coffeA - Columnar Object Framework For Effective Analysis

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Physics - The motivation

• The present challenge:
  - Analyze all LHC Run 2 data: $O(10 \text{ billion})$ events
  - Investigate data quality issues with fast time-to-insight
  - Optimize complex (e.g. deep learning) algorithms
• Multiply by $O(1000)$ data analysts
• These challenges magnified 20x in HL-LHC

• Solutions must be:
  - Easy to use
  - Scalable
  - Fast
Columnar analysis - The paradigm

• 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
  - Evaluate several array programming expressions
    • Implicit inner loops
  - Store derived values

• Coffea started 1 year ago with one goal: perform CMS analyses at scale using columnar analysis techniques
Coffea - The solution

Coffea is:
- A package in the scientific python ecosystem
  - $ pip install coffea
- A user interface for columnar analysis
  - With missing pieces of the stack filled in
- A minimum viable product
  - We are data analyzers too #dogfooding
- A really strong glue
  - To be glued in:

Coffea - The solution

Visualizaion

Coffea

matplotlib

SciPy

Numba

Awkward Array

Coiffe

Laurelin

ServiceX

Array API

Data ingestion

Task scheduler

Resource provisioning

Boost Histogram

pyhf

fast-carpenter
Coffea - The solution

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  - Boost Histogram
  - pyhf
  - fast-carpenter

= CHEP contribution (link)
User experience

• User time more expensive than CPU time
  - Any working analysis code can scale up on condor (for now)
  - c.f. usage of PyROOT event loops despite dismal performance

• Profit from wider user base
  - Excellent ‘google-ability’
  - More time exploring physics data
  - Less duplicated effort writing common algorithms
  - Skills transfer to data science industry

• Profit from wider developer base
  - Follow established conventions in the scientific python ecosystem
  - User interface more likely to be intuitive
Domain of applicability

• Is columnar analysis always the best approach? No:
  - Too complex or too much intra-event data makes array programming a headache
  - When intra-event data is large, we can already use vectorized approaches in event loop

• What is the limit on complexity?
  - In principle, none—missing array programming primitives can easily be implemented
  - In practice, on IRIS-HEP analysis benchmark tasks, only one required a new primitive
    - [https://nbviewer.jupyter.org/github/mat-adamec/coffea-benchmarks/tree/master/benchmarks/](https://nbviewer.jupyter.org/github/mat-adamec/coffea-benchmarks/tree/master/benchmarks/)
  - CMS NanoAOD schema (incl. cross-references) is fully describable with awkward-array

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### Event loop

- **Event Reconstruction**
  - 1 MB/evt
  - Complex algorithms operating on large per-event inputs
  - Intra-event vectorization

- **Analysis Objects**
  - 40-400 kB/evt
  - Fewer complex algorithms, smaller per-event inputs

- **Filtering & Projection**
  - (skimming & slimming)
    - 1 kB/evt
  - Few complex algorithms, O(10) column inputs

### Columnar

- **Empirical PDFs**
  - (histograms)
  - No event scaling
  - Trivial operations
Analyst interface

- Jupyter notebooks
  - Combine source code and results in one document
  - More effective for data exploration
- Traditional CLI, scripts
  - Best for established processing workflows
  - Can integrate user python libraries
Scalability - The coffea processor

- User is provided data frame of columns they wish to process
  - Lazily evaluated access in uproot-based executors
- User fills a defined set of accumulators
  - Histograms, dictionaries of counts, appendable arrays, …
- Coffea executor takes care of the rest
  - Row chunking (a.k.a. partitioning or job splitting)
  - Scale-out to many workers
  - Input caching (support varies by executor)
  - Tree reduction of accumulators
- Supported executors:
  - Local machine, dask cluster, spark cluster, parsl cluster (and condor)

```python
from coffea import hist, processor

class MyProcessor(processor.ProcessorABC):
    def __init__(self, flag=False):
        self._flag = flag
        self._accumulator = processor.dict_accumulator(
            {'sumw': processor.defaultdict_accumulator(float)},
        )

    @property
def accumulator(self):
        return self._accumulators

def process(self, df):
    output = self.accumulator.identity()
    # PHYSICS GOES HERE
    return output

def postprocess(self, accumulator):
    return accumulator

p = MyProcessor()
```

