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Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

The Case for Columnar Analysis (a two-part series)

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iris hep

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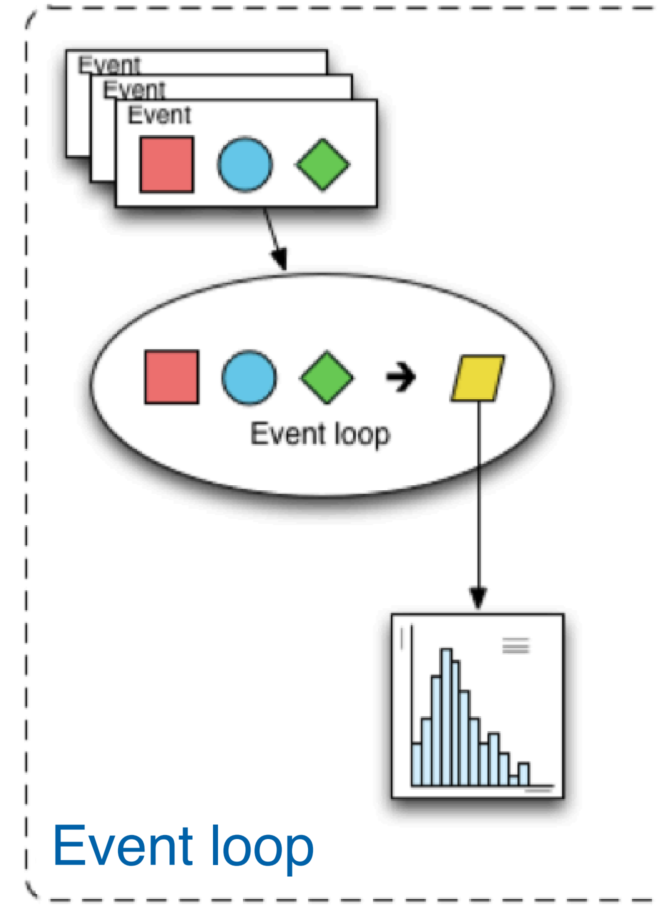
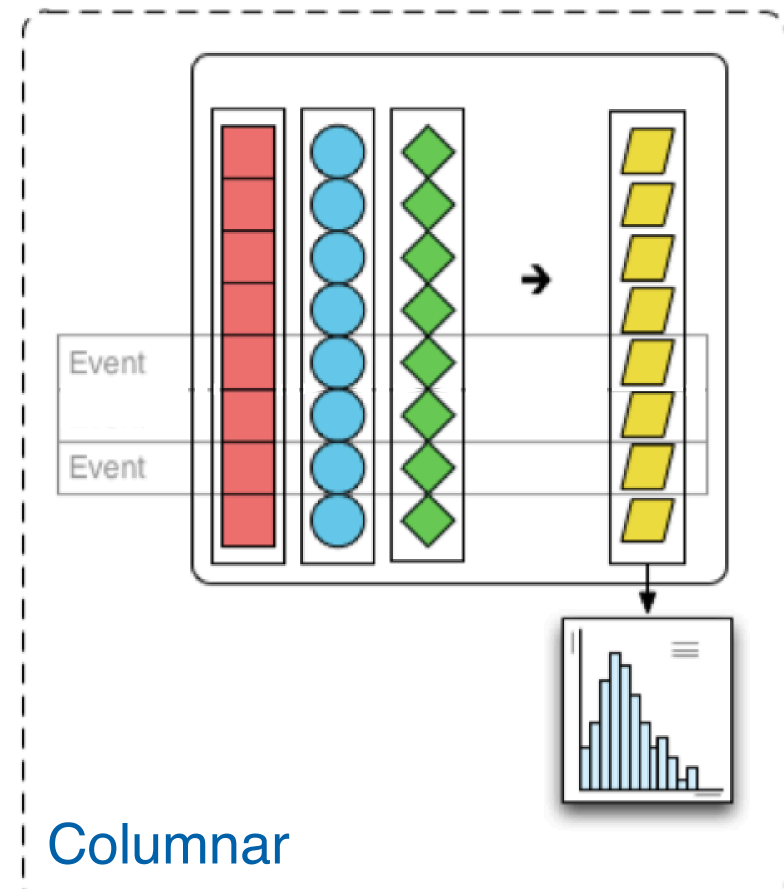
Prologue: terminology

