Nested data structures in array and SIMD frameworks

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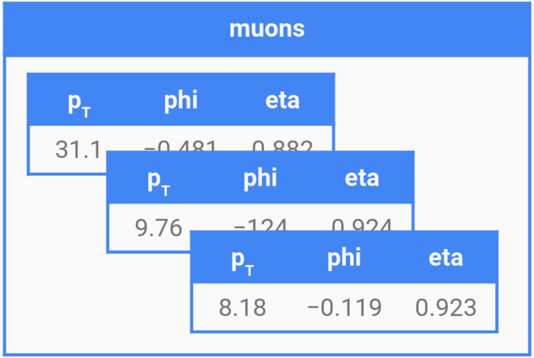
Nested, variable-sized data structures are crucial in HEP



mu1 p_T	mu1 phi	mu1 eta	mu2 p_T	mu2 phi	mu2 eta
31.1	−0.481	0.882	9.76	−0.124	0.924
5.27	1.246	−0.991	n/a	n/a	n/a
4.72	−0.207	0.953	n/a	n/a	n/a
8.59	−1.754	−0.264	8.714	0.185	0.629

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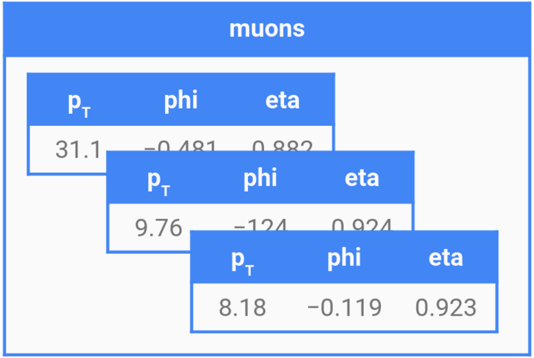

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Analysis datasets are big lists of variable-length lists of structs/objects/records.

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 ...
```

Columnar representation

But they don't have to be "structs," pointers to contiguous p_T, η, ϕ triples.

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```

They can be contiguous by field with counts or offsets or starts/stops or parents arrays.

counts	3,			1,	1,	2	
p_T	31.1,	9.76,	8.18,	5.27,	4.72,	8.59,	8.714
phi	-0.481,	-0.123,	-0.119,	1.246,	-0.207,	-1.754,	0.185
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```

They can be contiguous by field with counts or offsets or starts/stops or parents arrays.

offsets	0,			3,	4,	5,	7
p_T	31.1,	9.76,	8.18,	5.27,	4.72,	8.59,	8.714
phi	-0.481,	-0.123,	-0.119,	1.246,	-0.207,	-1.754,	0.185
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parents	0,	0,	0,	1,	2,	3,	3
p_T	31.1,	9.76,	8.18,	5.27,	4.72,	8.59,	8.714
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```

"Remove the first muon from each event." $\longrightarrow$ increase all starts by 1.

starts	1,			4,	5,	6	
stops	3,			4,	5,	7	
p_T	31.1,	9.76,	8.18,	5.27,	4.72,	8.59,	8.714
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We didn't need to touch any contents (read them from disk, decompress them...).

Library for manipulating non-standard array types

Awkward Array

https://github.com/scikit-hep/awkward-array

- variable-length subarrays: "jagged arrays"
- struct-of-arrays viewed as array-of-structs
- nullable types
- heterogeneous types (tagged unions)
- cross-references or even cyclic references
- sparse, non-contiguous, lazy

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Fully composable: any awkward array can be placed within any other awkward array.

Not lacking for data types

Nullable, heterogeneous, multiple levels of depth, nested records...

