



Marcel Rieger for the **C**/f Team

columnflow: Fully automated analyses via flow of columns over distributed resources

ACAT 2024

15.3.2024



#### **General idea**

- Python-based framework for nano-like inputs
- End-to-end orchestration & automation
- No reliance on single local cluster or local storage
- Adapt to any remote cluster and storage system
  - ▶ HTCondor, Slurm, CMS-CRAB, LSF
  - ▶ Store via file://, xrootd://, gsiftp://, webdav://
- Persistent intermediate outputs
  - ▷ Debugging, reuse, sharing across groups

#### **Automation stack**





workflow engine (originally by Spotify)

### Example graph\*

MergeSele

#### Parallelization over ...

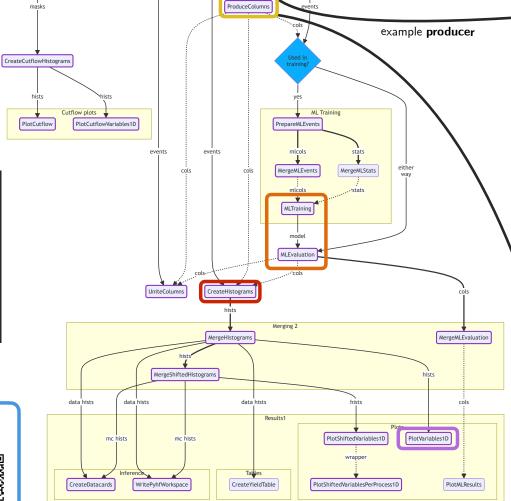
- Campaigns & datasets
- Files
- Systematics
- ▷ Typically  $\mathcal{O}(10k)$  60min jobs, **however**, on standard resources
- ▶ HTCondor, CRAB, ...

#### **Graph execution**

- Single command can trigger the full pipeline from **inputs to plots**
- Example
- Law run cf.PlotVariables1D \ --version dev1  $\setminus$ --datasets ttbar,dy  $\$ --calibrators jec,jer  $\setminus$ --selector full  $\setminus$ --producers muon\_weights  $\setminus$ --variables --workflow {crab,htcondor,...}

#### Documentation





CLUSTER OF EXCELLENCE QUANTUM UNIVERSE

# columns over distributed resources

Marcel Rieger on behalf of the ¢∕f -Team



#### Key concepts

- Experiment **agnostic core** 
  - ▷ Organize experiment-specific recipes in extensions
- Use awkward arrays as interface, parquet as file format
  - ▶ Give **users full control** over processing tools (NumPy, TensorFlow, coffea-nano-format, pandas, ...)
- High degree of **code-reuse** and collaboration
- Define **workflows** with luigi + law, metadata with order
- Control and execution via **CLI**, **scripts** and **notebooks**



(experiment independent)





analysis code

A PAG

factors

(\* Just a suggestion, can be easily altered or amended by analyses)

#### Simple customization

- Provide simple functions, producers, to create
  - calibrated (updated) columns
  - selection masks
  - new columns
  - ML training & evaluation
  - variables
- **Nesting** enables for easy reuse and capsulation



Using bare **awkward arrays** • Implementation and choice of tools fully up to user

layer for HEP & scale-out (experiment independent)

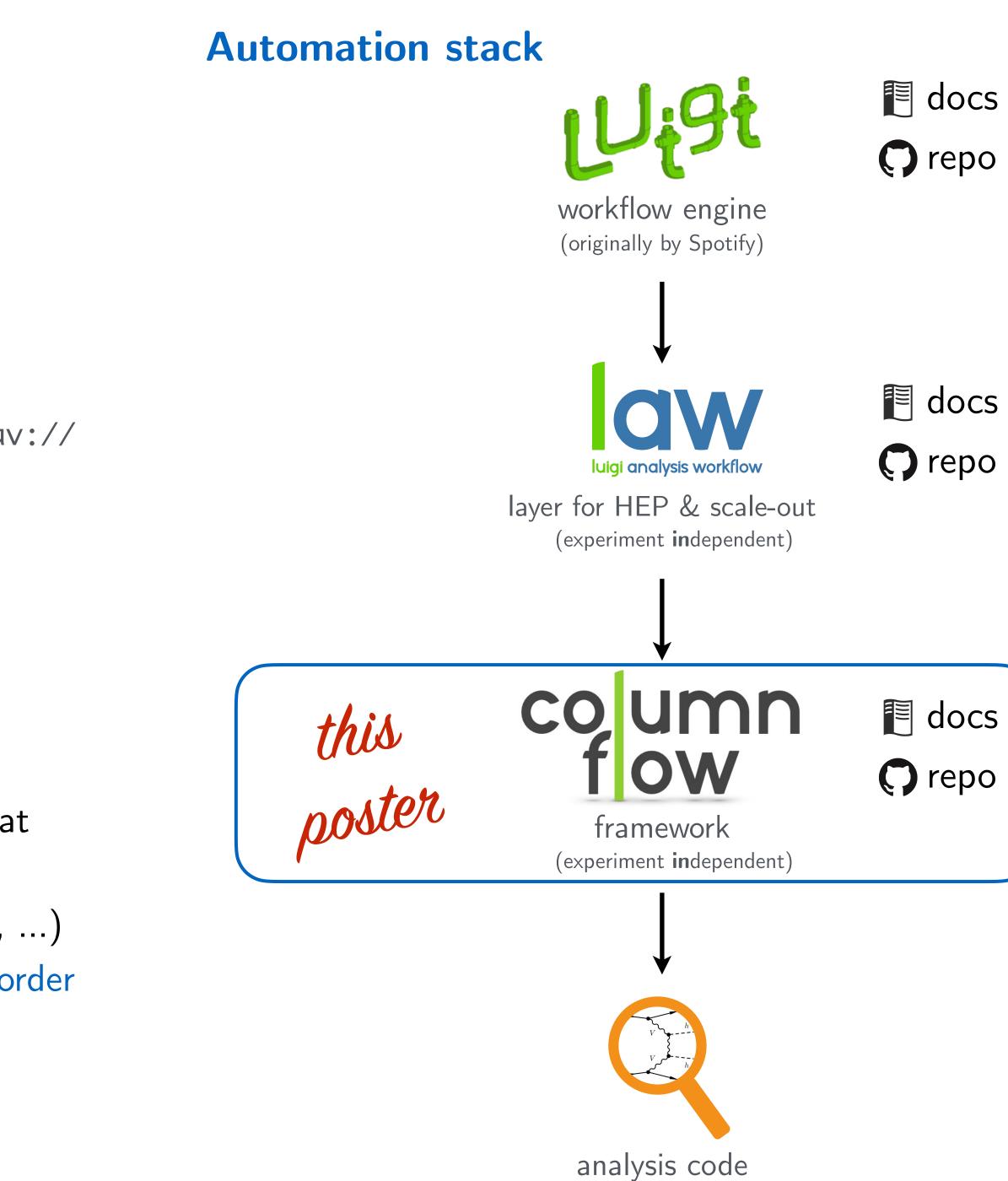
# General idea

- Python-based framework for nano-like inputs
- End-to-end orchestration & automation
   From events to plots in a single command
- No reliance on single local cluster or local storage
- Adapt to any remote cluster and storage system
   ► HTCondor, Slurm, CMS-CRAB, LSF
   ► Store via file://, xrootd://, gsiftp://, webdav://
- Persistent intermediate outputs

▷ Debugging, reuse, sharing across groups

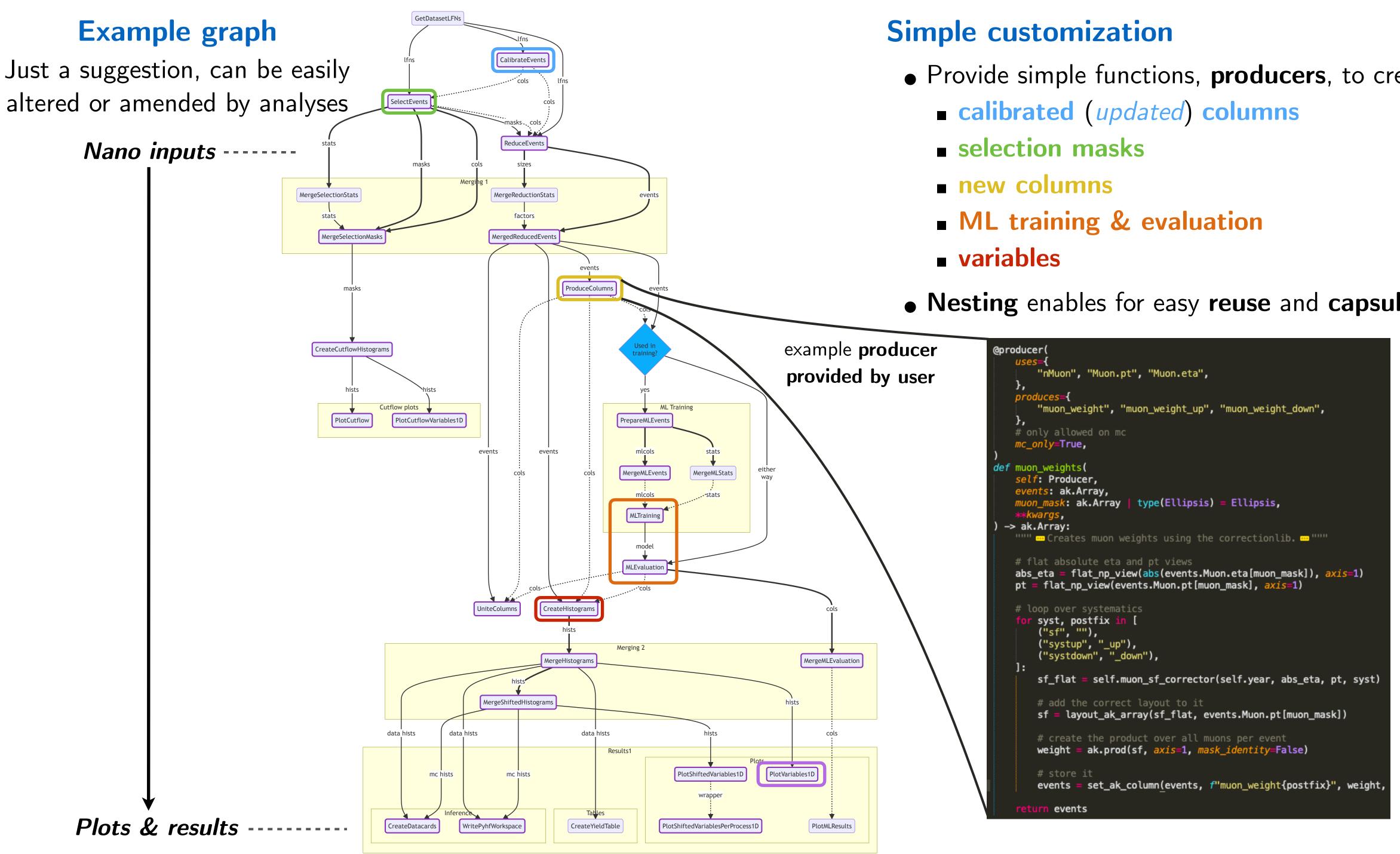
# Key concepts

- Experiment-agnostic core
- Use awkward arrays as interface, parquet as file format
   ▷ Give users full control over tools used (NumPy, TensorFlow, coffea-nano-format, pandas, ...)
- Define **workflows** with luigi + law, metadata with order
- Capsulation of standard recipes
   High degree of code-reuse & collaboration





