YAML as an ADL: YADL (?) The F.A.S.T. analysis tools





Software Sustainability Institute Ben Krikler 7th May 2019

Analysis Description Languages for the LHC: indico.cern.ch/event/769263/

Outline of this talk

Why YAML?

How do the tools work?

What's next?

Why focus on YAML?

- An existing markup: many parsers exist
- A superset of JSON
 - Static object description (dicts, lists, numbers, strings)
 - Adds anchors and references: reuse common occurrences
- Easier to read than JSON:
 - Can write without brackets and braces
 - Indentation to imply nesting (c.f. python)
- Naturally declarative: No "control flow" (e.g. no for loops)
- Widely used to describe pipeline configuration:
 - gitlab-Cl, travis-Cl, Azure Cl/CD, Ansible, Kubernetes, etc
 - HEPData: YAML for reproducible Data

How do we use YAML at this point?

Four separate types of YAML file, to answer:

- 1. What are your datasets?
- 2. How to process them into tables (histograms and cut-flow efficiencies)?
- 3. How to convert histograms into fitting inputs?
- 4. How to visualise outputs?

"Hang on Ben, isn't that just a set of configuration files?" Much of this project is building towards a DSL but that's something of a secondary consequence of the key goal behind all of this....

Ask not "what does my code need me to do for it"

but "what do I want my code to do for me"

The F.A.S.T tools...

FAST codebase

A minimal-viable product to develop these ideas

- Changing rapidly and often
- Some sizeable changes on the roadmap

Developed largely by myself and a couple of others

But being used in some form for 2 CMS analyses and students on DUNE, FCC, LUX-ZEPLIN experiments

• Have seen students copy snippets verbatim into talks to other collaboration members

Code to handle configs and execute all written in Python

- Use existing tools as much as possible
- My goal: code written by $me \rightarrow 0$

Where to find the code

- Docs: <u>fast-carpenter.readthedocs.io/</u>
- All on CERN's gitlab, likely to move to github soon
 - <u>https://gitlab.cern.ch/fast-hep/public</u>
 - Main package: gitlab.cern.ch/fast-hep/public/fast-carpenter
- Demo repository where most examples in this talk come from: <u>gitlab.cern.ch/fast-hep/public/fast cms pu</u> <u>blic tutorial</u>

A fast-carpenter

Docs » fast-carpenter

View page source

Search docs

CONTENTS:

Installing Key Concepts

Command-line Usage

The Processing Config Example repositories

Glossary

CODE REFERENCE

fast_carpenter package fast_carpenter.define_package

fast_carpenter.define.reductions module

fast_carpenter.define.systematics module

fast_carpenter.define.variables module fast_carpenter.event_builder module fast_carpenter.expressions module fast_carpenter.help module fast_carpenter.masked_tree module fast_carpenter.selection.package fast_carpenter.selection.filters module fast_carpenter.selection.stace module

fast_carpenter.summary package

fast_carpenter.summary.binned_dataframe module

fact comontor cummon chinning con

Read the Docs



Turns your trees into tables (ie. reads ROOT TTrees, writes summary Pandas DataFrames)

pypi v0.9.1 pipeline passed coverage 71.00% docs passing chat on gitter

fast-carpenter can:

- Be controlled using YAML-based config files
- Define new variables
- Cut out events or define phase-space "regions"
- Produce histograms stored as CSV files using multiple weighting schemes
- Make use of user-defined stages to manipulate the data

Powered by:

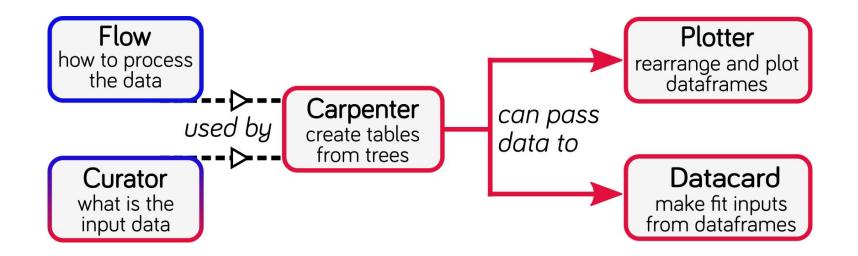
- AlphaTwirl (presently): to run the dataset splitting
- Atuproot: to adapt AlphaTwirl to use uproot
- uproot: to load ROOT Trees into memory as numpy arrays
- fast-flow: to manage the processing config files
- fast-curator: to orchestrate the lists of datasets to be processed
- coffee: to help the developer(s) write code