```
>>> import awkward
>>> array = awkward.fromiter(
...     [[1.1, 2.2, None, 3.3, None],
...      [4.4, [5.5]],
...      [{"x": 6, "y": {"z": 7}}, None, {"x": 8, "y": {"z": 9}}]])
```

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>>> print(array)                # internally, these are all arrays
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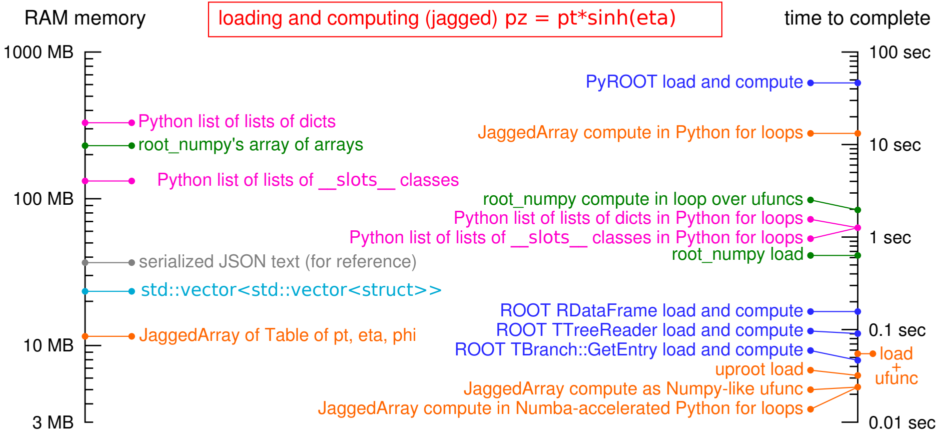
>>> (array + 100).tolist()   # element-wise function applied to arrays
[[101.1, 102.2, None, 103.3, None],
 [104.4, [105.5]],
 [{'x': 106, 'y': {'z': 107}}, None, {'x': 108, 'y': {'z': 109}}]]
```

Columnar data structures minimize memory use and time

Example of one operation, deriving p_z of a variable number of p_T and η per event, using awkward-array, ROOT, pure Python, and root_numpy.



Real life

a single operation $\neq$ a physics analysis

Beyond toy studies

Coffea

Columnar **O**bject **F**ramework **F**or **E**fficient **A**nalysis

Matteo Cremonesi, Lindsey Gray, Oliver Gutsche, Allison Hall, Bo Jayatilaka, Igor Mandrichenko, Kevin Pedro, Nick Smith [FNAL], and me [Princeton] https://github.com/CoffeaTeam

Performing two complete CMS analyses with columnar tools:

- Dark Higgs search
- Boosted SM $H \to b\bar{b}$

Also developing `fnal-column-analysis-tools`, a HEP layer on awkward-array, and a distributed query processing system with Ben Galewsky, Mark Neubauer [Illinois], and Andrew Melo [Vanderbilt].

First finished analysis: Z peak

Z peak is the "hello world" of analysis frameworks.

This implementation is realistic: run-lumi mask, pile-up correction, ID scale factors, and $ee/\mu\mu/e\mu$ channels. 350 lines in a Jupyter notebook, accessing 25 columns.

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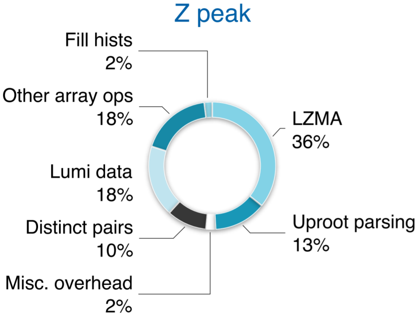
columnar analysis:

6 μs/event/thread (165 kHz)

ROOT C++:

4 μs/event/thread (250 kHz)

Columnar analysis is about 50% slower than its C++ equivalent.



Second near-complete analysis

Prototype of boosted $H \to b\bar{b}$ has

- recursive gen parent-finding
- gen-reco matching
- binned corrections
- parametric corrections
- systematics

70 μs/event/thread (14 kHz)

Uses about 100 columns.