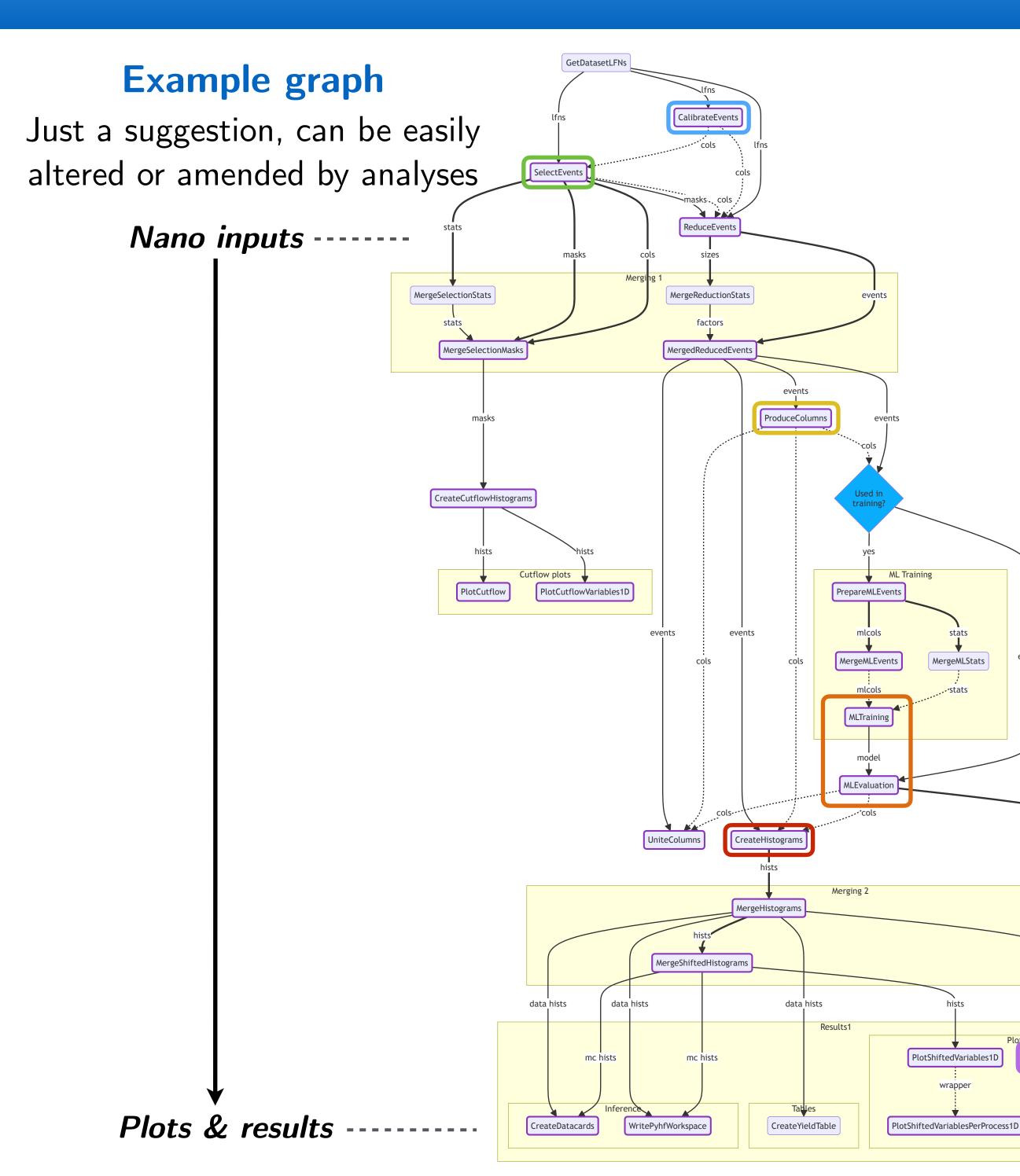
#### Workflow, customization & execution 4



- Provide simple functions, **producers**, to create
- Nesting enables for easy reuse and capsulation



#### Workflow, customization & execution 4



# **Simple customization**

- Provide simple functions, **producers**, to create
  - calibrated (updated) columns
  - selection masks
  - new columns
  - ML training & evaluation
  - variables
- **Nesting** enables for easy **reuse** and **capsulation**

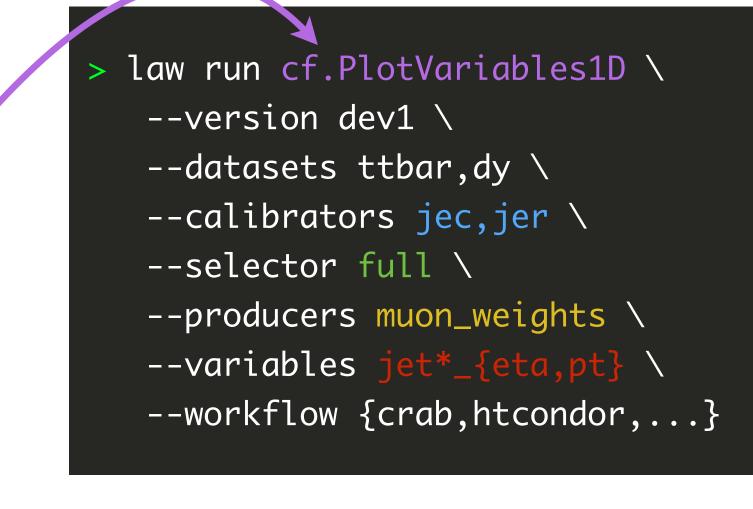
# **Graph execution**

- **Single command** can trigger the full pipeline from **inputs** to **plots**, or any intermediate task
- Example

MergeMLEvaluation

PlotMLResults

PlotVariables1D





Backup

columnflow in depth

# Project overview

# Python framework for vectorized, columnar HEP analysis with flat (nano-like) inputs

- Mostly experiment agnostic **core**, plenty of CMS-related **specializations** on top
- Using awkward arrays + coffea nano-scheme, parquet as file format Workflows with luigi/law, metadata definition using order

# Our initial wishlist

- End-to-end orchestration & automation ▷ One command can trigger the entire workflow
- Highly parallel execution on **any remote batch system** ▶ HTCondor, Slurm, LSF, WLCG, CMS-CRAB, ...
- Seamless integration of any remote storage system
  - ▷ Storage: file://, xrootd://, gsiftp://, webdav://, ...
- No reliance on custom, local hardware
  - ▶ We need to be able to invite external collaborators
  - ▷ Reduction in speed ( ) to be compensated with high parallelism
- **Persistent** intermediate outputs
  - ▶ Easy reuse across groups, ML applications, working with students ...

columnflow Marcel Rieger for the CF team

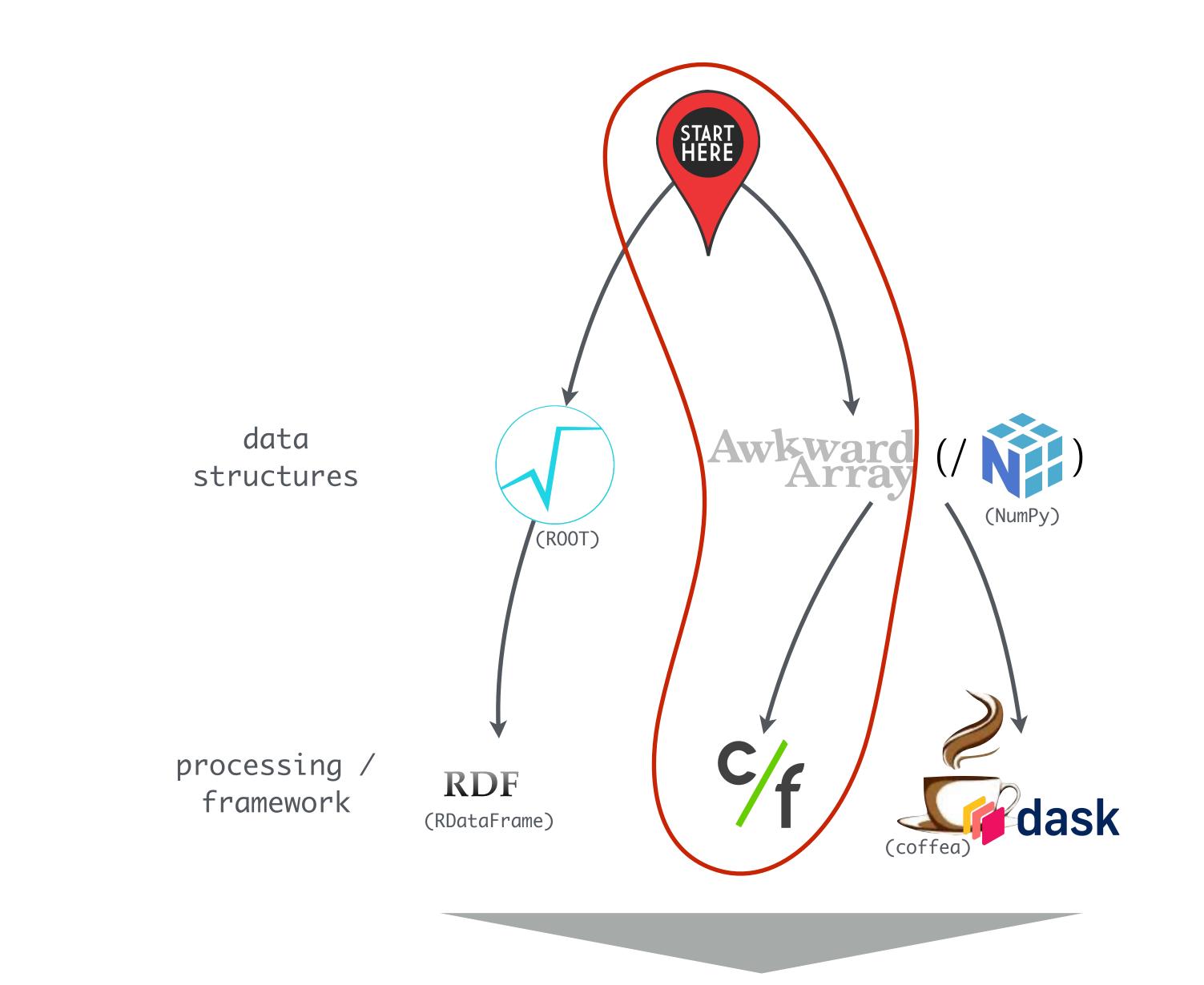
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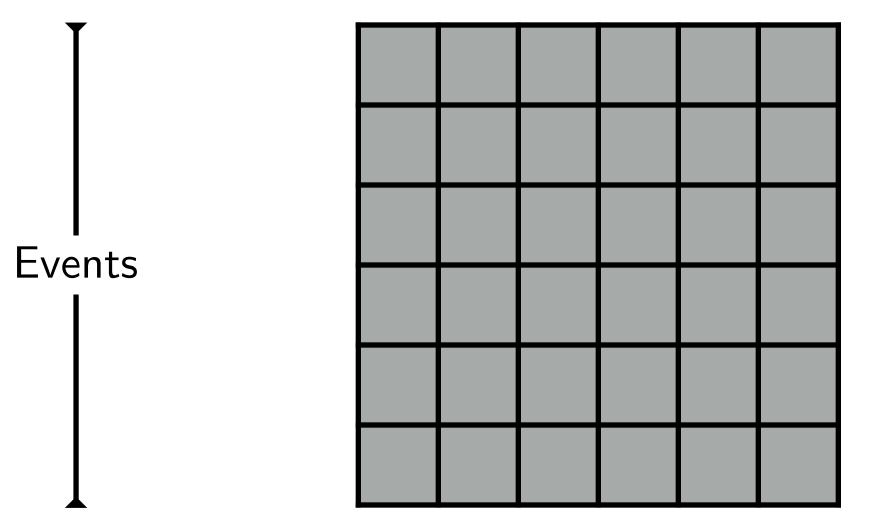


