Data analysis tools from within HEP and from industry

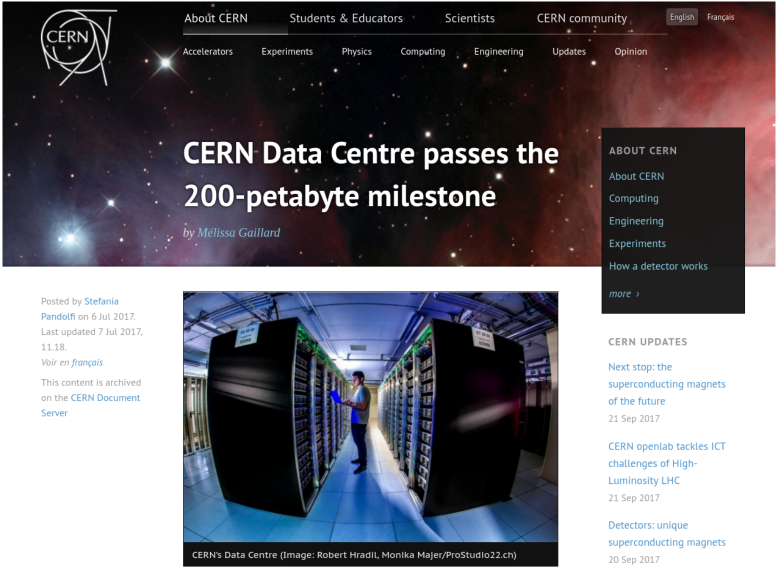
Jim Pivarski

Princeton University – DIANA-HEP

July 12, 2018

I'm going to start with a dumb comparison, to make a point.

We measure globally distributed data in hundreds of PB



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CERN Data Centre passes the 200-petabyte milestone

by Mélissa Gaillard

Posted by Stefania Pandolfi on 6 Jul 2017. Last updated 7 Jul 2017, 11.18.

Voir en français

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CERN's Data Centre (Image: Robert Hradil, Monika Majer/ProStudio22.ch)

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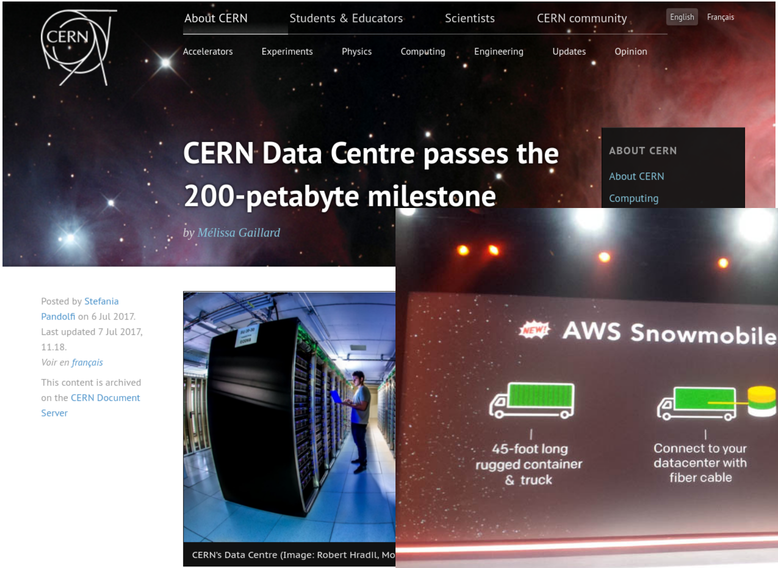
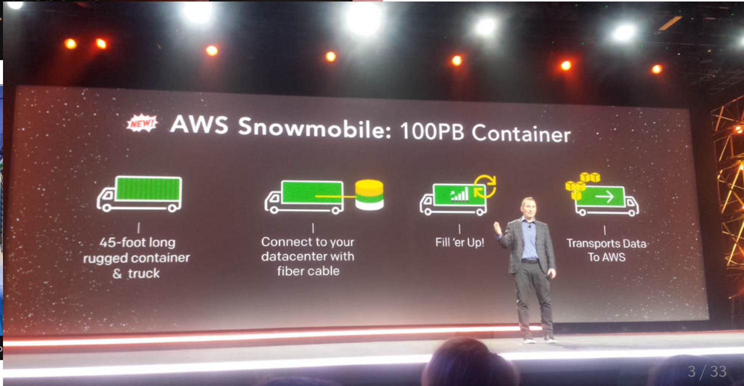
But for “web scale” companies, 100 PB = 1 truck