- **Root files**
- **Parquet files**
- **…**
- **map**
- **reduce**
- **Histories**
- **Event lists**
- **…**
Scaling out - lessons learned

• Every cluster is unique!
  - Executor + resource provisioning combinatorics leads to new issues at each site
  - Examples: network firewall between workers; filesystem parallel read limits; user code packaging.
  - **However, no issue required changes to user code**

• We run real-world analyses at a range of scales
  - 10 GB up to 10 TB demonstrated

• Factorizing the data delivery enables
  - Fast local prototyping
  - Seamless scale-out

• Intermediate scale resources are more important
  - An O(100) core-hour resource can execute a full CMS Run 2 columnar analysis
  - If executor is to provide <10 min time-to-insight, **resources must be dedicated or provisioned quickly!**
Looking forward

• As ecosystem matures, coffea will be factorized into separate packages
  - Subpackages that remain useful will stay
  - Some subpackages will be replaced by better alternatives

• The next frontier for resource and productivity gains is a multi-user analysis facility
  - Shared input cache at column granularity
  - Intermediate result cache
  - Unified metadata and schema database
  - Exportable derived columns
  - “slim and skim” with coffea, do the rest however you like
  - And more

• Coffea farms!
  - Plan to transition from current user-provisioned resources to a simple-to-deploy multi-user cluster
  - Primary technology focus has been Spark, but plans in place to test other schedulers
Conclusions

• Columnar analysis is effective for HEP analyst use cases
  - 10 CMS analysis groups have implemented or are implementing their analysis in coffea
    • Opportune moment: switch from private nTuples to NanoAOD
  - Prototype efforts in ATLAS, DUNE ongoing

• Columnar analysis enables performant code
  - Users write high-level operations, vectorized code stays in library

• Coffea simplifies interface to scale-out mechanisms

• Try it yourself: pip install coffea
  - Or poke around: [link]
Code samples I

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

```python
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)

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

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

```python
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)

```python
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

```python
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:

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

h = uproot.open("histo.root")["a2dhisto"]
xedges, yedges = h.edges
xcens, ycens = np.meshgrid(centers(xedges), centers(yedges))
points = np.hstack([xcens.flatten(), ycens.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**
Per-thread performance

- Z peak benchmark compared to ROOT
  - 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
  - Half the time spent in the uproot reading
  - Other executors may have different performance
  - Some awkward-array kernels are expensive
  - Work ongoing to port awkward-array to C++
    - https://github.com/scikit-hep/awkward-1.0
Scale-out performance

- Spark tests at FNAL show MHz-level performance with 500 cores for a full analysis code
  - Reading ~500 GB of ROOT TTree data over xrootd through laurelin

```
In [6]:
import time
from coffea.processor import run_spark_job
from coffea.processor.spark.spark_executor import spark_executor

tic = time.time()
final_accumulator = run_spark_job(datasets_spark, processor_instance, spark Executor,
  spark=spark, partitions=partitionsize, thread_workers=thread_workers,
  executor_args={'file_type': 'root', 'cache': True})
dt = time.time() - tic

loading: 0/44 [00:00<?, ?datasets/s]
```

- Parsl tests at 500-core scale already show <10m turnaround, more work to be done here

```
In []:
import time
from fnalColumnType_analysis_tools.processor import run_parsl_job
from fnalColumnType_analysis_tools.processor.parsl.parsl_executor import parsl_executor

tic = time.time()
treename = ['otree', 'Events'] # deal with mixed skims and full derived trees
final_accumulator = run_parsl_job(datasets, treenames, processor_instance, parsl_executor, 
  executor_args={'config':None}, data_flow='dfk, chunksize=chunksize')
dt = time.time() - tic

Processing: 0/44 [00:00<?, ?datasets/s]
```