- Event loop analysis:
  - Load relevant values for a specific event into local variables
  - Evaluate several expressions
  - Store derived values
  - Repeat (explicit outer loop)



- Columnar analysis:
  - Load relevant values for many events into contiguous arrays
    - Nested structure (array of arrays) → flat content + offsets
      - This is how TTree works!
  - Evaluate several **array programming** expressions
    - Implicit *inner* loop**s**
  - Store derived values



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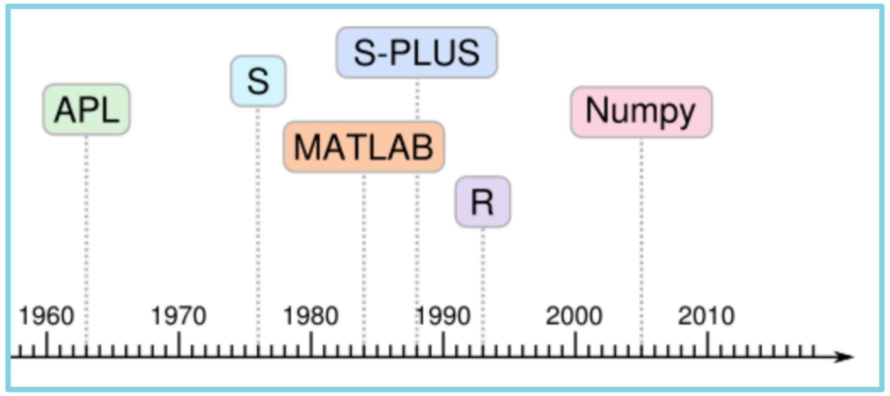
Prologue: technology

- Array programming:
  - Simple, composable operations
  - Extensions to manipulate offsets
  - *Not declarative* but towards goal



- Awkward array programming:
  - Extension of numpy syntax
  - Variable-length dimensions: “jagged arrays”
  - View SoA as AoS, familiar object syntax, e.g. p4.pt()
  - References, masks, other useful extensions
  - See awkward, talk by J. Pivarski at ACAT2019

- Coffea framework:
  - Prototype analysis framework utilizing columnar approach
  - Provide lookup tools, histogramming, other ‘missing pieces’ usually f
  - See fnal-column-analysis-tools
    - Functionality will be factorized as it matures