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- x FTEs in HEP developing open source analysis tools
- y FTEs outside of HEP developing open source analysis tools (not sure of x and y, but $x \ll y$)

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→ There's a lot of good data analysis software out there!
  → Could adopting it reduce in-house maintenance burdens?
    → More training examples and career options for users?

Show of hands: are you currently using data analysis software created outside of HEP?

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Are you planning to or want to?

On the other hand. . .

Another important metric: experience!

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The simple prescription of "just use Spark" would leave analyzers without some necessary tools.

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Continue developing our own everything.

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#3 is my opinion, but it begs the question: what's HEP-specific and what's not?

Three examples each:

What they've got

1. Distributed DAG processing
2. Indexed analysis
3. Machine learning

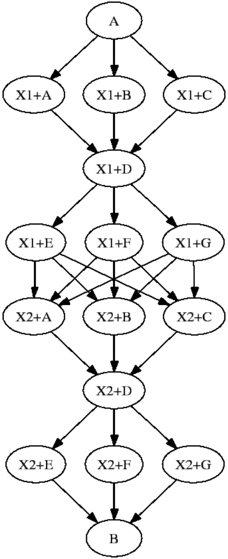
What we'd need

1. Nested data structures
2. Advanced histogramming
3. Ansatz fitting

Distributed DAG processing

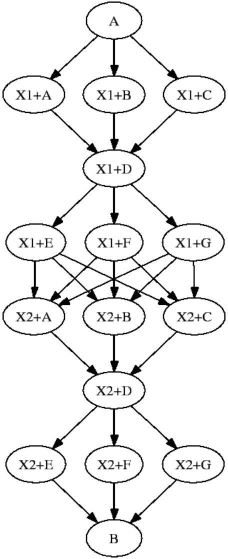
not HEP-specific

Distributed DAG processing



DAG: Directed Acyclic Graph of dependencies between subtasks.
Some would say this is what big data processing *is*.

Distributed DAG processing



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Spark (JVM), Dask, Joblib, Parsl (Python), Storm (continuous), Thrill (C++), DAGMan (HTCondor), TensorFlow (fitting)...

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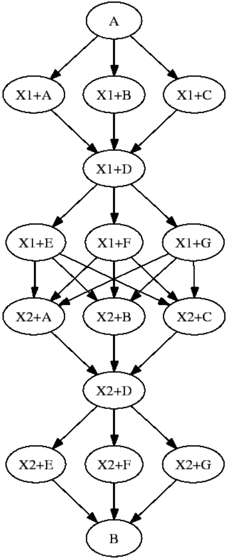

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To use these frameworks, one must

- express user tasks as DAG nodes (e.g. ROOT RDataFrame);
- serialize user functions on the driver and load user data on the workers in accordance to the framework's way of doing things.

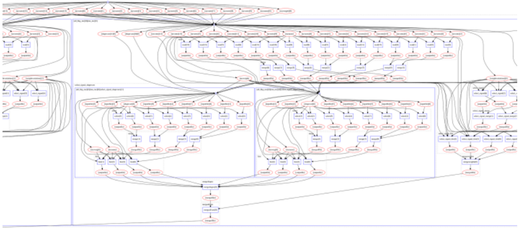
From "REANA: A System for Reusable Research Data Analyses"