analyses





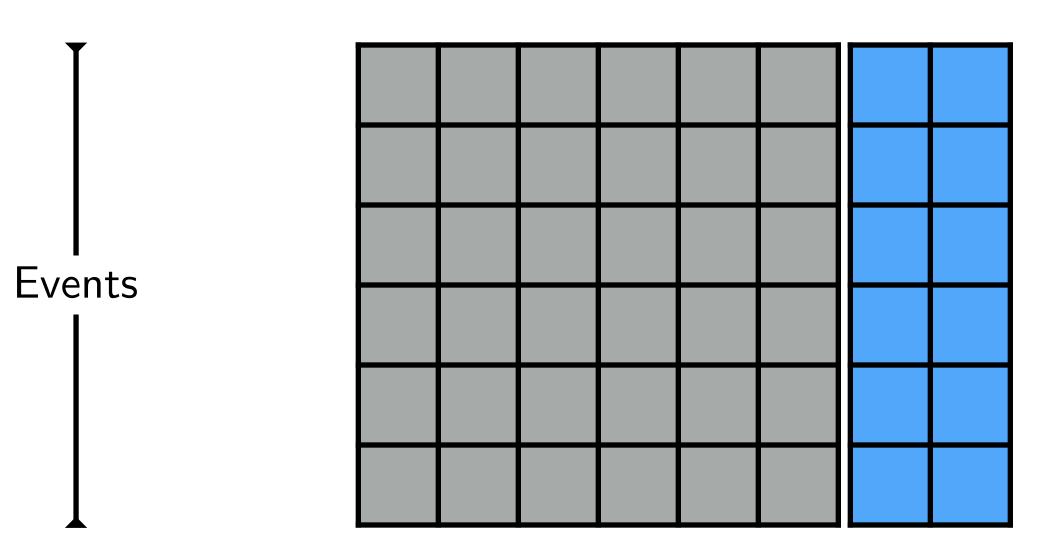




- □ Extension
- Selection (*creating* masks)
- Reduction (*applying* masks)
- □ Extension
- □ Merge



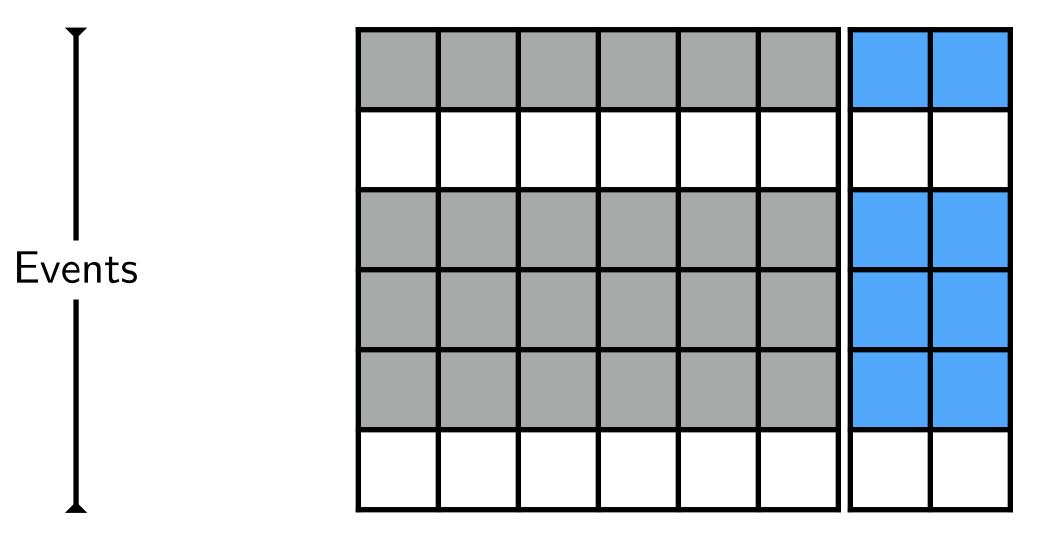




- Extension
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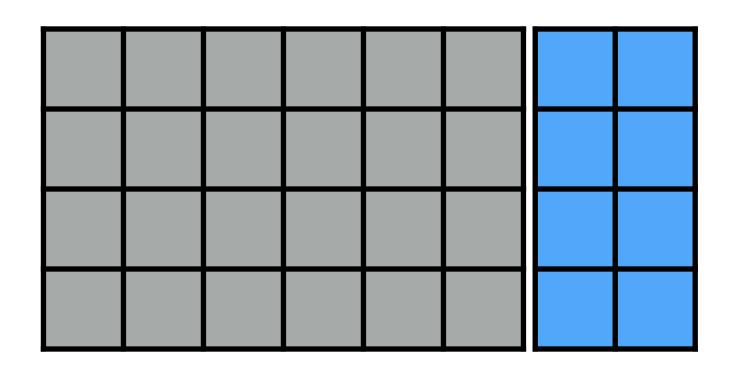






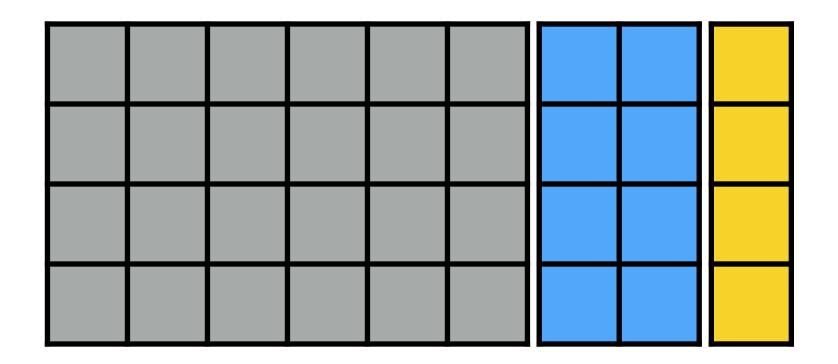
- Extension
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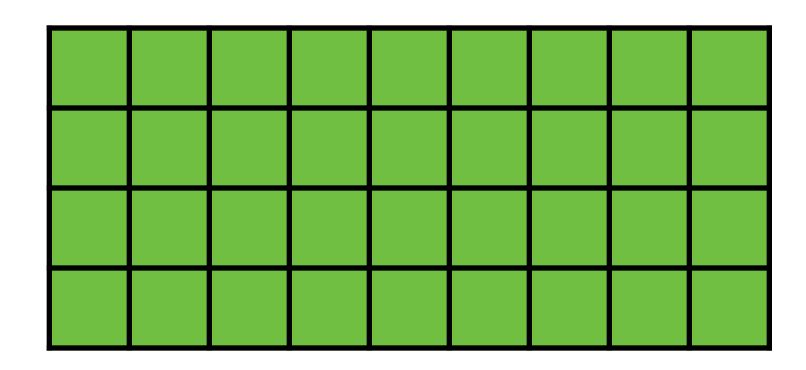
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- Selection (*creating* masks)
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- □ Extension
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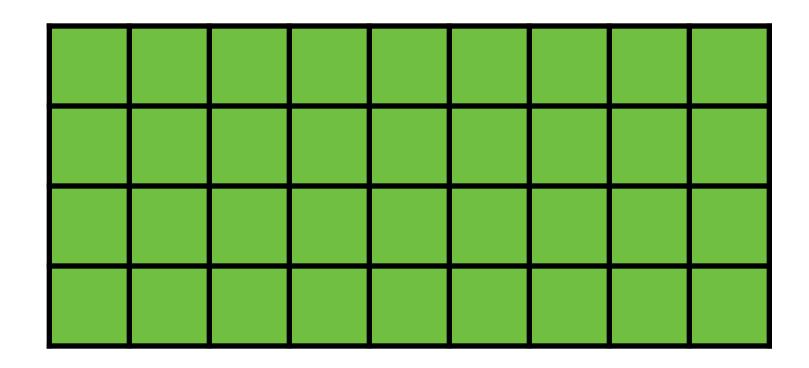
- Extension
- Selection (*creating* masks)
- Reduction (*applying* masks)
- **Extension**
- □ Merge





- Extension
- Selection (*creating* masks)
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- **Extension**
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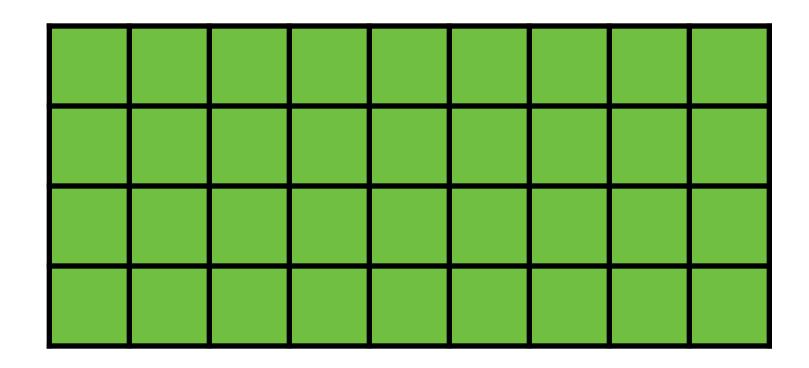
- Extension
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# In-memory

- Trivial
- NumPy / awkward array provide all necessary tools and helpers
- Across a large scale analysis with persistent intermediate files