A tool from the Faster Analysis Software Taskforce: http://fast-hep.web.cern.ch/

Contents:

- Installing
 - From Pypi
 - From Source
- Key Concepts
 - Goals of fast-carpenter

FAST codebase interplay





Changes since IRIS-HEP presentation (4th March)

https://indico.cern.ch/event/802182/contributions/3334624/

1 Documentation on readthedocs



Stage to produce a ghast



Import mechanism for processing description

Optimisation of various stages behind the scenes

How it works...

Anatomy of the processing description

What type of action to take at each step:

- Stage1 = A built-in stage of fast-carpenter
- Stage2 = A stage imported from a python module
- IMPORT = Import a list of stages and their descriptions from another YAML file

For each stage named above:

- Provide a dictionary of keyword arguments
- Passed through to stage's init method

stages:

- Stage1: StageFromBackend
- Stage2: module.that.provides.some.Stage
- IMPORT: "{this_dir}/another_description.yaml"

```
Stage1:
   keyword: value
   another_keyword: [a, list, of, values]
```

```
Stage2:
   arg1: 35
   arg2:
      takes: ["a", "dict"]
      with: 3
      different: keys
```

Stages section: What do you want to do with the data?

stages:

- # Just defines new variables
- BasicVars: fast_carpenter.Define
- # A custom class to form the invariant mass of a
- # two-object system
- DiMuons: cms_hep_tutorial.DiObjectMass
- # Filled a binned dataframe
- NumberMuons: fast_carpenter.BinnedDataframe
- # Select events by applying cuts
- EventSelection: fast_carpenter.CutFlow
- # Fill another binned dataframe
- DiMuonMass: fast_carpenter.BinnedDataframe

(Currently) a *sequence* of stages and their descriptions.

Each stage:

- Can be any python importable class
- Should implement three or four key processing methods
- Fast-carpenter provides several stages

For example:

- 1. Define some variables
- 2. Make a histogram
- 3. Cut out some events
- 4. Make another histogram

Define Stage: fast_carpenter.Define

BasicVars:

variables:

- Muon_Pt: "sqrt(Muon_Px ** 2 + Muon_Py ** 2)"
- IsoMuon_Idx: (Muon_Iso / Muon_Pt) < 0.10
- # This next variable will create a single
 # number for each event, using a set of inputs
 # whose length varies for each event
- NIsoMuon:

formula: IsoMuon_Idx
reduce: count_nonzero

- HasTwoMuons: NIsoMuon >= 2
- # Capture first muon's Pt, padded
- # with NaNs if NMuon < 1</pre>
- Muon_lead_Pt: {reduce: 0, formula: Muon_Pt}
- # Capture second muon's Pt, padded
- # with NaNs if NMuon < 2</pre>
- Muon_sublead_Pt: {reduce: 1, formula: Muon_Pt}

- Combines uproot + numexpr (v2)
 - Presents a dict-like object to numexpr, containing uproot tree and other new variables
 - <u>https://gitlab.cern.ch/fast-hep/public/fast-ca</u> <u>rpenter/blob/master/fast_carpenter/express</u> <u>ions.py</u>
 - All input variable in expression need same "jaggedness"
 - In future: numpy-like broadcasting across jaggedness
- Additional reductions: object-level variables (jagged arrays) to event-level
- Adds variables into tree using replaced `itervalues` method
- Can some of this become central functionality within uproot(-methods) in the future?