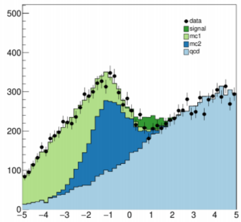
reana

Reproducible research data analysis platform

http://www.reana.io/

Example: BSM search

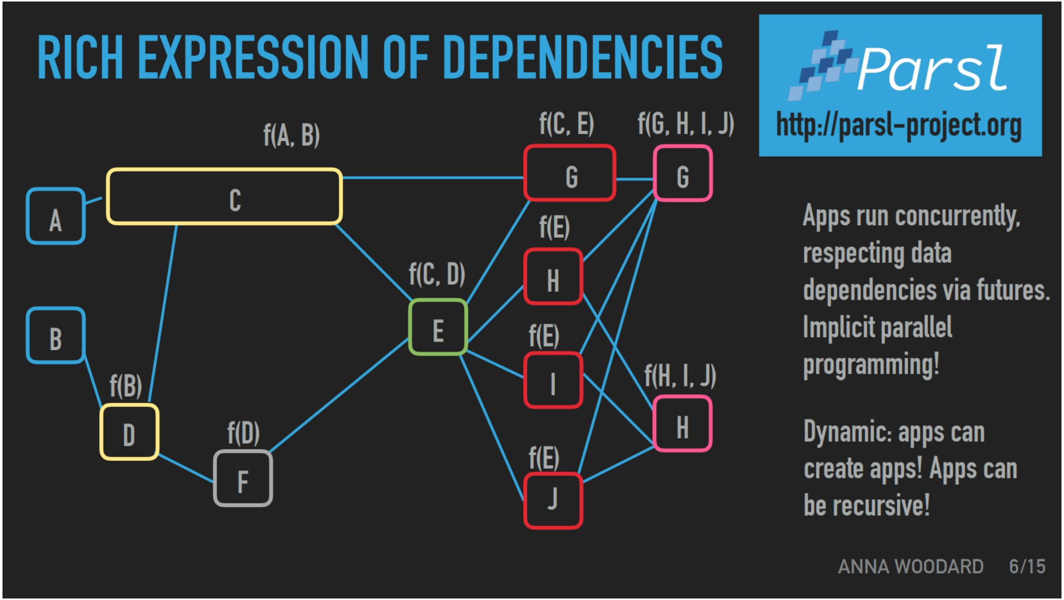




https://github.com/reanahub/reana-demo-bsm-search/

Complex computational workflows typical in particle physics analyses.

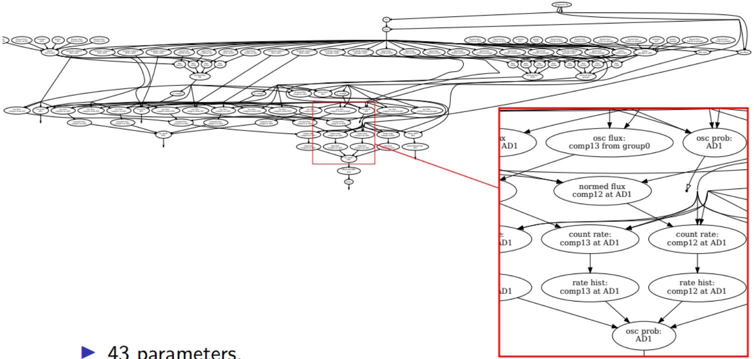
From “Interactive, scalable, reproducible data analysis with con. . .



From "GNA: new framework for statistical data analysis"

Computational graph example

The whole JUNO graph



- 43 parameters.
- The JUNO graph contains 110 nodes and 174 edges.
- It produces a histogram of 280 bins.

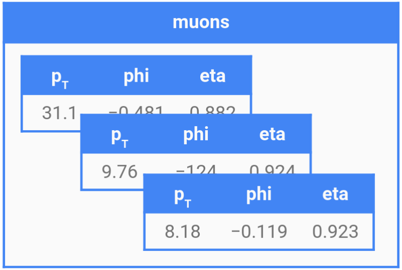
HEP has adopted the idea of DAGs, but will we be developing our own DAG-processors or using what we find?

(*Can* we? Why or why not?)

Nested data structures

strangely HEP-specific

Nested data structures



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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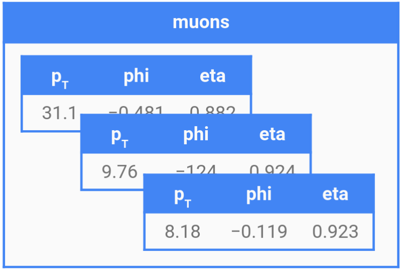

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Objects are essential in HEP analysis.

