Lessons learned in Python-C++ integration

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This talk is about **lessons learned in Python-C++ integration**.

Awkward Array is the case study.
What is Awkward Array?

Efficient representation of variable length, nested, JSON-like data with NumPy-like functions to quickly compute and restructure data in Python.
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```python
array = ak.Array([{
    "x": 1.1, "y": [1],
}, {
    "x": 2.2, "y": [1, 2],
}, {
    "x": 3.3, "y": [1, 2, 3],
}, [], {
    "x": 4.4, "y": [1, 2, 3, 4],
}, {
    "x": 5.5, "y": [1, 2, 3, 4, 5]
}])
```
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{
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}])

NumPy-like expression

output = np.square(array["y", ..., 1:])
output.to_list()
[
    [[], [4], [4, 9]],
    [],
    [[4, 9, 16], [4, 9, 16, 25]]
]
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])
```

NumPy-like expression

```
output = np.square(array["y", ..., 1:])
```

equivalent Python

```
output = []
for sublist in python_objects:
    tmp1 = []
    for record in sublist:
        tmp2 = []
        for number in record["y"][1:]:
            tmp2.append(np.square(number))
        tmp1.append(tmp2)
    output.append(tmp1)
```
History of the project

Prehistory: Femtocode (21 kLOC Python) and OAMap (8 kLOC Python)

Awkward 0.x: first users, first API, pure Python + NumPy (9 kLOC Python)

Awkward 1.x: rewrite for stability & API (22 kLOC Python, 70 kLOC C++, 14 kLOC C)

Awkward 2.x: refactor for maintainability (29 kLOC Python, 10 kLOC C++, 9 kLOC C)

name switch: awkward1 → awkward0
awkward0

Development
Released
Deprecated
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Language changes

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Also had to replace some NumPy function calls with precompiled C functions, so we built the infrastructure in C++ with Python only for the high-level front-end.

Awkward 1.x → 2.x: we are now porting the C++ infrastructure back to Python.
(For reasons described later in this talk.)

<table>
<thead>
<tr>
<th>Language</th>
<th>Decrease in KLOC</th>
<th>Increase in KLOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Python</td>
<td>-19.6</td>
<td>+26.9</td>
</tr>
<tr>
<td>C++</td>
<td>-59.8</td>
<td>+0</td>
</tr>
<tr>
<td>C</td>
<td>-4.9</td>
<td>+0</td>
</tr>
</tbody>
</table>

kLOC = thousands of non-blank, non-comment lines of code counted by cloc

Awkward 2.x is 75% done; the above is a projection
Evolution of architecture: Awkward 0.x

- tree structures, user interface
- manipulation of 1D buffers
Evolution of architecture: Awkward 1.x

- **user interface**
  - ak.Array in Python
  - operates on CPU pointers
  - registered as a type in Numba
  - compiled in dlopen
  - extern "C" interface

- **tree structures**
  - C++ classes
  - Numba models
  - operates on GPU pointers
  - cuda-kernels
  - cpu-kernels

- **manipulation of 1D buffers**
  - overrides NumPy’s ufuncs
  - pybind11 user interface
  - tree structures
  - Numba models
  - C++ classes
Evolution of architecture: Awkward 2.x

- **ak.Array in Python**
  - registered as a type in Numba
  - overrides NumPy's ufuncs

- **Python classes**
  - Numba models
  - extern "C" interface
  - ctypes

- **user interface**
  - pybind11

- **tree structures**
  - manipulate

- **manipulation of 1D buffers**
  - cpu-kernels: operate on CPU pointers
  - cuda-kernels: operate on GPU pointers
This language choice is unrelated to performance

All $O(n)$ operations for arrays of length $n$ are performed in the kernels layer (C). Porting the tree structures from C++ to Python has no $O(n)$ impact.
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Porting the tree structures from C++ to Python has no $O(n)$ impact.

For an array of 30 million lists of records:

NumPy-like expression

```python
output = np.square(array["y", ..., 1:]
```

equivalent Python

```python
output = []
for sublist in python_objects:
    tmp1 = []
    for record in sublist:
        tmp2 = []
        for number in record["y"][1:]:
            tmp2.append(np.square(number))
        tmp1.append(tmp2)
    output.append(tmp1)
```

Awkward 0.15.5: 4.6 seconds
Awkward 1.5.1: 2.4 seconds
Awkward 2.0.0a: 1.5 seconds

equivalent Python: 140 seconds

because $O(n)$ operations are performed in Python
Lessons learned in Python-C++ integration
Awkward 1.x design goal: connect to C++ HEP libraries through the C++ layer. Awkward 2.x removes this capability.