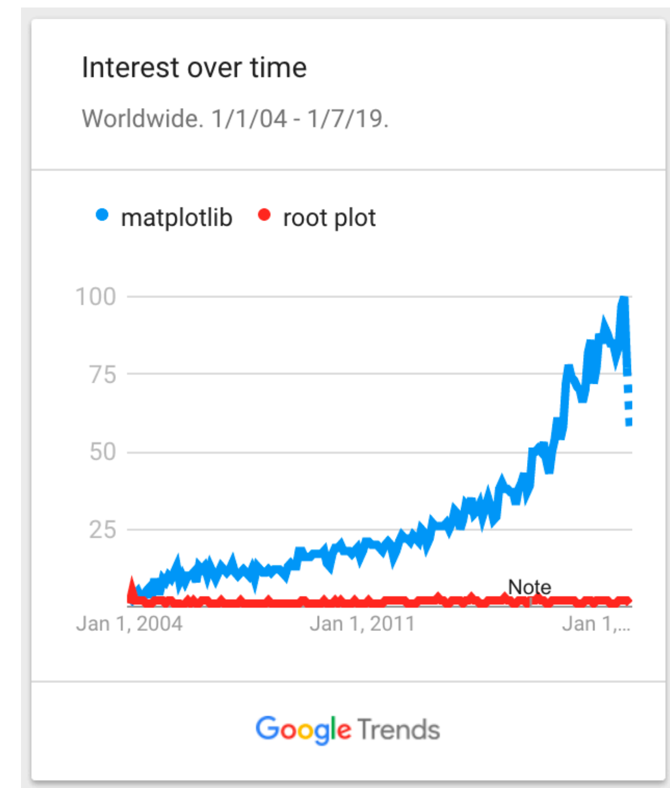
Part I:
Analyzer Experience

User experience

- Unsurprisingly, #1 user priority
  - Any working analysis code can scale up…for now
  - c.f. usage of PyROOT event loops despite dismal performance
    - (this will *never* change)

- Fast learning curve for scientific python stack
  - Excellent 'google-ability'
  - The quality and quantity of off-the-shelf components is impressive—many analysis tool implementations contain very little original code
  - Essentially all functions available in a vectorized form

- Challenge: re-frame problem in array programming primitives rather than imperative style (for+if)
  - User [interviews]() conducted:
    - "its different, not necessarily harder"
    - "easier to read than write" ?!



Code samples I

- Idea of what Z candidate selection can look like
- Python allows very flexible interface, under-the-hood data structure is columnar

```
ele = electrons[(electrons.p4.pt > 20) &
                                   (np.abs(electrons.p4.eta) < 2.5) &
                                   (electrons.cutBased >= 4)]

mu = muons[(muons.p4.pt > 20) &
                          (np.abs(muons.p4.eta) < 2.4) &
                          (muons.tightId > 0)]
```

- Selects good candidates (per-entry selection)

```
ee = ele.distincts()
mm = mu.distincts()
em = ele.cross(mu)
```

- Creates pair combinatorics (creates new pairs array, also jagged)

```
channels['ee'] = good_trigger & (ee.counts == 1) & (mu.counts == 0)
channels['mm'] = good_trigger & (mm.counts == 1) & (ele.counts == 0)
channels['em'] = good_trigger & (em.counts == 1) & (ele.counts == 1) & (mu.counts == 1)
```

- Selects good events, partitioning by type (per-event selection)

```
dileptons['ee'] = ee[(ee.i0.pdgId*ee.i1.pdgId == -11*11) & (ee.i0.p4.pt > 25)]
dileptons['mm'] = mm[(mm.i0.pdgId*mm.i1.pdgId == -13*13)]
dileptons['em'] = em[(em.i0.pdgId*em.i1.pdgId == -11*13)]
```

- Selects good pairs, partitioning by type (per-entry selection on pairs array)

Code samples II

- Enable expressive abstractions without python interpreter overhead
  - e.g. storing boolean event selections from systematic-shifted variables in named bitmasks: each add() line operates on O(100k) events

```
shiftSystematics = ['JESUp', 'JESDown', 'JERUp', 'JERDown']
shiftedQuantities = {'AK8Puppijet0_pt', 'pfmet'}
shiftedSelections = {'jetKinematics', 'jetKinematicsMuonCR', 'pfmet'}
for syst in shiftSystematics:
    selection.add('jetKinematics'+syst, df['AK8Puppijet0_pt_'+syst] > 450)
    selection.add('jetKinematicsMuonCR'+syst, df['AK8Puppijet0_pt_'+syst] > 400.)
    selection.add('pfmet'+syst, df['pfmet_'+syst] < 140.)
```

- Columnar analysis is a lifestyle brand
  - Opens up scientific python ecosystem. e.g. interpolator from 2D ROOT histogram:

```
def centers(edges):
    return (edges[:-1] + edges[1:])/2

h = uproot.open("histo.root")["a2dhisto"]
xedges, yedges = h.edges
xcenters, ycenters = np.meshgrid(centers(xedges), centers(yedges))
points = np.hstack([xcenters.flatten(), ycenters.flatten()])
interp = scipy.interpolate.LinearNDInterpolator(points, h.values.flatten())
x, y = np.array([1,2,3]), np.array([3., 1., 15.])
interp(x, y)
```