Many physicists consider TTrees with `std::vector<float>` branches to be “minimal” or “flat.”

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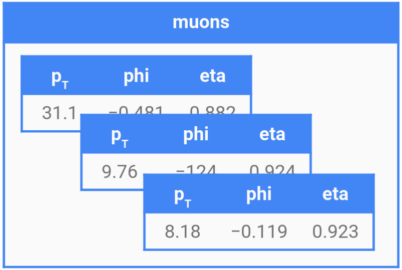

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Most data analysis tools have an SQL mindset, with rectangular data tables.

Objects $\to$ rectangular tables is lossy!

Performance claims often start the stopwatch after this “data cleaning.”

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- HDF5 has lists of compounds, but they're rowwise ("unsplit").
- Pandas can put arbitrary Python objects in DataFrames, but most operations only apply to numbers.

Nested data structures

```
>>> import uproot
>>> t = uproot.open("tests/samples/HZZ.root")["events"]
>>> t.pandas.df(["MET_px", "Muon_Px", "Electron_Px"], entrystart=-20, flatten=False)

           MET_px                 Muon_Px             Electron_Px
2401     2.998099             [-1.492689]                      []
2402    27.944883             [-4.560287]                      []
2403     3.787466             [-9.715589]                      []
2404     9.378232            [-31.072098]                      []
2405   -17.310106  [47.484627, 4.6953125]                      []
2406   -81.965927  [74.75617, -20.911081]                      []
2407    -9.059591 [25.786427, -29.265024]                      []
2408    25.649775                      []                      []
2409    29.691553             [-24.7368]                      []
2410   -25.754967 [53.005814, -30.208649] [-37.681973, 18.453588]
2411    -2.426847   [55.7203, -26.914448]                      []
2412   -15.611773             [14.896802]                      []
2413    18.921183            [-24.158083]                      []
2414   -11.730723             [-9.204197]                      []
2415   -10.648725  [34.506527, -31.56778]                      []
2416   -14.607650            [-39.285824]                      []
2417    22.208313             [35.067146]                      []
2418    18.101646            [-29.756786]                      []
2419    79.875191             [1.1418698]                      []
2420    19.713749             [23.913206]                      []
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In some cases, maybe we're using the wrong idiom: instead of working with structured values, Pandas prefers structured indexes.

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                   MET_px    Muon_Px  Electron_Px
entry subentry
2401  0          2.998099  -1.492689          NaN
2402  0         27.944883  -4.560287          NaN
2403  0          3.787466  -9.715589          NaN
2404  0          9.378232 -31.072098          NaN
2405  0        -17.310106  47.484627          NaN
      1               NaN   4.695312          NaN
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2415  0        -10.648725  34.506527          NaN
      1               NaN -31.567780          NaN
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This is my main project now: fast manipulation of columnar data.

General programming model

```
@numba.jit      # LLVM-compiled Python
def deltaphi(event):
    metphi = event.MET.phi
    for jet in event.jets:
        yield metphi - jet.phi
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Numpy-like broadcasting