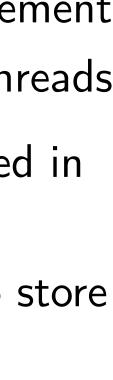


- **Extension**
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# In-memory

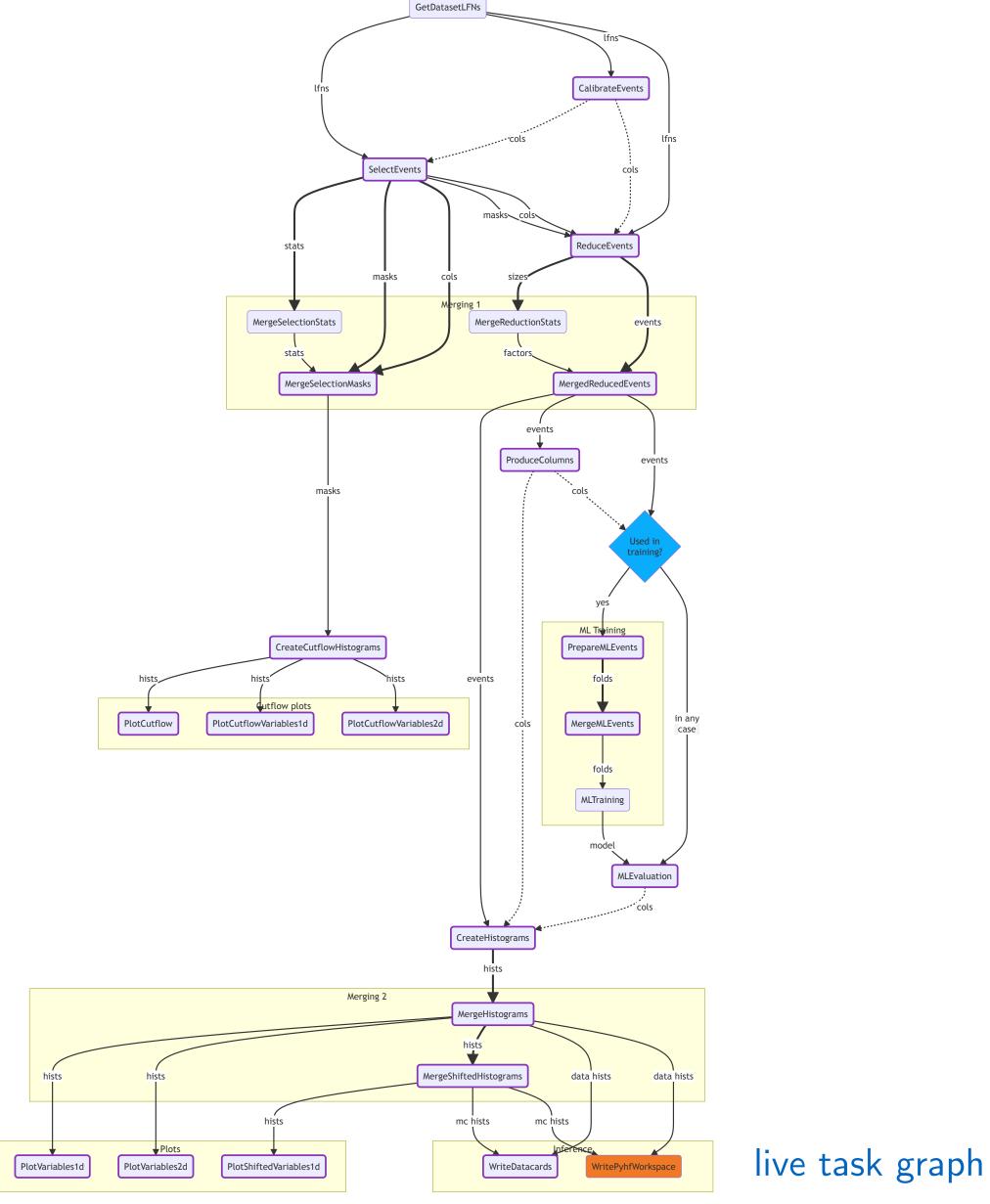
- Trivial
- NumPy / awkward array provide all necessary tools and helpers
- Across a large scale analysis with persistent intermediate files
  - **H** represent input files
    - $\triangleright$  Typically  $\mathcal{O}(1k 10k)$
    - High parallelism, only **single-core** requirement  $\triangleright$
    - Chunked reading with IO offloading to threads
  - and represent columns, potentially stored in additional files and same event order
    - ▷ Flexible decisions by analyses whether to store columns and when to load them
    - ▷ Can be written & read in multi-threaded IO





#### **1** Fully orchestrated workflow

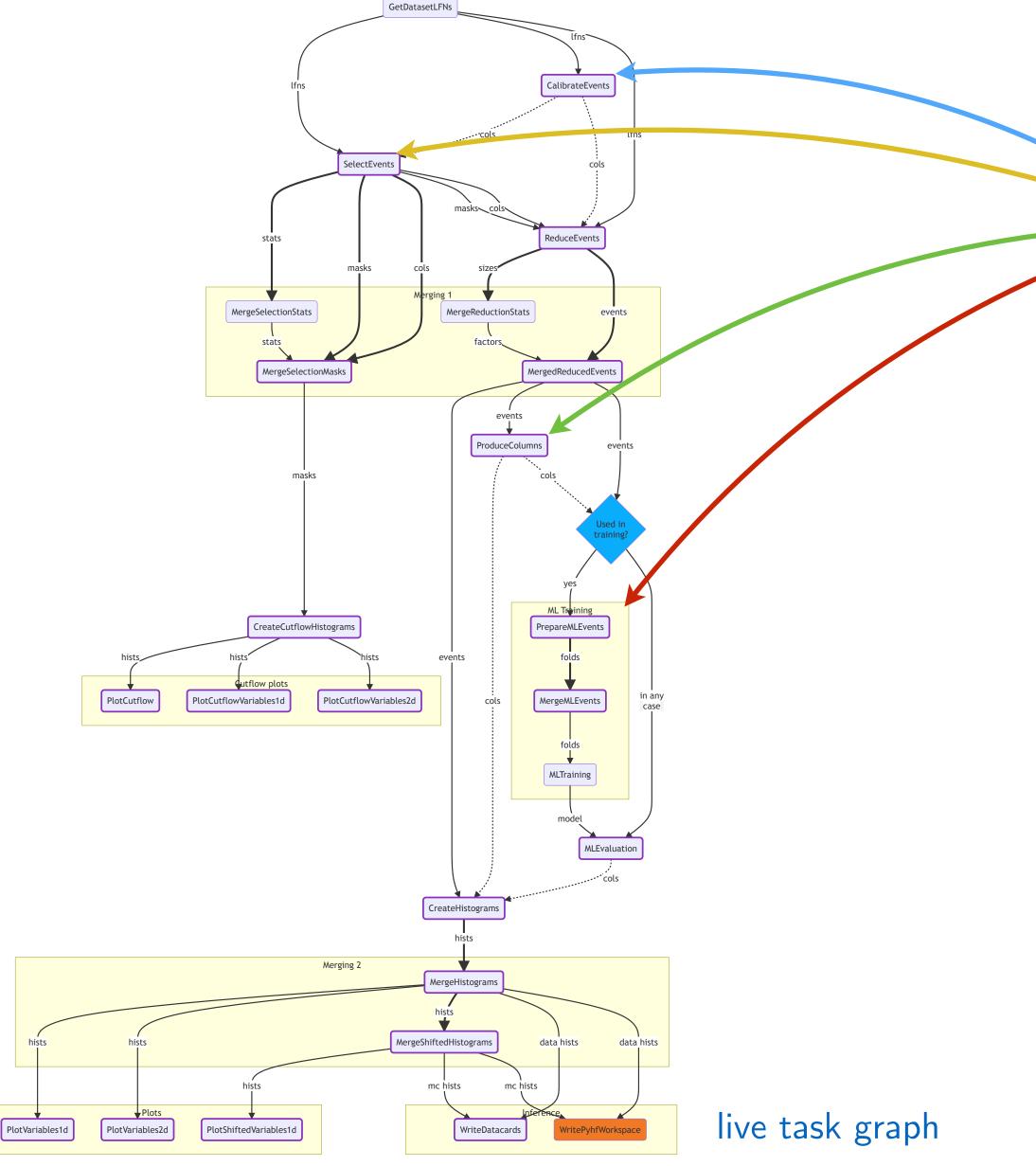
- Only a *suggestion*, but able to model majority of analyses
- Can be altered or created from scratch by analyses





# **I** Fully orchestrated workflow

- Only a *suggestion*, but able to model majority of analyses
- Can be altered or created from scratch by analyses



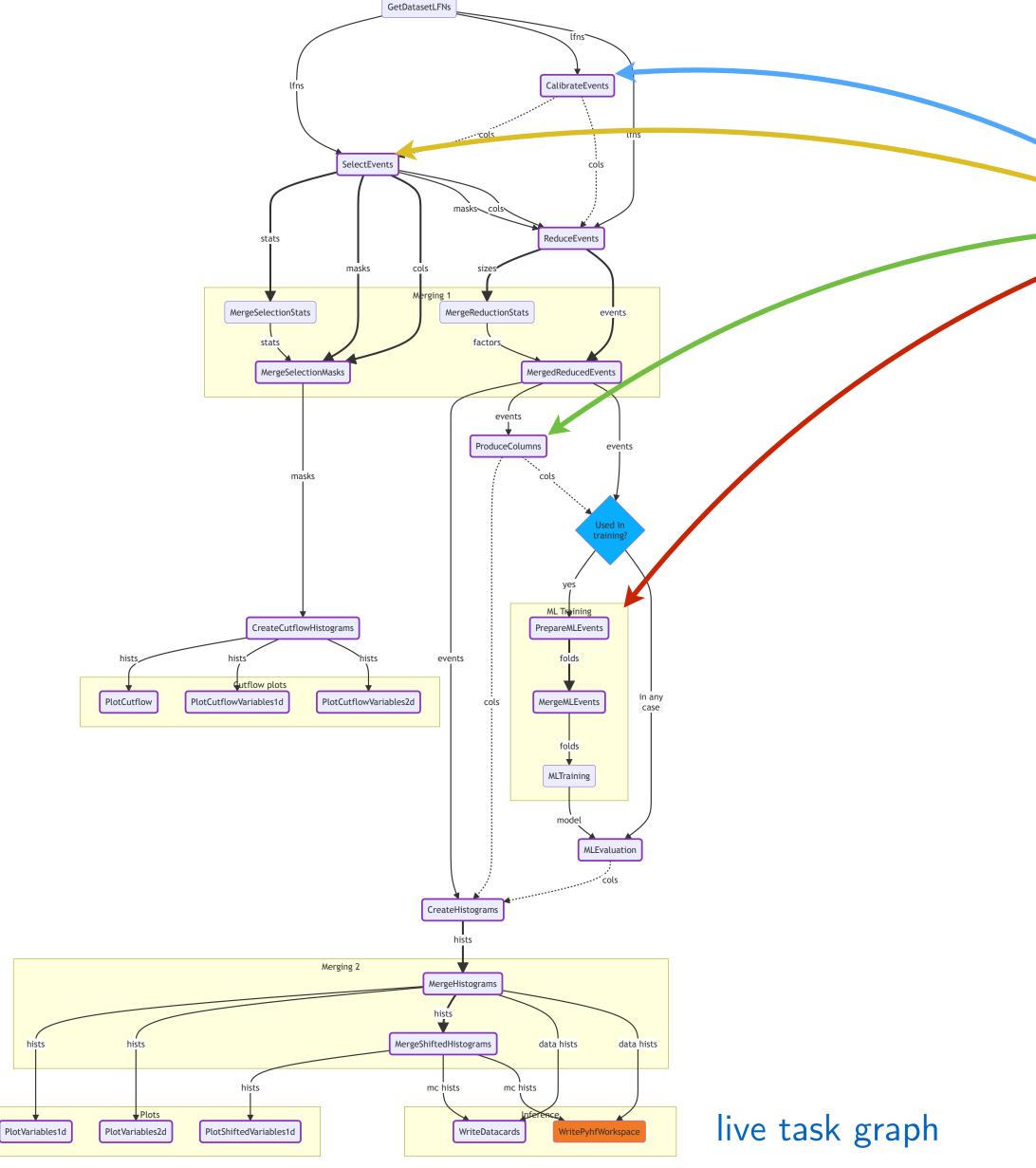
# **Z** Tools for on-demand column retrieval / production

