Spark-like and query-like analysis systems and tools

(what works, what doesn’t work, what’s needed, and what we’re building to fill that need)

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“Analysis system” is a data access optimization scenario

The following are often true about end-user data analysis:

▶ Only need a small fraction of the event and particle attributes, like a few dozen.  
  (A handful of trigger flags, details on two or three particle types, maybe a veto on another’s kinematics, but nowhere close to the thousands of available attributes.)

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Consider this request: “Please submit a GRID job to plot the muon $p_T$ spectrum. Then we’ll think about what we want to look at next.” Is that unreasonable?
An example of what I have in mind: Google BigQuery

### New Query

<table>
<thead>
<tr>
<th>SELECT timestamp, country_code, file.name, file.version, file.type, url, details.distro.name, details.distro.version, details.system.name, details.system.release, details.cpu</th>
</tr>
</thead>
<tbody>
<tr>
<td>FROM TABLE DATE_RANGE</td>
</tr>
<tr>
<td>[the pg/pypi_downloads], TIMESTAMP('2017-01-28'), CURRENT_TIMESTAMP()</td>
</tr>
<tr>
<td>WHERE file.project = 'uproot' and details.installer.name = &quot;pip&quot; and details.distro.name = &quot;Raspberry GNU/Linux&quot;</td>
</tr>
</tbody>
</table>

#### Run Query

- **Save Query**
- **Save View**
- **Format Query**
- **Show Options**
- **Save to Table**
- **Save to Google Sheets**

#### Results

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<th>file.version</th>
<th>file.type</th>
<th>url</th>
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#### Table

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<th>Rows 1 - 17 of 37</th>
<th>Next</th>
<th>Last</th>
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<th>Download as JSON</th>
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<th>Save to Google Sheets</th>
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<tbody>
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So we can just use BigQuery, then?

No!!!

Reason #1: SQL. Simple HEP problems translate into complex SQL and moderate-to-complex HEP problems would be unreasonably difficult to express. Non-SQL languages in this problem space, such as SparkSQL's column expressions or Apache Drill's internal query language, are just as restrictive in the ways that matter.

Reason #2: Data model. The BigQuery paper (“Dremel”), Parquet & Drill (open source versions of the same), Apache Arrow, and SparkSQL all describe rich, nested data models sufficient to describe HEP events. However, for every one of these, you quickly encounter “not implemented yet” messages when you try to use them for HEP events.

Reason #3: User interface. The web form is fun, but we need queries embedded in an interactive, programmable environment with plotting and statistics libraries: ROOT or Python or both (probably both).
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HEP is both simpler and more complex than relational analytics

**HEP analysis is simpler**

HEP functions never have to cross events.

Common elsewhere: e.g. market basket analysis.
HEP is both simpler and more complex than relational analytics

HEP analysis is more complex

HEP data are variable-length, nested data structures, and we typically need to loop over combinations of particles.

In many fields, data are not considered ready for analysis until they’re in a tabular form. (Earlier steps are called “tidying.”)

<table>
<thead>
<tr>
<th>column 1</th>
<th>column 2</th>
<th>column 3</th>
</tr>
</thead>
<tbody>
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HEP is both simpler and more complex than relational analytics

<table>
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<th>Tabular Data</th>
<th>Independent Events</th>
<th>All-to-All Shuffle</th>
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<tr>
<td>Basic Spreadsheets</td>
<td>Relational Analytics</td>
<td></td>
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<td>HEP Analysis</td>
<td>Graph Analytics</td>
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</tr>
</tbody>
</table>

Variable-length, nested data
What should our data source be?

Identically typed, variable-length, nested data can be split into columns:

- All attribute values at a given level of hierarchy are stored together and may be retrieved independently of the rest.
- Good for reading only the dozen interesting attributes.
- ROOT has been doing this for years.
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- **Share cache**: column popularity distribution is steeper than the file popularity distribution; most popular columns could remain in memory for all users.
- **Avoid touching disk**: sorted partitions do not need to be fully read if a cut is being applied to the sorted variable (most likely $p_T$).
Object Array Map: columnar, hierarchical data as runtime objects

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- Arrays can come from anywhere: ROOT (through uproot), raw data files, remote network calls, HDF5, etc.

