev/)
• [Differentiable programming in C++, CppCon21](https://github.com/vgvassilev/)

https://github.com/vgvassilev/

https://www.linkedin.com/in/vgvassilev/