Select events fast_carpenter.CutFlow

DiMu_controlRegion:

weights: {nominal: weight}
selection:

All:

- {reduce: 0, formula: Muon_pt > 30}
- leadJet_pt > 100
- All:
 - DiMuon_mass > 60
 - DiMuon_mass < 120
- Any:
 - nCleanedJet == 1
 - DiJet_mass < 500
 - DiJet_deta < 2

Masks events from subsequent stages

Produces a cut-flow summary with:

- Raw and weighted yields
- Inclusive and exclusive yields to each cut

Selection is specified as a nested dictionary of All and Any and a list of cuts

 Inspired by Tai Sakuma's approach in AlphaTwirl

Individual cuts use same scheme as variable definition

EventSelection: weights: {weighted: EventWeight} selection:

All:

- NIsoMuon >= 2
- triggerIsoMu24 == 1
- {reduce: 0, formula: Muon_Pt > 25}

Select events fast_carpenter. CutFlow

Resulting cut-flow outputs from EventSelection config on last slide

>>> import pandas as pd >>> pd.read_csv("cuts_EventSelection-weighted.csv", header=[0, 1], index_col=[0, 1, 2])								
			passed_incl		passed_excl		totals_excl	
6.03			unweighted	EventWeight	unweighted	EventWeight	unweighted	EventWeight
dataset	deptl							
data	Θ	All	15995.0	15995.000000	15995.0	15995.000000	469384.0	469384.000000
	1	NIsoMuon >= 2	16208.0	16208.000000	16208.0	16208.000000	469384.0	469384.000000
		triggerIsoMu24 == 1	469384.0	469384.000000	16208.0	16208.000000	16208.0	16208.000000
		{'formula': 'Muon_Pt > 25', 'reduce': 0		229710.000000	15995.0	15995.000000	16208.0	16208.000000
dy	Θ	All	37263.0	16628.843750		16628.843750	77729.0	34115.511719
	1	NIsoMuon >= 2	37559.0	16829.451172	37559.0	16829.451172	77729.0	34115.511719
		triggerIsoMu24 == 1	77729.0	34115.511719	37559.0	16829.451172	37559.0	16829.451172
		{'formula': 'Muon_Pt > 25', 'reduce': 0		32168.121094	37263.0	16628.843750	37559.0	16829.451172
qcd	Θ	All	0.0	0.00000	0.0	0.000000	142.0	79160.507812
		NIsoMuon >= 2	0.0	0.00000	0.0	0.00000	142.0	79160.507812
		triggerIsoMu24 == 1	142.0	79160.507812	0.0	0.00000	0.0	0.00000
		{'formula': 'Muon_Pt > 25', 'reduce': 0		6014.819336	0.0	0.00000	0.0	0.00000
single_top		All	110.0	5.676235	110.0	5.676235	5684.0	311.622986
	1	NIsoMuon >= 2	111.0	5.748312	111.0	5.748312	5684.0	311.622986
		triggerIsoMu24 == 1	5684.0	311.622986	111.0	5.748312	111.0	5.748312
		{'formula': 'Muon_Pt > 25', 'reduce': 0		290.494965	110.0	5.676235	111.0	5.748312
ttbar	Θ	All	206.0	47.293686	206.0	47.293686	36941.0	7929.475586
		NIsoMuon >= 2	226.0	51.629749	226.0	51.629749	36941.0	7929.475586
		triggerIsoMu24 == 1	4515.0	1001.804932	206.0	47.293686	226.0	51.629749
		{'formula': 'Muon_Pt > 25', 'reduce': 0		1109.433960	206.0	47.293686	206.0	47.293686
wjets	Θ	All	1.0	0.311917	1.0	0.311917	109737.0	209603.531250
		NIsoMuon >= 2	1.0	0.311917	1.0	0.311917	109737.0	209603.531250
		triggerIsoMu24 == 1	109737.0	209603.531250	1.0	0.311917	1.0	0.311917
		{'formula': 'Muon_Pt > 25', 'reduce': 0		191354.781250	1.0	0.311917	1.0	0.311917
ww	Θ	All	243.0	12.577849	243.0	12.577849	4580.0	229.949570
	1	NIsoMuon >= 2	244.0	12.639496	244.0	12.639496	4580.0	229.949570
		triggerIsoMu24 == 1	4580.0	229.949570	244.0	12.639496	244.0	12.639496
		{'formula': 'Muon_Pt > 25', 'reduce': 0		212.997131	243.0	12.577849	244.0	12.639496
wz	Θ	All	623.0	13.157759	623.0	13.157759	3367.0	69.927917
		NIsoMuon >= 2	623.0	13.157759	623.0	13.157759	3367.0	69.927917
		triggerIsoMu24 == 1	3367.0	69.927917	623.0	13.157759	623.0	13.157759
		{'formula': 'Muon_Pt > 25', 'reduce': 0		65.436157	623.0	13.157759	623.0	13.157759
zz	Θ	All	1232.0	8.985804	1232.0	8.985804	2421.0	16.922522
	1	NIsoMuon >= 2	1235.0	8.998816	1235.0	8.998816	2421.0	16.922522
		triggerIsoMu24 == 1	2421.0	16.922522	1235.0	8.998816	1235.0	8.998816
		{'formula': 'Muon_Pt > 25', 'reduce': 0	} 2325.0	16.362473	1232.0	8.985804	1235.0	8.998816