The same object can have attributes served from all of the above, so an official dataset can be served from ROOT files while a user’s modification (cuts or partial calculations applied) can be these ROOT files augmented by raw arrays.
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    \textit{The same object} can have attributes served from all of the above, so an official dataset can be served from ROOT files while a user’s modification (cuts or partial calculations applied) can be these ROOT files augmented by raw arrays.
  \item Array fetching is through an arbitrary dict-like object: may defer to disk, network, or per-column cache.
  \item OAMap has enough indirection that different particle types can be \textit{independently sorted} by their own $p_T$s. Thus, a filter like “muon $p_T > X$ and jet $p_T > Y$” may touch disk for only half the muon data and half the jet data.
\end{itemize}
```python
>>> import uproot

>>> import oamap.source.root

>>> url = "http://scikit-hep.org/uproot/examples/HZZ.root"

>>> events = uproot.open(url)['events'].oamap()

>>> events.schema.content['muons'].show()
List(
    starts = 'NMuon', # schema maps object attributes to array names
    stops = 'NMuon',
    content = Record( # at all levels of nesting
        fields = {
            'px': Primitive(dtype('float32'), data='Muon_Px'),
            'py': Primitive(dtype('float32'), data='Muon_Py'),
            'pz': Primitive(dtype('float32'), data='Muon_Pz'),
            'energy': Primitive(dtype('float32'), data='Muon_E'),
            'charge': Primitive(dtype('int32'), data='Muon_Charge'),
            'isolation': Primitive(dtype('float32'), data='Muon_Iso')
        }
    )
)```
The dataset looks like a nested Python list.

```python
>>> events
[<Event at index 0>, <Event at index 1>, <Event at index 2>, ..., <Event at index 2418>, <Event at index 2419>, <Event at index 2420>]

>>> events[0].muons
[<Muon at index 0>, <Muon at index 1>]

>>> [x.px for x in events[0].muons]
[-52.899456, 37.73778]

But it is generated on demand from arrays.

"NMuon": array([2, 1, 2, ..., 1, 1, 1], dtype=int32)
"Muon_Px": array([-52.899456, 37.73778, -0.81645936, ..., -29.756786, 1.1418698, 23.913206 ], dtype=float32)
```
OAMap example

It can also be included in compiled code with no change in syntax.

```python
>>> import numpy
>>> import numba
>>> import oamap.compiler
>>> @numba.njit # declares the following function to be compiled
... def compute(events, out):
...     i = 0
...     for event in events: # "event" and "event.muons" are a compiler fiction
...         if len(event.muons) == 2:
...             mu1, mu2 = event.muons[0], event.muons[1]
...             px = mu1.px + mu2.px
...             py = mu1.py + mu2.py
...             pz = mu1.pz + mu2.pz
...             energy = mu1.energy + mu2.energy
...             out[i] = sqrt(energy**2 - px**2 - py**2 - pz**2)
...             i += 1

>>> out = numpy.empty(1371)
>>> compute(events, out) # compilation and array-fetching happen on first call
>>> out
array([ 90.22780609,  74.74654388,  89.75765991, ...,  92.06494904,
        85.44384003,  75.96061707])
```
Current thinking...

outside

user query

reduced output

inside

data source

processing

new sources
Current thinking...

outside

Python function

reduced output

inside

ROOT/array OAMap

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new arrays
What should our reduced output be?

Simplest case: histograms, but that would get restrictive as analyses develop.
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- Until recently, I’ve had the wrong idea about what a Pandas DataFrame is: I thought it was a TTree (set of events) with egregious limitations:
  - Tabular, with little support for variable-length, nested data.
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- I had been missing an important fact: most of Pandas’s functionality is in its handling of *indexes*.
  - TTrees/events are indexed only by entry or run/event number.
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- Pandas has more in common with *histograms* than it does with *event sources*. 
Just an example...

I'll illustrate these operations through a series of examples. Consider a small DataFrame with string arrays as row and column indexes:

```python
In [94]: data = DataFrame(np.arange(6).reshape((2, 3)),
                      index=pd.Index(['Ohio', 'Colorado'], name='state'),
                      columns=pd.Index(['one', 'two', 'three'], name='number'))
```

```python
In [95]: data
Out[95]:
number  one  two  three
state
Ohio    0     1     2
Colorado 3     4     5
```

Using the `stack` method on this data pivots the columns into the rows, producing a Series:

```python
In [96]: result = data.stack()
```

```python
In [97]: result
Out[97]:
state number
Ohio one  0
two    1
three  2
Colorado one  3
two    4
three  5
```
Pandas generalizes what we do with histograms