- Configurable functions creating new columns at certain points of the workflow
- Can be selected at execution time, e.g. btag\_weight, pu\_weight
- Carry information on **used** and **produced** columns,  $\rightarrow$  open & save only necessary columns (see backup)



# Fully orchestrated workflow

- Only a suggestion, but able to model majority of analyses
- Can be altered or created from scratch by analyses



#### **Tools for on-demand column retrieval / production** 2

- Configurable functions creating new columns at certain points of the workflow
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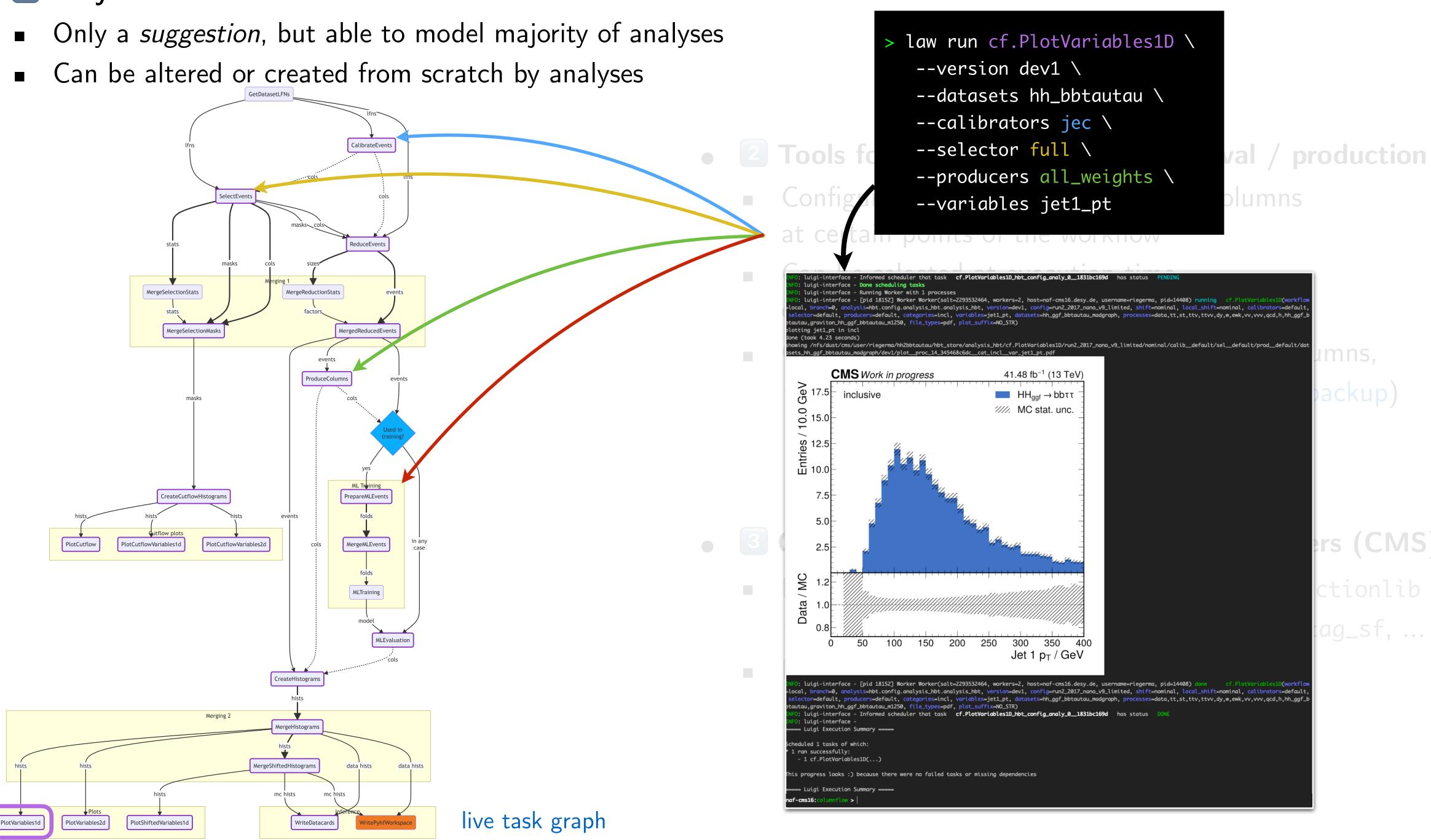
#### Collection of standardized column producers (CMS) 3

- Mostly SF and weight production using correctionlib → jec, jer, tec, e\_sf, mu\_sf, trigger\_sf, btag\_sf, ...
- Plug-in mechanism for analyses