Fill a histogram

fast_carpenter.BinnedDataFrame fast_carpenter.BuildAghast

NumberMuons:

dataset_col: true
binning:

- {in: NMuon, out: nMuons}
- {in: NIsoMuon, out: nIsoMuons}
 weights: [EventWeight, EventWeight_NLO_up]

DiMuonMass:

dataset_col: true

binning:

- in: DiMuon_Mass

out: dimu_mass

```
bins: {low: 60, high: 120, nbins: 60}
weights: {weighted: EventWeight}
```

• Binning scheme:

- Assume variable already discrete (eg. NumberMuons)
- Equal-width bins over a range (eg. DiMuonMass)
- List of bin edges
- Special: bin by dataset name
- Weighting schemes:
 - None
 - Single weight variable
 - List of weight variables
 - $\circ \quad \text{Mapping of names to input variable} \\$
- Output written to disk:
 - Pandas to produce a dataframe (csv)
 - $\circ \quad \ \ \text{Also to a Ghast for future tooling}$

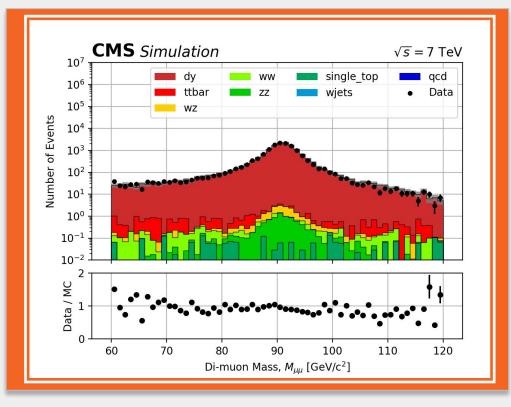
Fill a histogram: Resulting CSV from DiMuonMass

Showing only first three rows for each dataset (using groupby operation) >>> import pandas as pd >>> df = pd.read csv('tbl dataset.dimu mass--weighted.csv') >>> print(df.groupby('dataset').nth([0, 1, 2]).set_index('dimu_mass', append=True)) n weighted:sumw weighted:sumw2 dimu mass dataset data (-inf, 60.0] 993.0 NaN NaN (60.0, 61.0] 38.0 NaN NaN (61.0, 62.0] 25.0 NaN NaN dy (-inf, 60.0] 821.0 655.570801 1017.549133 (60.0, 61.0] 56.0 23.963226 12.091142 (61.0, 62.0] 56.0 25.572840 13.094129 acd (-inf, 60.0] 0.0 0.000000 0.000000 (60.0, 61.0] 0.0 0.000000 0.000000 0.0 0.000000 (61.0, 62.0] 0.000000 single top (-inf, 60.0] 32.0 0.100682 1.741041 (60.0, 61.0] 1.0 0.065288 0.004263 1.0 (61.0, 62.0] 0.005831 0.000034 ttbar (-inf, 60.0] 49.0 11.392980 3.072051 (60.0, 61.0] 3.0 0.840432 0.236490 (61.0, 62.0] 2.0 0.319709 0.075986 wjets (-inf, 60.0] 1.0 0.311917 0.097292 (60.0, 61.0] 0.0 0.000000 0.000000 (61.0, 62.0] 0.0 0.000000 0.000000 (-inf, 60.0] 61.0 3.600221 0.221474 WW (60.0, 61.0] 1.0 0.063284 0.004005 0.005617 (61.0, 62.0] 2.0 0.102053 0.007842 ωz (-inf, 60.0] 15.0 0.320914 (60.0, 61.0] 2.0 0.053328 0.001424 (61.0, 62.0] 0.0 0.000000 0.000000 ZZ (-inf, 60.0] 47.0 0.360053 0.002981 (60.0, 61.0]0.0 0.000000 0.000000 (61.0, 62.0] 0.0 0.000000 0.000000