Analysts' "favorite stanzas" of the boosted $H \to b\bar{b}$ analysis

VBF signal region definition:

```
AK4jet_AK8jet_matches = ak4_goodjets.fastmatch(leadingak8jet)
unmatched_ak4     = ak4_goodjets[~AK4jet_AK8jet_matches]
vbf_ak4_pairs     = unmatched_ak4.p4.distincts(nested=True)
vbf_ak4_detas     = np.abs(vbf_ak4_pairs.i0.eta - vbf_ak4_pairs.i1.eta).flatten()
vbf_ak4_maxdetas = vbf_ak4_detas.argmax()
vbf_ak4_masses    = (vbf_ak4_pairs.i0 + vbf_ak4_pairs.i1).mass.flatten()[vbf_ak4_maxdetas]
vbf_ak4_pass      = (vbf_ak4_detas[vbf_ak4_maxdetas] > 3.25) & (vbf_ak4_masses > 975.0)
```

Leading fat-jet selection with vetos:

```
k8puppijet_pt200 = ak8puppijet[
                       passLooseJetSel(ak8puppijet) &
                       (ak8puppijet.pt > 200) &
                       (np.abs(ak8puppijet.eta) < 2.5)]
ak8veto = ~(
    ak8puppijet_pt200.fastmatch(vetoMuons,deltaRCut=0.4) |
    ak8puppijet_pt200.fastmatch(vetoElectrons,deltaRCut=0.4) |
    ak8puppijet_pt200.fastmatch(vetoPhotons,deltaRCut=0.4) )
ak8jets_veto = ak8puppijet_pt200[ak8veto]
leadingak8jet = ak8jets_veto[ak8jets_veto.pt.argmax()]
```

Syntax is an extension of Numpy

Numpy arrays must all be rectangular: vectors, matrices, and tensors. Awkward arrays reproduce this behavior in rectangular cases and generalize in jagged cases.

- Multidimensional slices: `rgb_pixels[0, 50:100, ::3]`
- Elementwise operations: `all_pz = all_pt * sinh(all_eta)`
- Broadcasting: `all_phi - 2*pi`
- Masking (list compaction): `data[trigger & (pt > 40)]`
- Fancy indexing (gather/scatter): `all_eta[argsort(all_pt)]`
- Row/column commutativity (hides AoS $\leftrightarrow$ SoA): `table["column"][7]` (row 7 of column array)
`table[7]["column"]` (field of row tuple 7)
- Array reduction: `array.sum()` $\rightarrow$ scalar

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Numpy arrays must all be rectangular: vectors, matrices, and tensors. Awkward arrays reproduce this behavior in rectangular cases and generalize in jagged cases.

- Multidimensional slices: `events["jets"][:, 0]` → first jet per event
- Elementwise operations: `jetpt * sinh(jeteta)` → keep jagged structure
- Broadcasting: `jetphi - metphi` → expand `metphi` from one-per-event to one-per-jet before operation
- Masking (list compaction): `data[trigger]` → drop whole events
  `data[jetpt > 40]` → drop jets from events
- Fancy indexing (gather/scatter): `a = argmax(jetpt)` → `[[2], [], [1], [4]]`
  `jeteta[a]` → `[[3.6], [], [-1.2], [0.4]]`
- Row/column commutativity (hides AoS ↔ SoA): `events["jets"]["pt"][7, 1]`,
  `events["jets"][7]["pt"][1]`,
  `events[7]["jets"]["pt"][1]`, ...
- Jagged array reduction: `jetpt.max()` → array of max jet p_T per event

Structure for most physics data: multiple candidates per event

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JaggedArray(ObjectArray(Table(px, py, pz, E), LorentzVector))
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- `px`, `py`, `pz`, `E` are flat Numpy arrays (all particles, all events).
- `Table` to present contiguous columns as an array of rows
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Individual `LorentzVector` objects have kinematic methods—`pt`, `eta`, `mass`, etc.—but so do the `ObjectArray` and `JaggedArray`. Whole-array methods are vectorized.