- Don't want linear interpolation? Try one of several other options

Domain of applicability

- Domain of applicability depends on:
  - Complexity of algorithms
  - Size of per-event input state
- Examples:
  - JEC (binned parametric function): use binary search, masked evaluation: **columnar ok**
  - Object gen-matching, cross-cleaning: min(metric(pairs of offsets)): **columnar ok**
  - Deterministic annealing PV reconstruction: large input state, iterative: **probably not**
- How far back can columnar go?
  - *Missing array programming primitives not a barrier, can always implement our own*

Event loop **Columnar**

Event Reconstruction	Analysis Objects	Filtering & Projection	Empirical PDFs
1 MB/evt Complex algorithms operating on large per-event input state Inter-event SIMD	40-400 kB/evt Fewer complex algorithms, smaller per-event input state	(skimming & slimming) 1 kB/evt Few complex algorithms, O(1 column) input state	(histograms) No event scaling Trivial operations

Scalability

- Present a unified data structure to analysis function or class
  - Dataframe of awkward arrays
  - Decouple data delivery system from analysis system
- We can run real-world analyses at a range of scales
  - With home-grown and commercial scheduler software
- Lessons learned so far:
  - Fast time-to-backtrace as important as time-to-insight, keep in mind for analysis facilities!
  - Physics-driven bookkeeping (dataset names, cross sections, storage of derived data, etc.) is nontrivial in all cases, *needs to be decoupled*
  - Inherently higher memory footprint, solved by adjusting partitioning (chunking) scheme
    - Tradeoff with data delivery overhead

Data delivery system	*Z peak wall-time throughput*	*Subjective 'ease of use'*
uproot on laptop	*~ 100 kHz*	*5/5*
uproot + xrootd + multiprocessing	*~ 250 kHz @ 10 cores **	*5/5*
uproot + condor jobs	*Arbitrary*	*3/5*
striped system	*~ 10 MHz @ 100 cores*	*2/5*
Apache spark	*~ 1 MHz @ 100 cores ***	*4/5*

* constrained by bandwidth

** pandas_udf issue

Part II:
Technical Underpinnings

Theoretical Motivation

- Aligned with strengths of modern CPUs
  - Simple instruction kernels aid pipelining, branch prediction, and pre-fetching
  - Event loop = input data controlling instruction pointer = less likely to exploit all three!
  - *Unnecessary work is cheaper than unusable work*
- Inherently SIMD-friendly
  - Event loop cannot leverage SIMD unless inter-event data sufficiently large
- In-memory data structure *exactly* matches on-disk serialized format
  - Event loop must transform data structure - significant overhead
  - Memory consumption managed by chunking (event groups, or baskets)
- Array programming kernels form computation graph
  - Could allow query planning, automated caching, non-trivial parallelization schemes