Turning outputs into plots: fast-plotter

- Philosophy of: easy to produce basic plots, tools to support final publication-quality:
 - Command-line tool with good defaults and simple configuration
 - Written in lots of small functions that can help a user in a dedicated script / notebook
- Plot on the right with:

```
fast_plotter -y log \
-c plot_config.yml \
-o tbl_*.csv
```



Plot of DiMuonMass binned dataframe from last slide

User-defined stages

stages:

- BasicVars: fast_carpenter.Define
- DiMuons: cms_hep_tutorial.DiObjectMass
- Histogram: BinnedDataframe

• This is a growing MVP

- Previous steps not able to capture all analysis needs (yet), eg:
 - More complex variable definition (e.g. invariant masses)
 - Scale factor look-ups
- But a stage needn't belong to fast_carpenter
 - Break out of declarative YAML to full, imperative python
- Any importable python class with the correct interface can be used:
 - __init__ method accepts at least a name and output directory path
 - An event method
 - Optionally: begin, end, and collector methods
 - Collector used to write to disk if wanted
- Example: <u>fast cms public tutorial/cms hep tutorial/ init .py</u>

Describe your datasets: fast-curator

import:

- "{this_dir}/WW.yml"
- "{this_dir}/WZ.yml"

datasets:

- eventtype: data

Files: [input_files/HEPTutorial/files/data.root]
name: data

nevents: 469384

- files: [input_files/HEPTutorial/files/dy.root]
 name: dy

nevents: 77729

- files: [input_files/HEPTutorial/files/qcd.root]
 name: qcd

nevents: 142

defaults:

eventtype: mc

nfiles: 1

tree: events

Ben Krikler

Mainly for scaling up to full analysis

- Many input files form a dataset
- Many datasets make up an analysis

Shouldn't need to produce dataset descriptions too often

• Analyses keep dataset files in repo, easy to review

Command line tool to help you:

• Eg. wild-card on the command line, <u>including xrootd</u> <u>files (contributed to pyxrootd</u>)

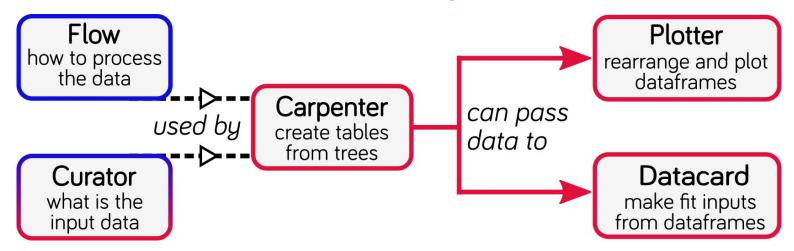
Dataset types can be "data" or "MC"

• Event weights only applied to MC

Can include additional meta-data e.g.:

- Cross-sections
- Number of original events (for processing skimmed inputs)
- Event tree name

FAST codebase interplay



- fast-flow: Library code only
- fast-curator: Executables to write and validate YAML
- fast-carpenter: Main entry-point. Default backend and stages
- fast-plotter: Executable with good defaults, small functions to assist custom scripts
- fast-datacard: Specific to CMS Higgs Combine inputs at this point

Just how "fast" is this?

Compared to C++ example analysis, single core

- Fast-carpenter: 6 seconds, ~100 lines of analysis-specific code
- C++ example: 3 seconds, >600 lines of code

Apples-to-apples comparison is tricky

Many places ripe for optimisation:

- Overly-general histogram filling using pandas
- Combining multi-processed jobs' output
- Caching and optimisation of variable definitions (a la histbook ?)

Going forwards...

Really using YAML as an ADL

YAML descriptions from previous slides specifically tied to fast-carpenter and friends.

Could this be "standardised" into a full language = YADL

Stage provides the same interface and outputs: its implementing the YADL standard for such a stage, e.g.:

- Variable definition expressions
- Cut-flows with nested dictionaries

Fast-flow already provides a "backend" mechanism

- Develop further: allow user to select backend
- E.g.: AlphaTwirl (current), Spark, RDataFrame

Roadmap for changes

- **1.** Generalised data-space concept:
 - Not just individual (jagged)-arrays
 - Tables, dataframes, ghasts, etc
 - Remove uproot tree "branch injection" hacks
- 2. Improved expressions:
 - **Pre-process on top of numexpr**
 - Move reductions into expressions
 - Separate package?