Python packages must be distributed as binaries, with compilation-on-install as a last resort! "pip install awkward" shouldn't have dependencies outside of pip, including the existence of a compiler.

Dynamically linking to precompiled C++ exposes a project to ABI dependencies. Awkward-enabled HEP libraries would depend on ABI version. (See PYBIND11_INTERNALS_VERSION in pybind11/include/pybind11/detail/internals.h.)

Not needed anyway: fastjet, a Python/Awkward interface to FastJet (C++), interfaces through C data types (raw arrays) easily. Awkward Array does not need to be C++ to interface with C++.

See Aryan Roy's poster!
Issue #1: Intention to use C++ as an ABI

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See Aryan Roy’s poster!
Issue #2: Reference cycles through C++

- **no reference cycle**
  - A → B → C

- **reference cycle**
  - A → B → C → D

- **reference cycle through Python/C++ boundary**
  - A → B → C

**Python**

- std::shared_ptr
- which calls PyDECREF when it is deleted

**C++**

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▶ Python garbage collector can detect reference cycles, immediately when a reference count goes to zero or during mark-and-sweep.
▶ But it can’t detect a reference cycle through C++.
▶ We tried to fix this by making the VirtualArray cache a weakref, but this had its own share of issues: #230, #400, #432, #479, #541, #560, #597, #603, #655, #679, #783, #865, #899, #940, #1052...
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Even sneakier: reference cycles can be created by function closures; VirtualArrays hold Python functions. (Anything mutable is an opening!)

Dropping C++ solves this, but we’re also replacing VirtualArrays with Dask.
If you’re using pybind11, be aware that it does not release Python’s GIL by default. The GIL undermines multithreading.

(See `py::gil_scoped_acquire`, `py::gil_scoped_release`, and `py::call_guard`.)
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Issue #3: Releasing the GIL

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Furthermore, you can’t release the GIL if you ever need to change any Python object, even a reference counter.

Awkward Array’s C++ objects hold references to Python objects (mostly NumPy arrays) and decrement the reference count if the C++ object is deleted. Since that could happen at any time, we can’t release the GIL without risking segfaults.
Issue #4: Algorithm visibility

The final reason for C++ → Python refactoring: third-party libraries like Dask and JAX couldn’t “see” enough of what Awkward Array was doing.

- ak.Array in Python
  - overrides NumPy's ufuncs registered as a type in Numba
  - Python can "see" down to this depth

- C++ classes
  - extern "C" interface

- Numba models

- cpu-kernels
  - operate on CPU pointers

- cuda-kernels
  - operate on GPU pointers
The *final* reason for C++ → Python refactoring: third-party libraries like Dask and JAX couldn’t “see” enough of what Awkward Array was doing.
These libraries use “tracers” to inspect a path through Python code, like this:

```python
>>> import numpy as np
>>> class Tracer(np.lib.mixins.NDArrayOperatorsMixin):
...     def __init__(self):
...         self.functions = []
...     def __array_ufunc__(self, ufunc, method, *inputs, **kwargs):
...         self.functions.append(ufunc.__name__)
...         return self
...
>>> t = Tracer()
>>> np.sin(t)**2 + np.cos(t)**2
<__main__.Tracer object at 0x7ff2a0f33e80>
>>> t.functions
['sin', 'power', 'cos', 'power', 'add']
```

Tracers can see binary ops and functions, but calls out of Python are black boxes.
Issue #4: Algorithm visibility

The “tree structures” (mid-level) of Awkward Array are too coarse for these libraries because the third-party libraries don’t recognize arrays of trees.

They do recognize simple arrays of numbers (our “kernels,” or low-level).

See Anish Biswas’s presentation at https://indico.cern.ch/event/1033648 for a heroic attempt to integrate Awkward Array and JAX using PyTrees.
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**This last problem with Awkward Array’s C++ layer is the one that finally convinced us to change.**
Awkward Array’s Python-C++ codebase was a bad design.
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Does that mean you shouldn’t mix Python and C++?
No!
Just watch out for these issues when you do.

1. Don’t plan on sharing stdlib (e.g. `std::vector`) or pybind11 objects between Python modules. Share data as basic C types.

2. Python and C++ can share references, but ensure no reference cycles! 100% immutability would prevent cycles.

3. You can only release the GIL in blocks of code that do not touch Python in any way, including reference counts.

4. Think about interoperability plans: how much of your code will third-party libraries need to see?
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(This may be an advertisement for Julia.)