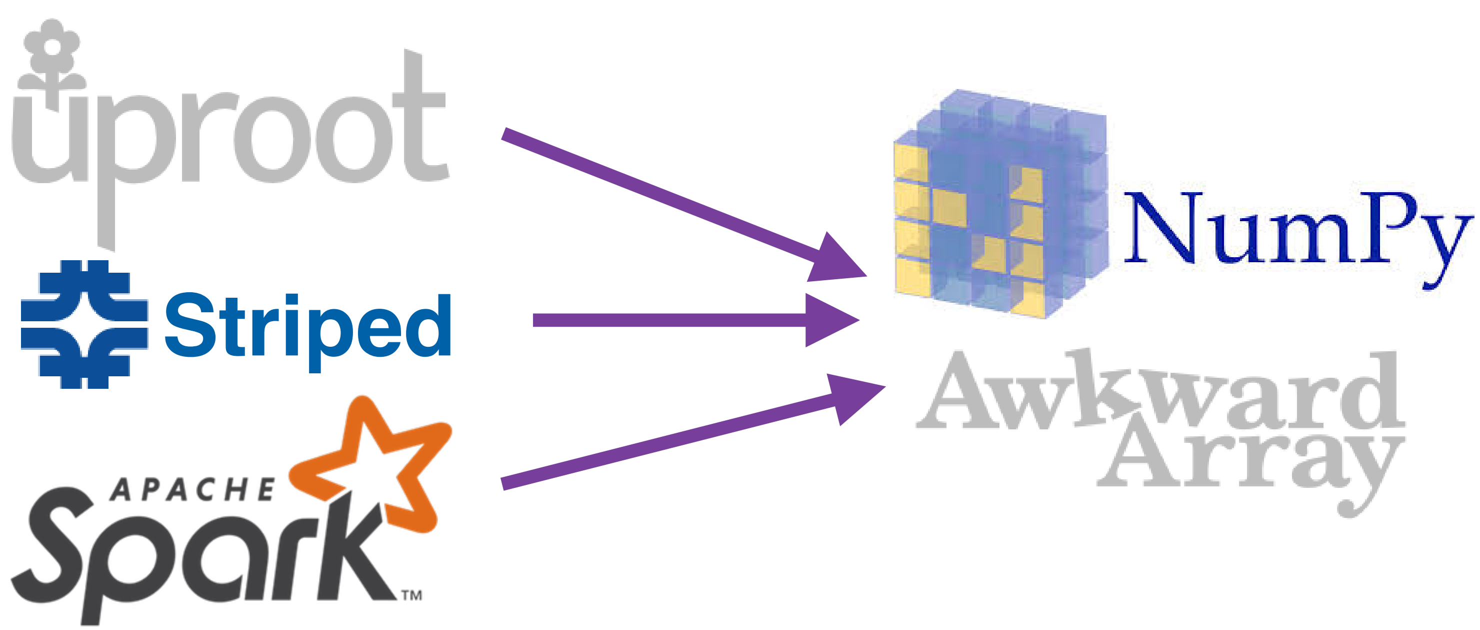
The Coffea framework

- Column Object Framework For Effective Analysis:
  - Prototype analysis framework utilizing columnar approach
  - Provides object-class-style view of underlying arrays
  - Implements typical recipes needed to operate on NANOAOD-like nTuples
  - One monolith for now: [fnal-column-analysis-tools]
    - Functionality will be factorized into targeted packages as it matures