Awkward Array

```
# one per event          one per particle
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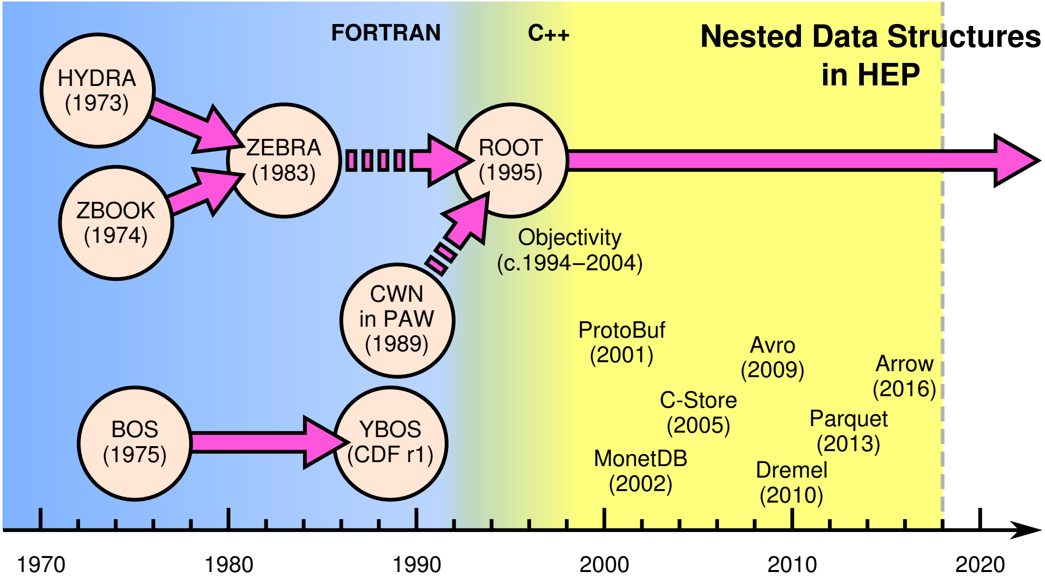
Also, this *should* be of wider interest than HEP: developers of Arrow, Dask, and XND (∼Numpy 2.0) are curious about it.

Missed opportunity



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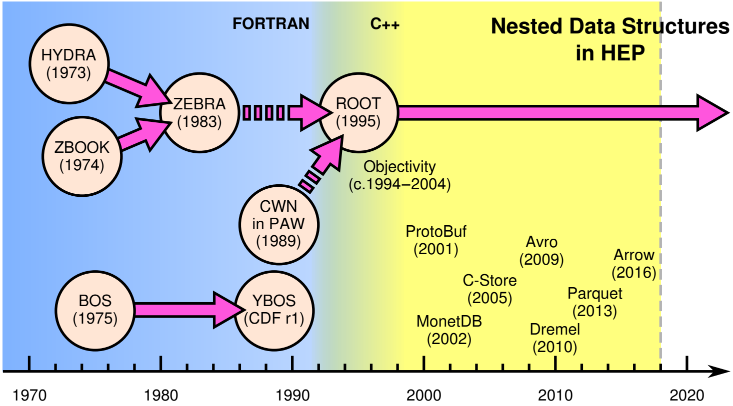

Google Dremel paper (2010):
(inspired Parquet)

storage and reduce CPU cost due to cheaper compression. Column stores have been adopted for analyzing relational data [1] but to the best of our knowledge have not been extended to nested data models. The columnar storage format that we present is supported by

Indexed analysis

not well-known in HEP

To understand what I mean by "indexed analysis," consider analysis with *less advanced indexing* than modern HEP.

Indexed analysis

```
h/cr/1d 201 'd0miss' 100 -0.5e-3 0.5e-3
h/cr/1d 202 'z0miss' 100 -0.015 0.015
h/cr/1d 203 'pxmiss' 100 -0.076 0.076
h/cr/1d 204 'pymiss' 100 -0.076 0.076
h/cr/1d 205 'pzmiss' 100 -0.076 0.076
nt/plot 2.d0 ! ! ! ! ! 201
nt/plot 2.z0 ! ! ! ! ! 202
nt/plot 2.px ! ! ! ! ! 203
nt/plot 2.py ! ! ! ! ! 204
nt/plot 2.pz ! ! ! ! ! 205

h/cr/1d 301 'normalized d0miss' 100 -10 10
h/cr/1d 302 'normalized z0miss' 100 -10 10
h/cr/1d 303 'normalized pxmiss' 100 -10 10
h/cr/1d 304 'normalized pymiss' 100 -10 10
h/cr/1d 305 'normalized pzmiss' 100 -10 10
nt/plot 2.d0/sqrt(ed0) ! ! ! ! ! 301
nt/plot 2.z0/sqrt(ez0) ! ! ! ! ! 302
nt/plot 2.px/sqrt(epx) ! ! ! ! ! 303
nt/plot 2.py/sqrt(epy) ! ! ! ! ! 304
nt/plot 2.pz/sqrt(epz) ! ! ! ! ! 305