# **I** Fully orchestrated workflow

- Can be altered or created from scratch by analyses



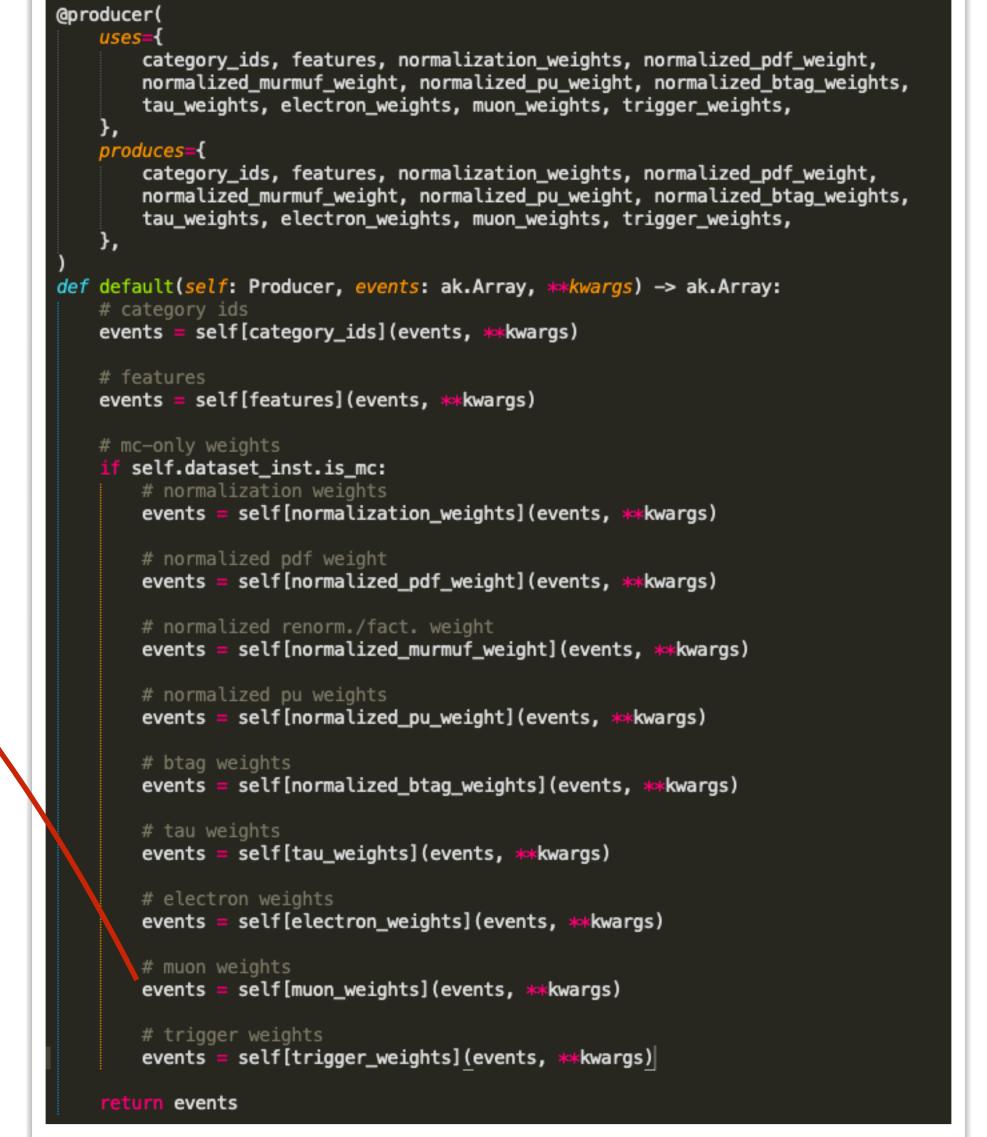


# 11 Example: single and nested producers

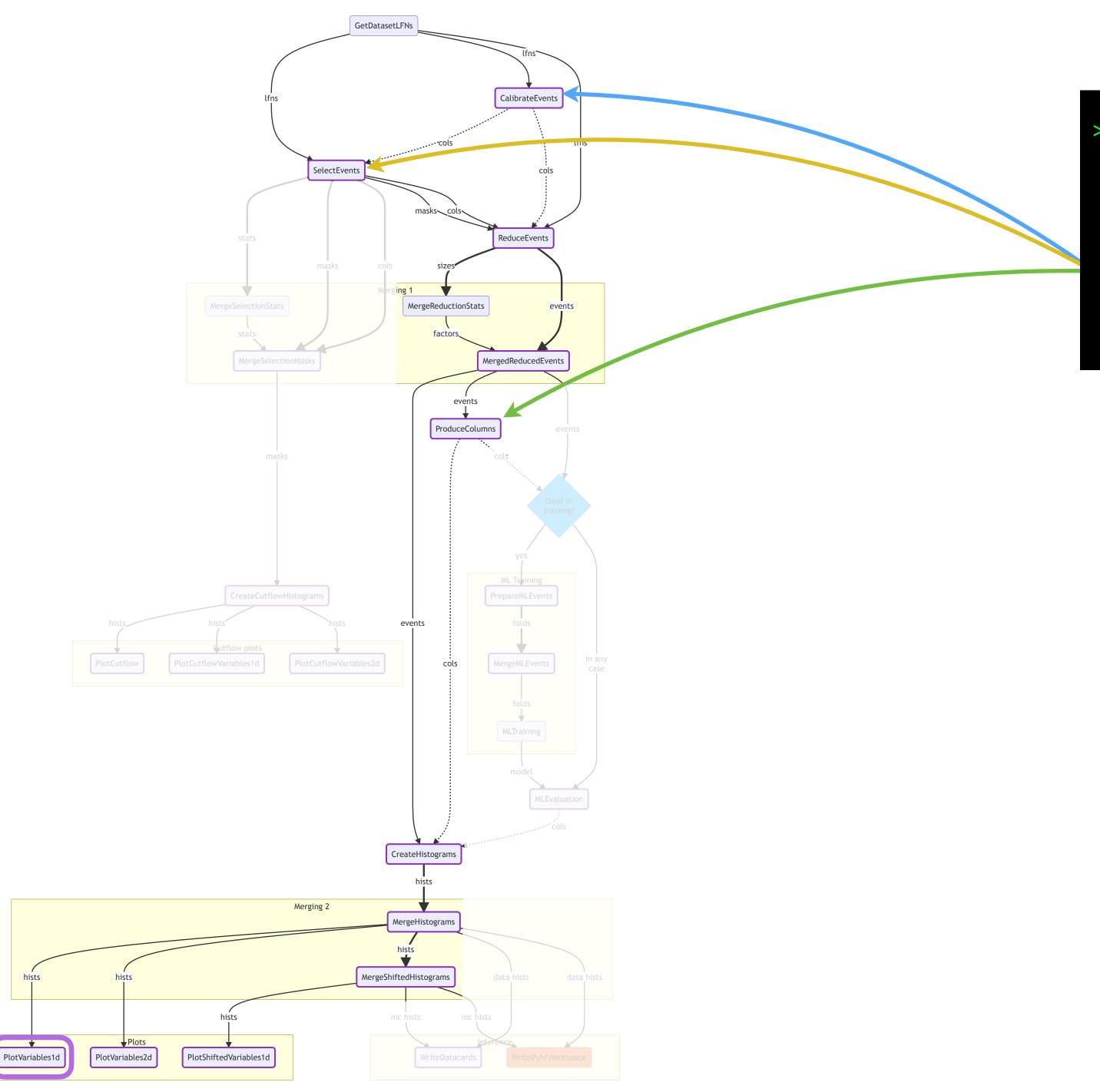
# Single producer

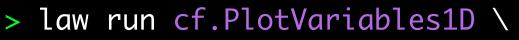
```
@producer(
     uses=
         "nMuon", "Muon.pt", "Muon.eta",
     3,
     produces={
         "muon_weight", "muon_weight_up", "muon_weight_down",
     },
    # only allowed on mc
    mc_only=True,
_def muon_weights(
    self: Producer,
    events: ak.Array,
    muon_mask: ak.Array | type(Ellipsis) = Ellipsis,
    **kwargs,
   -> ak.Array:
     """ - Creates muon weights using the correctionlib. - """
    # flat absolute eta and pt views
    abs_eta = flat_np_view(abs(events.Muon.eta[muon_mask]), axis=1)
    pt = flat_np_view(events.Muon.pt[muon_mask], axis=1)
    # loop over systematics
     for syst, postfix in [
         ("sf", ""),
         ("systup", "_up"),
         ("systdown", "_down"),
         sf_flat = self.muon_sf_corrector(self.year, abs_eta, pt, syst)
        # add the correct layout to it
        sf = layout_ak_array(sf_flat, events.Muon.pt[muon_mask])
         # create the product over all muons per event
        weight = ak.prod(sf, axis=1, mask_identity=False)
         # store it
        events = set_ak_column(events, f"muon_weight{postfix}", weight, value_type=np.float32)
     return events
```

### Nested producer



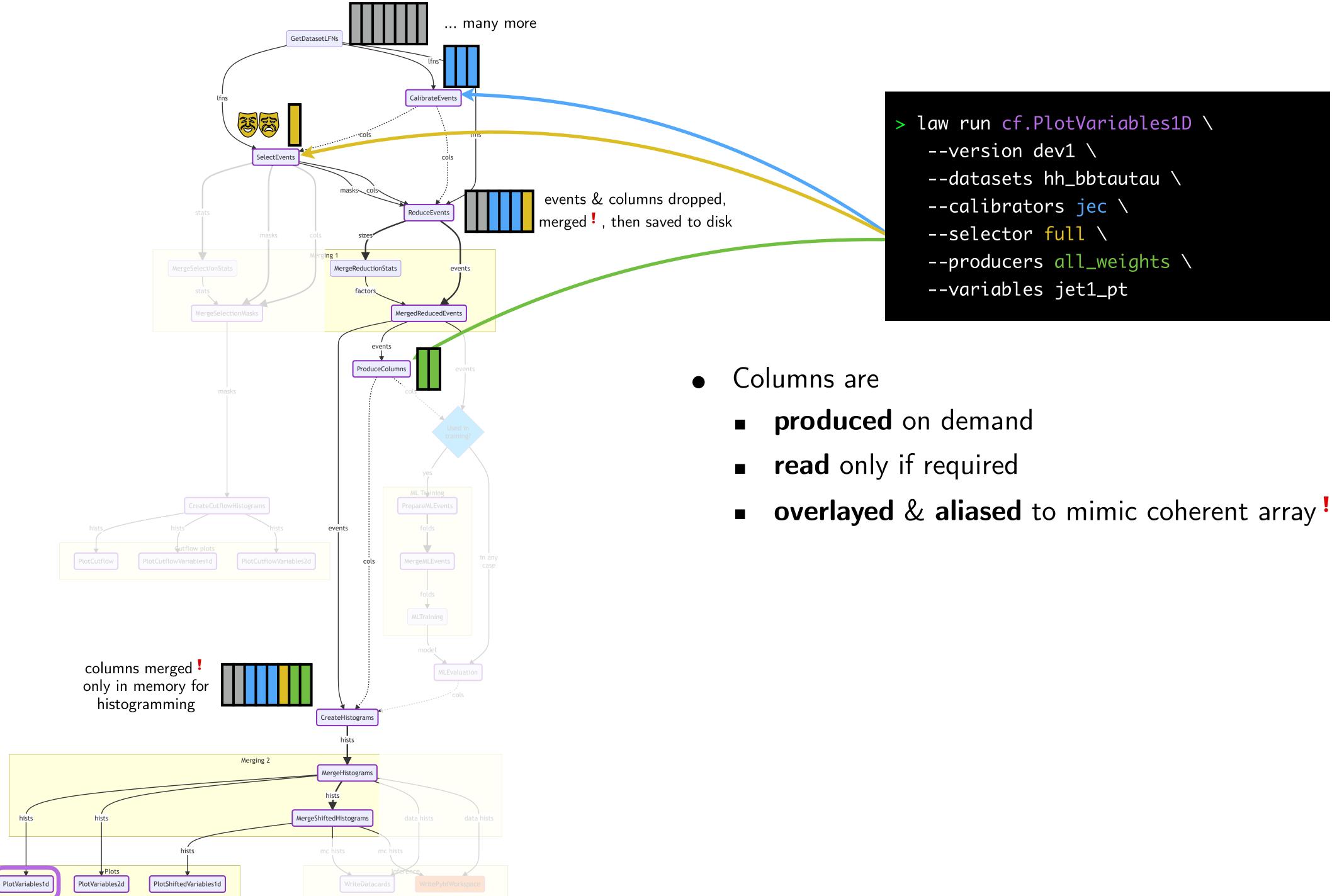




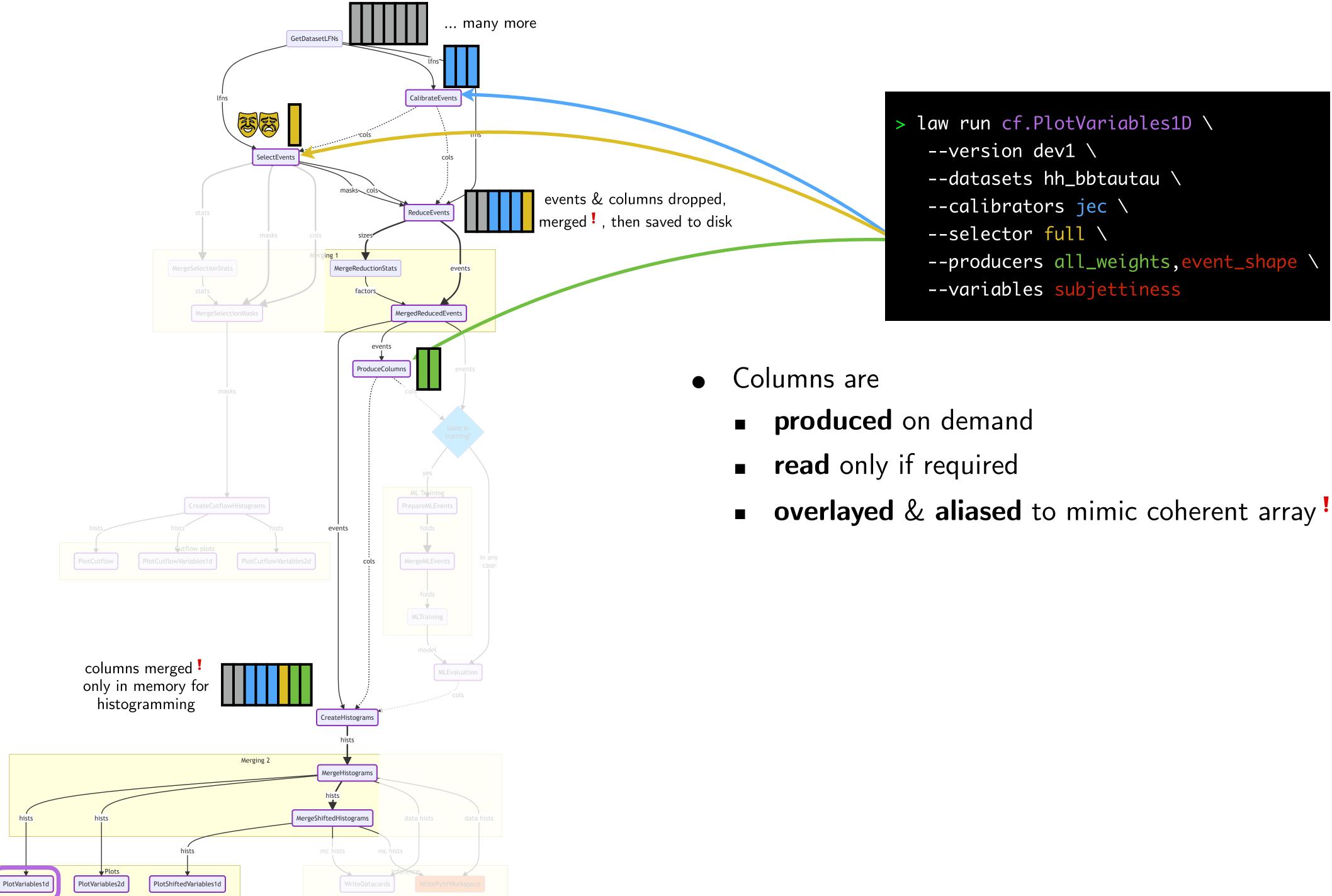


- --version dev1  $\setminus$
- --datasets hh\_bbtautau  $\setminus$
- --calibrators jec \
- --selector full  $\setminus$
- --producers all\_weights  $\land$
- --variables jet1\_pt