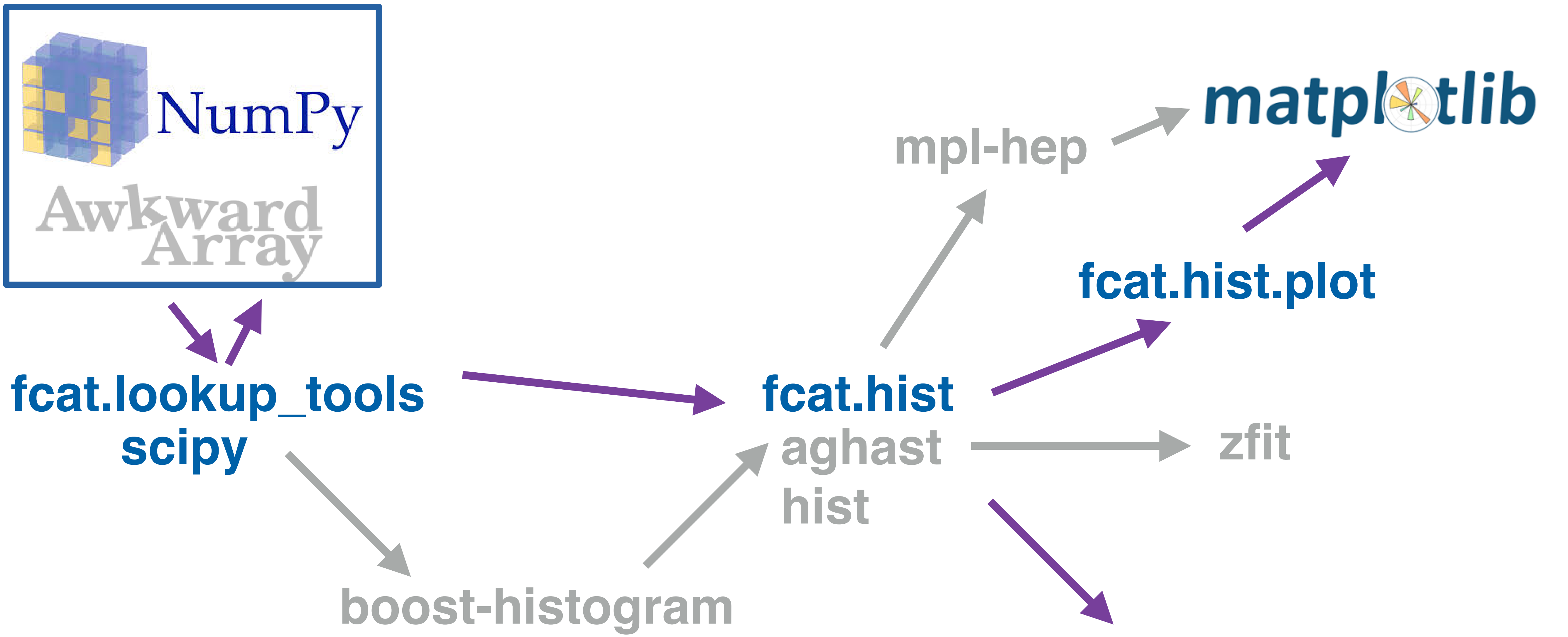
- Realized using scientific python ecosystem
  - numpy: general-purpose array manipulation library
  - numba: uses llvm to JIT-compile python code, understands numpy
    - Work ongoing to extend to awkward arrays as well
  - scipy: large library of specialized functions
  - cloudpickle: serialize arbitrary python objects, even function signatures
  - matplotlib: python visualization library

Factorized Data Delivery

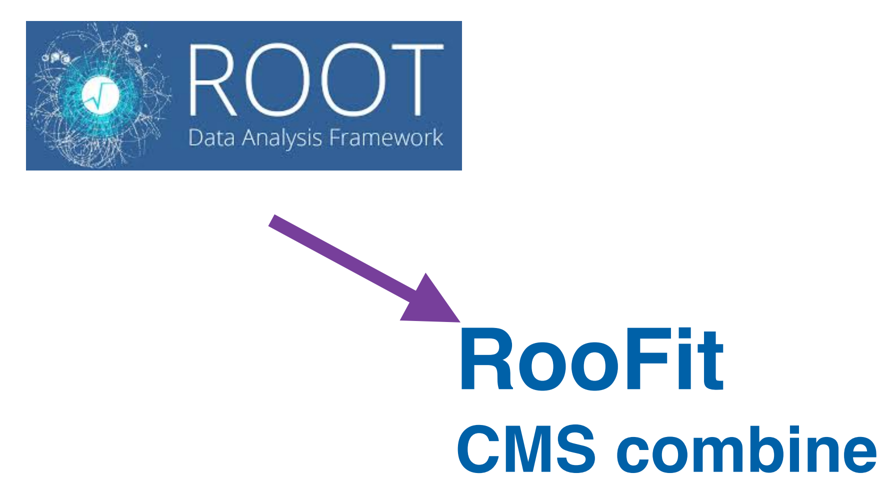
- Uproot
  - Direct conversion from TTree to numpy arrays and/or awkward JaggedArrays
- Striped
  - NoSQL database delivers ‘stripes’: numpy arrays
    - Re-assemble awkward structure via object counts + content
  - memcached layer, python job scheduler, ~150 core cluster
  - Derived columns persistable
- Spark
  - Interface using vectorized UDF (user-defined function)
  - Currently restricted to intermediate pandas format (pyarrow UDF to be implemented)
  - Derived columns persistable