h/cr/1d 401 'd0miss after constraint' 100 -0.1e-16 0.1e-16
h/cr/1d 402 'z0miss after constraint' 100 -0.1e-15 0.1e-15
h/cr/1d 403 'pxmiss after constraint' 100 -0.01 0.01
h/cr/1d 404 'pymiss after constraint' 100 -0.01 0.01
h/cr/1d 405 'pzmiss after constraint' 100 -0.01 0.01
nt/plot 2.ad0 ! ! ! ! ! 401
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To the left is a PAW script (pre-ROOT), creating and filling histograms.

Histograms were indexed by numbers because they didn't have *names* back then.

Indexed analysis

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h/cr/1d 304 'normalized pymiss' 100 -10 10
h/cr/1d 305 'normalized pzmiss' 100 -10 10
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The ability to name stuff was as fundamental to HEP data analysis as handwashing was to medical science!

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nt/plot 2.z0/sqrt(ez0) ! ! ! ! ! 302
nt/plot 2.px/sqrt(epx) ! ! ! ! ! 303
nt/plot 2.py/sqrt(epy) ! ! ! ! ! 304
nt/plot 2.pz/sqrt(epz) ! ! ! ! ! 305

h/cr/1d 401 'd0miss after constraint' 100 -0.1e-16 0.1e-16
h/cr/1d 402 'z0miss after constraint' 100 -0.1e-15 0.1e-15
h/cr/1d 403 'pxmiss after constraint' 100 -0.01 0.01
h/cr/1d 404 'pymiss after constraint' 100 -0.01 0.01
h/cr/1d 405 'pzmiss after constraint' 100 -0.01 0.01
nt/plot 2.ad0 ! ! ! ! ! 401
nt/plot 2.az0 ! ! ! ! ! 402
nt/plot 2.apx ! ! ! ! ! 403
nt/plot 2.apy ! ! ! ! ! 404
nt/plot 2.apz ! ! ! ! ! 405
```

To the left is a PAW script (pre-ROOT), creating and filling histograms.

Histograms were indexed by numbers because they didn't have *names* back then.

The ability to name stuff was as fundamental to HEP data analysis as handwashing was to medical science!

But we don't have to stop there. There's more to indexing than name-value pairs.

From “Pandas DataFrames for F.A.S.T. binned analysis at CMS”

Example Cut-flow Dataframe

component	depth	class	name	pass	total
data	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	16208	469384
		LambdaStr	ev: ev.triggerIsoMu24[0]	16208	16208
		LambdaStr	ev: ev.Muon_Pt[0] > 25	15995	16208
dy	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	37559	77729
		LambdaStr	ev: ev.triggerIsoMu24[0]	37559	37559
		LambdaStr	ev: ev.Muon_Pt[0] > 25	37263	37559
qcd	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	0	142
		LambdaStr	ev: ev.triggerIsoMu24[0]	0	0
		LambdaStr	ev: ev.Muon_Pt[0] > 25	0	0
single_top	1	LambdaStr	ev: len(ev.Muon_Iso_Idx) >= 2	111	5684
		LambdaStr	ev: ev.triggerIsoMu24[0]	111	111
		LambdaStr	ev: ev.Muon_Pt[0] > 25	110	111
ttbar	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
wjets	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
ww	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
wz	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev:		
		LambdaStr	ev:		
zz	1	LambdaStr	ev: len(ev.		
		LambdaStr	ev: ev.triggerIsoMu24[0]	1235	1235
		LambdaStr	ev: ev.Muon_Pt[0] > 25	1232	1235

```
# Apply an event selection
Selection:
    Selection:
        All:
            - len(ev.Muon_Iso_Idx) >= 2
            - ev.triggerIsoMu24[0]
            - ev.Muon_Pt[0] > 25
```


component	depth	class	name	pass	total
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Pandas DataFrames filled by AlphaTwirl, analyzed by F.A.S.T.

From "Pandas DataFrames for F.A.S.T. binned analysis at CMS"

Manipulating DFs: Long to wide form