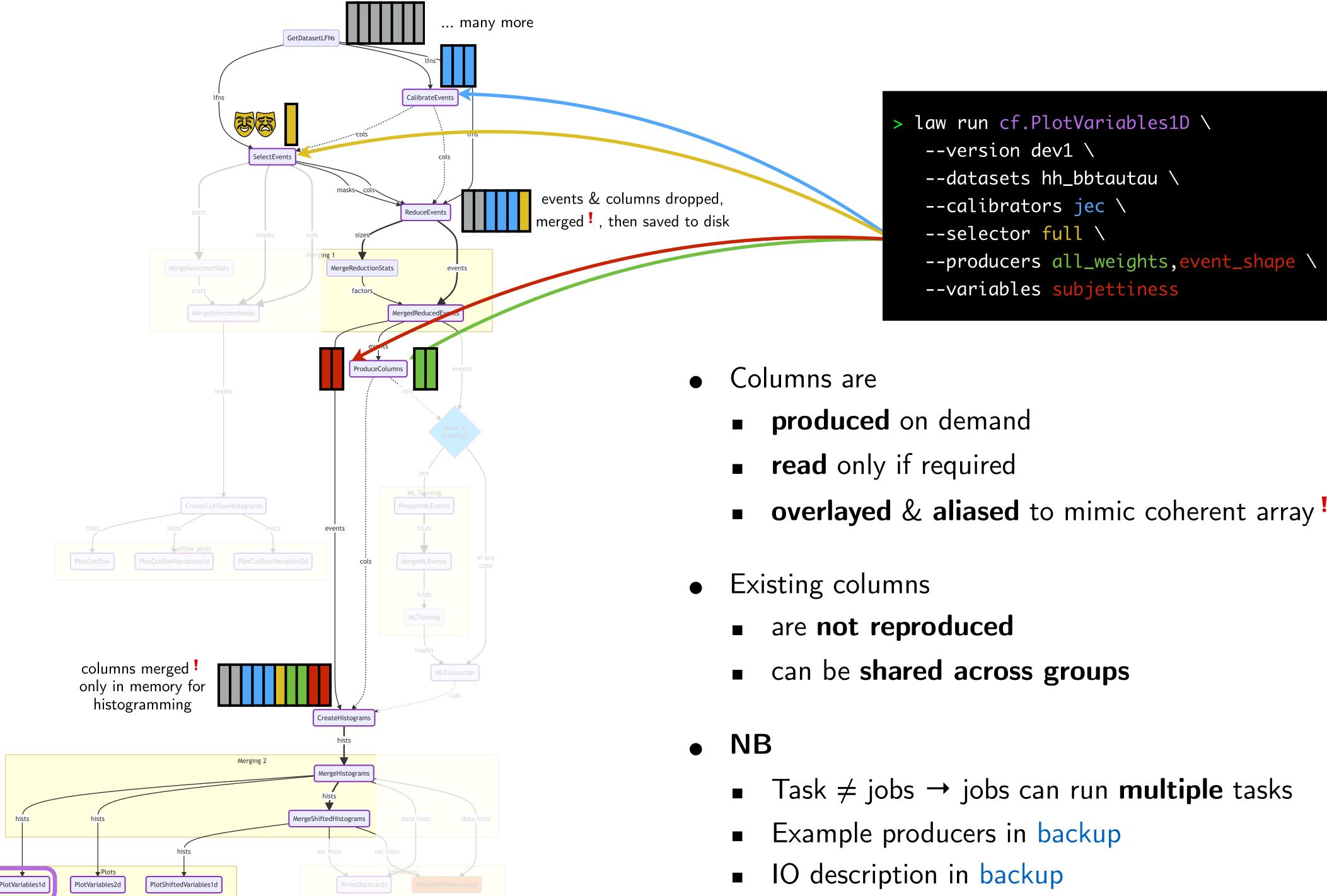












- **overlayed** & **aliased** to mimic coherent array



# Base Stack

micromamba with conda-forge packages
 → contains all required non-python packages,
 rarely updated

(python3.9, bash/zsh, git, gfal2)

"cf" Sandbox

→ All python packages needed to run tasks,
 moderately updated

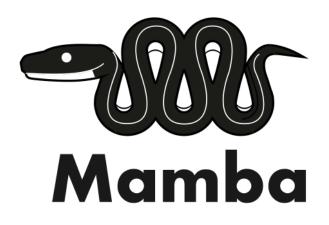
(luigi, law, pyyaml)

### Task sandboxes

Any type: venv, cmssw subshell, docker, ...

→ Python packages to run a specific task, frequently updated

(e.g. awkward, numpy, tensorflow, ...)













...

#### Writing your own producer (calibrator, selector, ...) (1) 14



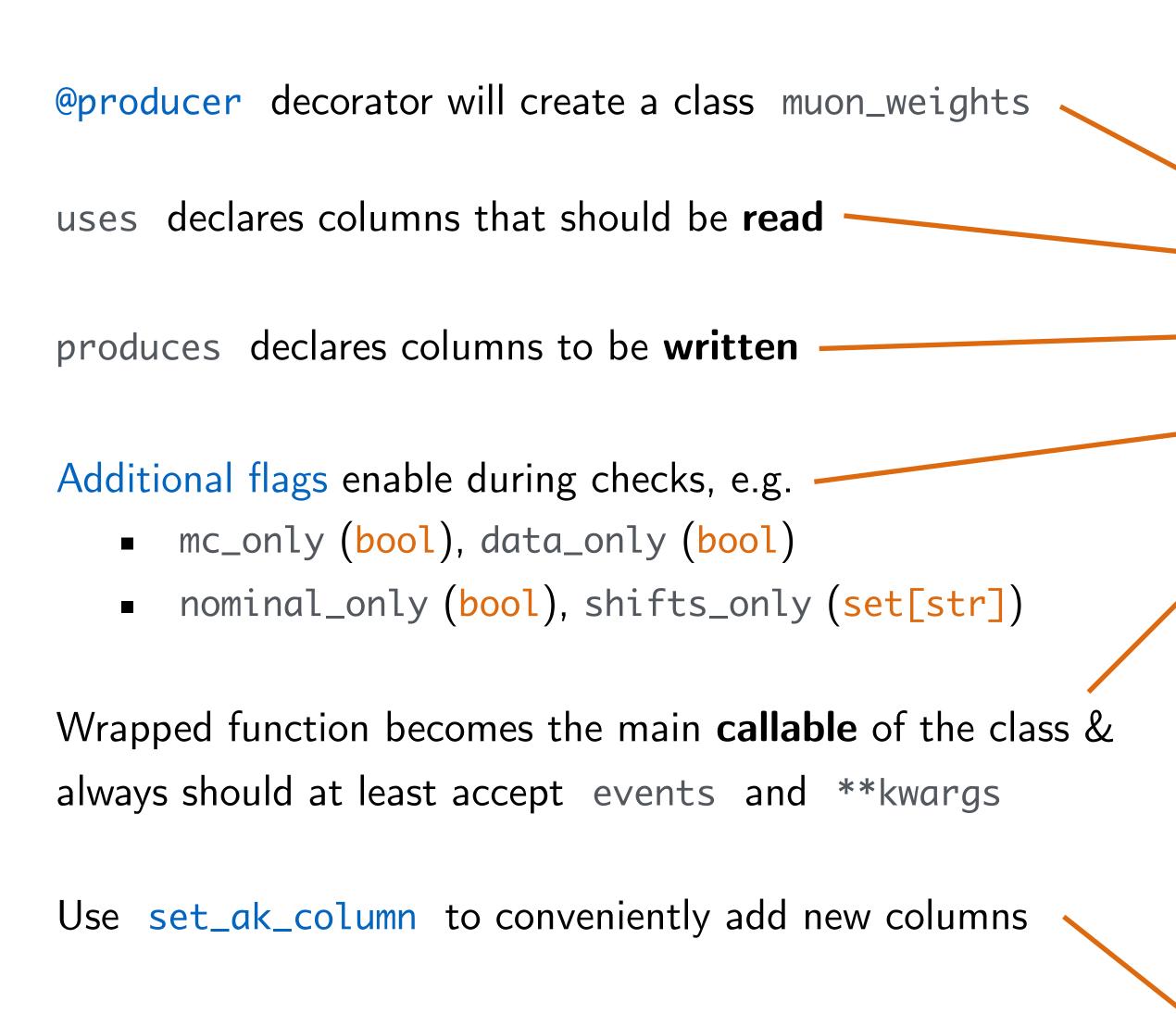
# *Example*: muon weight producer (as shown earlier)

```
@producer(
    uses=
        "nMuon", "Muon.pt", "Muon.eta",
    },
    produces={
        "muon_weight", "muon_weight_up", "muon_weight_down",
    ł,
   # only allowed on mc
   mc_only=True,
def muon_weights(
    self: Producer,
   events: ak.Array,
    muon_mask: ak.Array | type(Ellipsis) = Ellipsis,
   **kwargs,
 -> ak.Array:
    """ - Creates muon weights using the correctionlib. - """
    # flat absolute eta and pt views
    abs_eta = flat_np_view(abs(events.Muon.eta[muon_mask]), axis=1)
    pt = flat_np_view(events.Muon.pt[muon_mask], axis=1)
    # loop over systematics
    for syst, postfix in [
        ("sf", ""),
        ("systup", "_up"),
        ("systdown", "_down"),
    1:
        sf_flat = self.muon_sf_corrector(self.year, abs_eta, pt, syst)
        # add the correct layout to it
        sf = layout_ak_array(sf_flat, events.Muon.pt[muon_mask])
        # create the product over all muons per event
        weight = ak.prod(sf, axis=1, mask_identity=False)
        # store it
        events = set_ak_column(events, f"muon_weight{postfix}", weight, value_type=np.float32)
    return events
```





# 14 Writing your own producer (calibrator, selector, ...) (1)

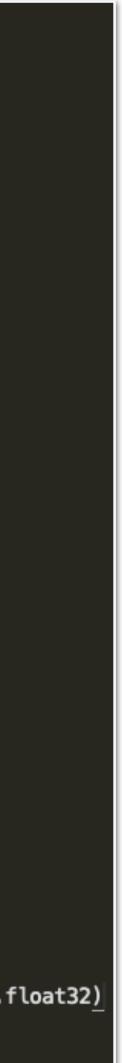


Return all events (selectors: return also a SelectionResult)