Package ecosystem

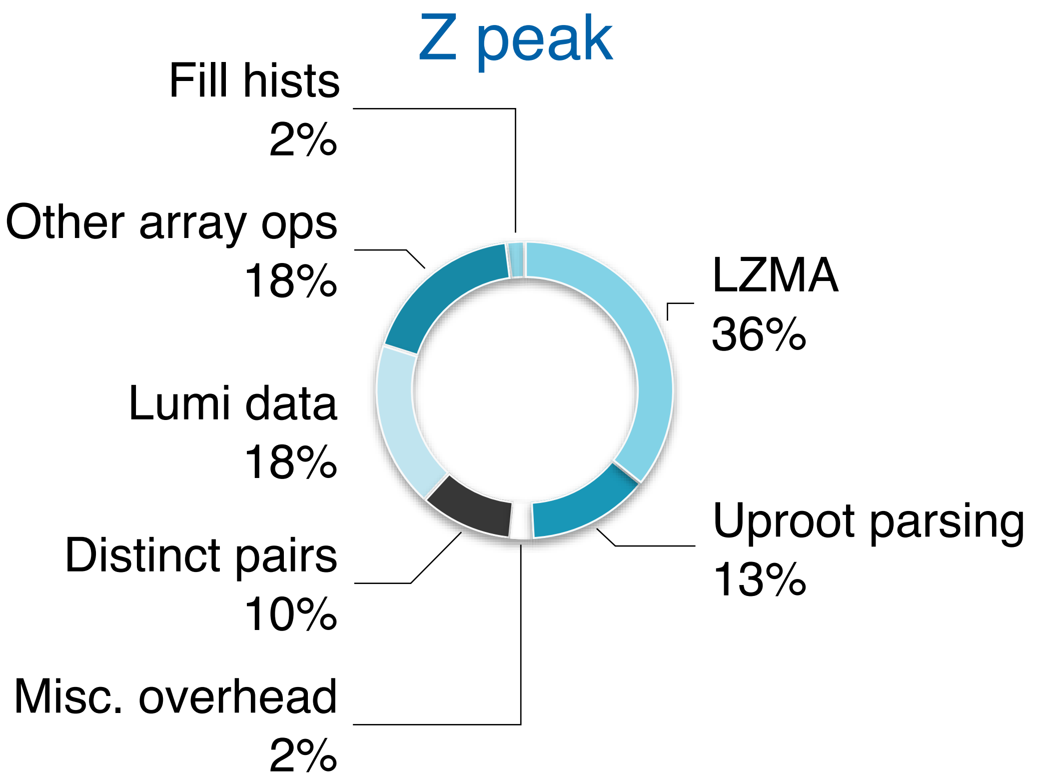


- Prototype analyses are using the workflow in blue
  - fcat = fnal-column-analysis-tools
  - Future pyHEP ecosystem analysis packages in grey



Performance

- Z peak benchmark
  - Includes many typical corrections: lumimask, PU correction, ID scale factors, flavor-categorized
  - 350 lines jupyter notebook, 25 columns accessed
  - 6 μs/evt/thread (125 kHz) wall time
    - ROOT C++ TBranch::GetEntry(): ~1.5x faster
- Two prototype analyses
  - “end-to-end” = NanoAOD-like nTuple to templates
  - Varies from 30-150 μs/evt/thread
  - Already being used to steer analysis, present results in analysis group meetings
- Many inefficiencies known
  - Can be removed with further development in awkward and helper libraries



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Future Directions

- As Coffea (& underlying libraries) matures, invite beta testers
  - I encourage everyone to try uproot+numpy now
- Target first release this summer
  - Two full analysis implemented
  - Data delivery mechanisms fully separated
  - User interface improvements and documentation

- Far future: analysis facility
  - This feeds towards the dream of a “short time-to-insight” “analysis as a service” facility
    - Tendering bids for additional buzzwords
  - Array programming allows easier construction of computation graphs
    - Query planning can detect common patterns and execute them once
    - By removing manual cache management, we can optimize throughput and storage

- First, lets see if we are happy and productive with the columnar approach
  - So far, the answer appears to be yes