3. Flow control model

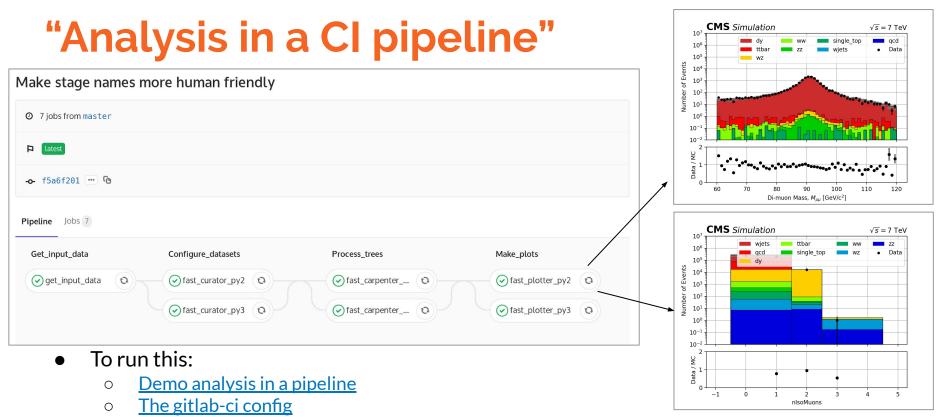
- Stages to become more functional
- Move to PARSL, SAGA-Python
- Support Spark integration
- 4. Type system for configurations
 - Via Python 3 type annotations?
- 5. Collaboration with similar efforts?
 - E.g. using functions from Coffea

Summary

- Have introduced the FAST codebase
 - Incorporating uproot, awkward array, numexpr, aghast
 - Being used on CMS and several other experiments
- YAML-based analysis description
 - Datasets, processing, plotting steps
 - Not too much work to "standardize" this beyond existing backend
- About twice as slow as equivalent C++ analysis (single core)
 - But lots of room for optimisation
- Resources
 - Code: <u>gitlab.cern.ch/fast-hep/public/fast-carpenter/</u>
 - Installing: pypi.org/project/fast-carpenter/
 - Docs: <u>fast-carpenter.readthedocs.io/</u>
 - Gitter: <u>gitter.im/FAST-HEP/community</u>



Thank You



- <u>Script tying the commands together</u>
- Feasible for huge datasets unclear, but can happily manage subsets of data for testing

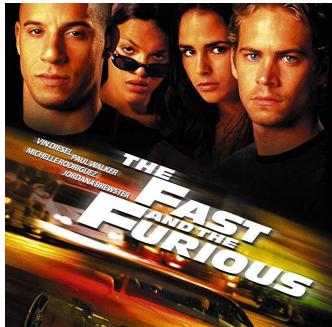
Fill a histogram: Technical implementation details

- First load necessary branches into pandas dataframe
- Then one highly general function to
 - Discretize (i.e. bin) variables if needed (using pandas.cut)
 - Aggregate (groupby) and produce counts, sum of (multiple) weights, and sum of square of (multiple) weights
- This covers all cases but not optimal in many common uses, e.g.:
 - $\circ \quad \ \ \, \text{Single variable to bin on}$
 - Unweighted counts
- Can optimise behind the scenes
 - <u>https://iscinumpy.gitlab.io/post/histogram-speeds-in-py</u> <u>thon/</u>
 - Config file doesn't have to change

FAST = Faster Analysis Software Taskforce

- Group of HEP researchers
- Primarily working for UK institutes
- Started around May 2017
- Use of 1 to 3-day "hack-shops" to test new ideas

- Goals: Try to help improve HEP analysis software
 - a. Simplicity
 - b. Speed
 - c. Documentation
 - d. Automation



No connection to this work, just an excuse to include an image

FAST Hack-shops



- Halfway between hackathon and a workshop
- Small (<10) group of people working together for 1 to 3 days
- People / pairs working on self-defined projects (eg. set up PARSL within fast-carpenter)
- Mainly for trying out new tools, experimenting with new ideas
- 4 hack-shops held throughout last two years, but only within FAST
- Would there be interest to extend this to HSF / IRIS-HEP / scikit-hep more broadly?

A little bit of context