```python
import pandhist

# define bins in many dimensions; we’ll think about how to plot later
muonhist = (pandhist
    .bin(100, 0, 500, "mass")
    .cut("q1*q2 < 0")
    .irrbin([0.2, 0.5], "mt1")
    .irrbin([0.2, 0.5], "mt2")
    .fillable())  # creates a fillable Pandas DataFrame

for muons, charge, mt2activity in uproot.iterate(
    "RA2Analysis/*.root", "TreeMaker2/PreSelection",
    ["Muons", "Muons_charge", "Muons_MT2Activity"], outputtype=tuple):
    for i in range(len(muons)):
        if len(charge[i]) == 2:
            mu1, mu2 = muons[i]
            q1, q2 = charge[i]
            mt1, mt2 = mt2activity[i]
            # fill method has an argument for each variable
            muonhist.fill((mu1 + mu2).mass, q1, q2, mt1, mt2)
```

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Pandas generalizes what we do with histograms

```python
>>> muonhist

| mass       | q1*q2 < 0 | mt1 | mt2         | count | # in this example, count is
|------------|-----------|-----|-------------|-------| # the only column; the rest
| [inf, 0.0) | fail      | [inf, 0.2) | [inf, 0.2) | 0.0   | # is a hierarchical index
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
| [0.2, 0.5) |           | [inf, 0.2) | 0.0        |
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
| [0.5, inf) |           | [inf, 0.2) | 0.0        |
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
| pass      | [inf, 0.2) | [inf, 0.2) | 0.0        | # if we asked for weights,
|           |           | [0.2, 0.5) | 0.0        | # sumw and sumw2 would be
|           |           | [0.5, inf) | 0.0        | # separate columns
| [0.2, 0.5) |           | [inf, 0.2) | 0.0        |
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
| [0.5, inf) |           | [inf, 0.2) | 0.0        |
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
|           |           |           |           | # but most of the work is done
|           |           | [0.2, 0.5) | 0.0        | # by the hierarchical index
|           |           | [0.5, inf) | 0.0        |
| [0.5, inf) |           | [inf, 0.2) | 0.0        |
|           |           | [0.2, 0.5) | 0.0        |
|           |           | [0.5, inf) | 0.0        |
|           |           |           |           | ...

[1836 rows x 1 columns]
```
Pandas generalizes what we do with histograms

```python
>>> pandhist.steps("mass").data(muonhist)
```

![Histogram](image.png)
Pandas generalizes what we do with histograms

```python
>>> pandhist.steps("mass").overlay("q1*q2 < 0").data(muonhist)
```
Pandas generalizes what we do with histograms

```python
>>> pandhist.area("mass").stack("q1*q2 < 0").data(muonhist)
```

![Histogram](chart.png)
Pandas generalizes what we do with histograms

```python
>>> pandhist.steps("mass").column("q1*q2 < 0").data(muonhist)
```
Pandas generalizes what we do with histograms

```python
>>> pandhist.steps("mass").row("mt1").column("mt2").data(muonhist)
```
Pandas generalizes what we do with histograms

```python
>>> pandhist.steps("mass").overlay("q1*q2 < 0").row("mt1").column("mt2").data(muonhist)
```
Current thinking...

outside

Python function

reduced output

inside

ROOT/array OAMap

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- **Dask** looks like a good choice: it’s in the C++/Python world, general enough to piece together what we need out of basic parts.

  (More about this in the concurrency session.)
Current thinking...
Current thinking...
What should our data storage be?

Again, no need for HEP to invent.
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- Using columns, rather than files, as the fundamental unit means keeping track of a much larger number of named entities.
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- **Ceph** is both an object store and a filesystem, and it minimizes metadata overhead by coordinating data placement through a static function, rather than a dynamic service.
  - Lets us experiment both ways.
  - We could use the static function to place executable tasks, improving data locality...
Current thinking...
Current thinking...
Conclusions

Though an analysis service should use as many open source parts as possible, some functionality is missing and we need to build our own.

Software products developed along the way:

- **uproot** Quickly access ROOT branches as arrays. mature, in use
- **oamap** Translate between object-oriented Python and low-level array operations. ready for testing
- **pandhist** Reinterpretation of Pandas DataFrames as super-histograms. (Plotting in Vega-Lite.) experimental
- **vegascope** Browser-based TCanvas for Vega/Vega-Lite, so that you don’t have to use Jupyter if you don’t want to. done (simple)
- ? OAMap as a collection in Dask.
- ? Column manager (for sharing data among datasets).
- ? All-in-one environment for query-based analysis.