```python
# Convert variance --> error
df["err"] = np.sqrt(df.nvar)

# Switch to long-form
df2 = df.pivot_table(index="dimu_mass", columns="component", values=["n", "err"])
df2 = df2.sort_index(axis=1, ascending=False)

# Sort components to match tutorial
order = ["data", "ttbar", "wjets", "dy", "ww", "wz", "zz", "qcd", "single_top"]
df2 = df2.reindex(order, axis=1, level="component")

# Show first 10 rows
df2.head(10)
```

	n								err			
component	**data**	**ttbar**	**wjets**	**dy**	**ww**	**wz**	**zz**	**single_top**	**data**	**ttbar**	**wjets**	**d**
dimu_mass												
-inf	993.0	11.392980	0.311917	655.570771	3.600221	0.320914	0.360053	1.741041	31.511903	1.752727	0.311917	3
60.000000	38.0	0.840432	0.000000	23.963227	0.063284	0.053328	0.000000	0.065288	6.164414	0.486302	0.000000	:
61.000000	25.0	0.319709	NaN	25.572841	0.102053	0.000000	NaN	0.005831	5.000000	0.275655	NaN	:
62.000000	22.0	0.274432	NaN	29.271624	0.068484	0.038697	NaN	0.000000	4.690416	0.274432	NaN	:
63.000000	28.0	0.000000	NaN	22.941727	0.194258	0.000000	0.009475	NaN	5.291503	0.000000	NaN	:
64.000000	29.0	0.847224	NaN	20.534599	0.065338	0.081642	0.009540	NaN	5.385165	0.490427	NaN	:
65.000000	17.0	0.352667	NaN	29.464412	0.130224	0.000000	0.004153	0.093700	4.123106	0.282423	NaN	:
66.000000	37.0	0.570011	NaN	27.861013	0.128668	0.059988	0.015375	0.000000	6.082763	0.403615	NaN	:
67.000000	34.0	0.817704	NaN	34.173523	0.063818	0.000000	0.017707	0.000652	5.830952	0.475827	NaN	.
68.000000	31.0	0.753107	NaN	26.971645	0.024008	0.042326	0.000000	0.000000	5.567764	0.440761	NaN	:

Depending on task, "wide-form" tables can be easier to work with

Pandas DataFrames filled by AlphaTwirl, analyzed by F.A.S.T.

I had the same thought: our primary examples of indexable data are histograms and systems of related histograms. Rich indexing would let us project/rebin/cut/transform histograms more fluidly.

```
>>> from histbook import *
>>> multihist = Hist(bin("mass", 100, 0, 500), cut("q1*q2 < 0"),
...                  split("mt1", [0.2, 0.5]), split("mt2", [0.2, 0.5]), fill=df)
>>> multihist.pandas()
                                                   count()  err(count())
mass           q1*q2 < 0 mt1         mt2
[-inf, 0.0)    fail      [-inf, 0.2) [-inf, 0.2)       0.0           0.0
                                     [0.2, 0.5)        0.0           0.0
                                     [0.5, inf)        0.0           0.0
                         [0.2, 0.5)  [-inf, 0.2)       0.0           0.0
                                     [0.2, 0.5)        0.0           0.0
                                     [0.5, inf)        0.0           0.0
                         [0.5, inf)  [-inf, 0.2)       0.0           0.0
                                     [0.2, 0.5)        0.0           0.0
                                     [0.5, inf)        0.0           0.0
               pass      [-inf, 0.2) [-inf, 0.2)       0.0           0.0
                                     [0.2, 0.5)        0.0           0.0
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                         [0.2, 0.5)  [-inf, 0.2)       0.0           0.0
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>>> multihist.step("mass")
```

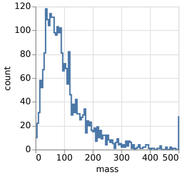

Indexed analysis

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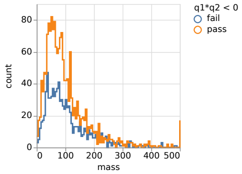
>>> multihist.overlay("q1*q2 < 0").step("mass")
```