To compute the mass of all particles in all events are pack it into per-event sublists, you say

```
>>> particles.mass
```

Putting it all together: a simple Z peak

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>>> hastwo = (array.counts >= 2)            # to select at least two muons
>>> leading = array[hastwo, 0]              # mask and select first
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>>> candidates = leading + subleading           # Lorentz vector sum across all
>>> candidates.mass                             # compute mass for all
array([90.22779777, 74.74654928, ..., 85.44384208, 75.96066262])
```

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- Interesting mistake: analysts must unlearn order-dependent coding habits!

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(nMuons > 0) & (Muons_pt[:, 0] > 30)  # intersection of masks
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  ```

  The latter might try to access the first of zero muons.

  Instead,

  ```
  Muons_pt[(nMuons > 0), 0] > 30        # mask first dim, pick 0
  ```

Is this making analysis easier?

If yes, great! Continue developing array operations, thinking about their "ergonomics," and optimize their implementations.

If no, it's still a useful abstraction layer, but we'll need a more user-friendly interface on top of it, such as a functional or declarative language.

Half-hour interviews with physicists about array syntax

1 grad student, 2 postdocs (beginning & advanced), and 1 advanced researcher

Everyone had most experience in C++ (5 years to decades), less in Python, which was primarily PyROOT (6 months to 3–4 years), very little in Numpy (2 to 5 months).

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Some motivated by execution speed, some by ease of use.

- "Thirty minutes is too long to wait for a plot."
- "Will be run order-of-a-hundred times over the course of the year; this is a big investment." but "For something that could be two times faster, I wouldn't do these optimizations."
- "Ease of use is paramount; I've always struggled with poorly written code." and "Making it fast to run it again and again is *going around* ease of use."
- "Ease of use is most important, even if execution speed decreases."

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Some found it easier, some more difficult.

- "Way, way much easier than applying cuts with for loops."
- "Surprised by how conceptually different you have to think about selections, combining objects." but "Not good or bad, just surprising that it has a learning curve."
- "Individual problems have been much more difficult than expected." and "Translating 'if' statements is where I get hung up." but "Not inherently harder; just harder now for those of us used to the 'for' loop version."

Half-hour interviews with physicists about array syntax

1 grad student, 2 postdocs (beginning & advanced), and 1 advanced researcher

Everyone had most experience in C++ (5 years to decades), less in Python, which was primarily PyROOT (6 months to 3–4 years), very little in Numpy (2 to 5 months).

One point came up multiple times: easier to read than write.

- "The good thing is, once you figure it out, it's clear why it works. It's not magic, you just have to get the mapping right."
- "If I ask a student to read my code, he'll be able to read it. But five minutes later, he'll try something similar and it won't work."

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~~Write-only~~ Read-only code???

Further developments

- Numba is a JIT-compiler for Python, but only for statically typed data. Awkward-array types are "statically typed at runtime," so I'm extending Numba to recognize and JIT-compile them.

  This will permit fast (compiled), imperative (for-loop style) calculations in Python.

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- Giuseppe Cerati (Fermilab) is investigating the use of jagged arrays in C++, to write reconstruction algorithms that are equally efficient on CPUs and GPUs.

  Status: implemented track-propagation in Python and switched from CPU to GPU with from "`import numpy as np`" → "`import cupy as np`".

  Reimplemented in C++ using xtensor (Numpy clone for C++).

Conclusions

Awkward-array is a library for complex data, presented as arrays. Jagged arrays are the most important for HEP. (Perhaps the only type *necessary* for HEP?)

We're beyond single-operation tests; we're implementing complete analyses. Performance is within a factor of two of C++, and there's low-hanging fruit for improvements.

Physicists find it hard to write, but easy to read.

This is an open area of development with many paths to follow!