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>>> multihist.stack("q1*q2 < 0").area("mass")
```

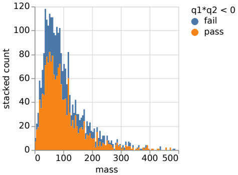

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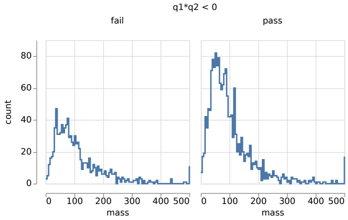
```



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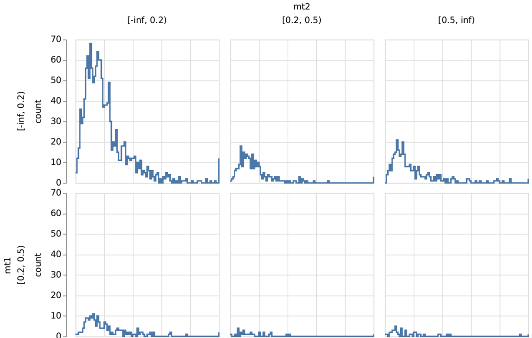

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```

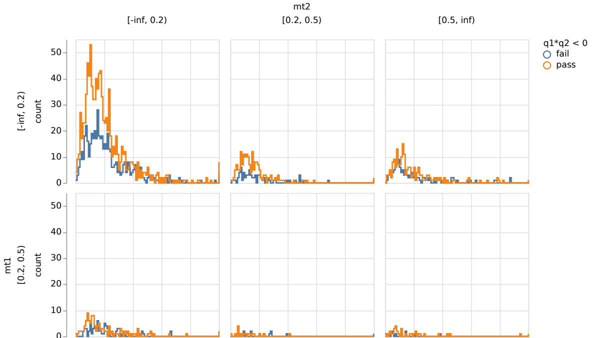

Indexed analysis

Using tools with rich indexing systemizes what we're already doing with naming conventions, splitting names on underscores, etc.

Pandas is not a TTree replacement— if anything, it's a histogram organizer!

Advanced histogramming

very HEP-specific

Advanced histogramming

The histograms themselves, however, are more sophisticated in HEP than elsewhere.

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These features aren't difficult, but they're our responsibility.

Machine learning versus ansatz fitting

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Qualitatively different purposes: **both needed.**

We can look to industry for machine learning innovations, but the best ansatz fitters are in HEP: RooFit, RooStats, GooFit, HistFitter, HistFactory, pyhf...

Areas of overlap

What they've got

1. Distributed DAG processing
2. Indexed analysis
3. Machine learning

What we'd need

1. Nested data structures
2. Advanced histogramming
3. Ansatz fitting

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What we'd need

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2. Advanced histogramming
3. Ansatz fitting

Nearly all ML techniques require flattened or sequences of flattened data, but we have real problems that need nested data: e.g. classifying N_i jets per event (nested, unordered sets). RNNs and LSTMs (for non-nested, ordered sequences) are designed for a different data type!

Areas of overlap

<u>What they've got</u>

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1. Nested data structures
2. **Advanced histogramming**
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F.A.S.T. and histbook are incorporating Pandas indexing into advanced histogramming.

Areas of overlap

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1. **Distributed DAG processing**
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1. Nested data structures
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3. **Ansatz fitting**

As fits get bigger, they may need to be distributed, for instance with iterative map-reduce.

Conclusions

Data analysis tools outside of HEP are mature but not a perfect fit to our needs.

- Some of what we need is available now: can we use it?
- Some exists only as HEP software: can it interoperate?
- Some of what's available is unlike anything we do now: an opportunity to do better physics?

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Data analysis tools outside of HEP are mature but not a perfect fit to our needs.

- Some of what we need is available now: can we use it?
- Some exists only as HEP software: can it interoperate?
- Some of what's available is unlike anything we do now: an opportunity to do better physics?
- The door swings both ways: we have things to teach the world!