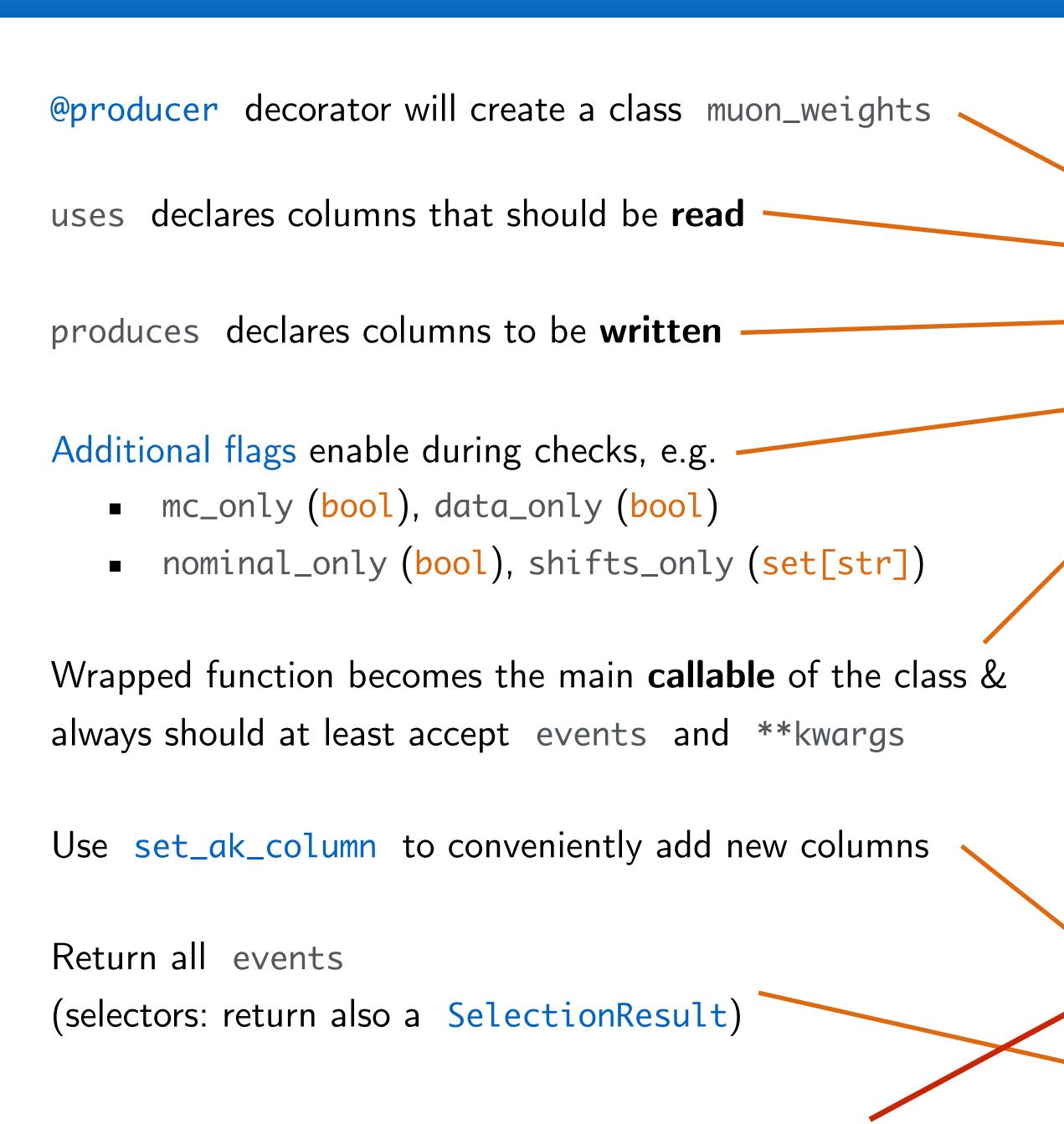






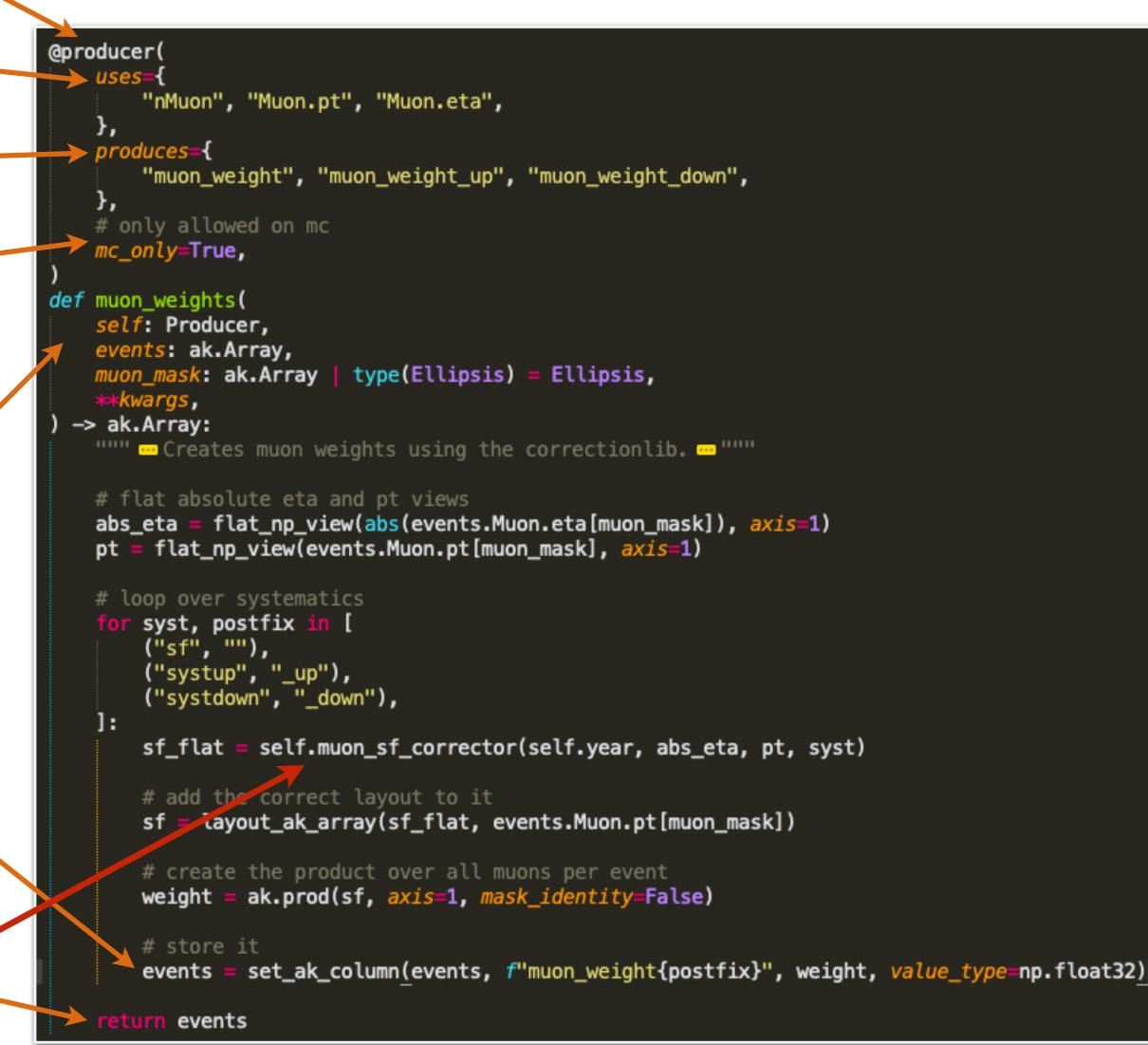


# 14 Writing your own producer (calibrator, selector, ...) (1)

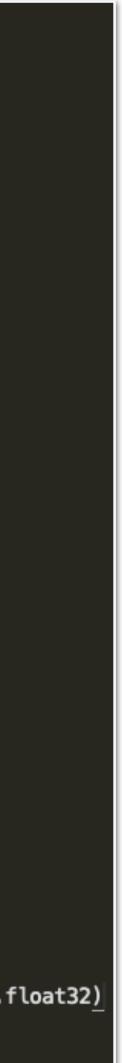


Where does the muon\_sf\_corrector come from?









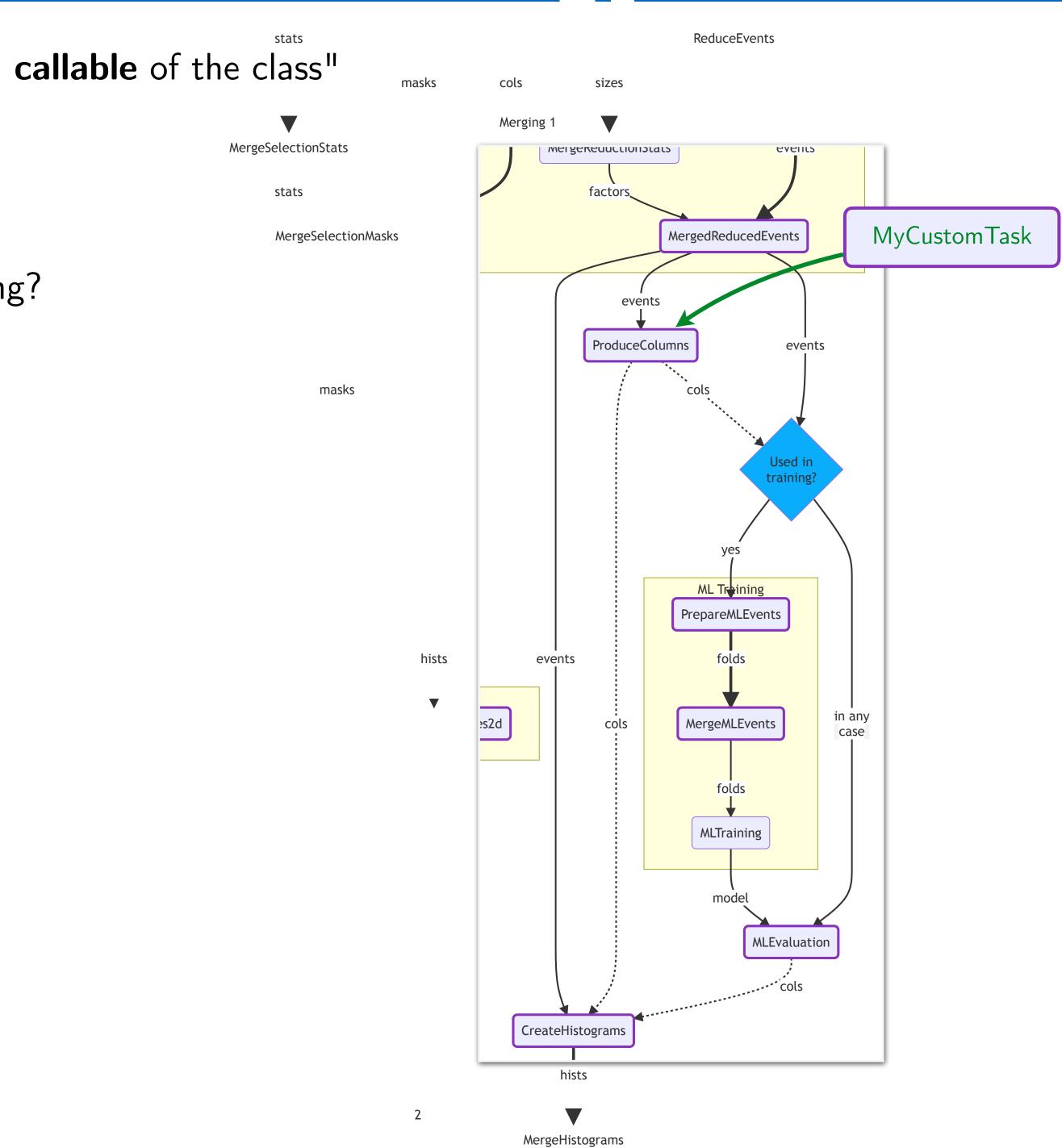
# 15 Writing your own producer (calibrator, selector, ...) (2)

- From previous slide: "Wrapped function becomes the main callable of the class"
   → Called for every chunk of events during processing
- But
  - How to setup objects **before** the actual event processing?
  - How to define a custom dependency?
     (i.e., task(s) on whose outputs the producer depends)

SelectEvents

### columousflow

### Marcel Rieger for the CF team





# 15 Writing your own producer (calibrator, selector, ...) (2)

- From previous slide: "Wrapped function becomes the main callable of the class"
  - → Called for every chunk of events during processing

# • But

- How to setup objects **before** the actual event processing?
- How to define a custom dependency?
   (i.e., task(s) on whose outputs the producer depends)

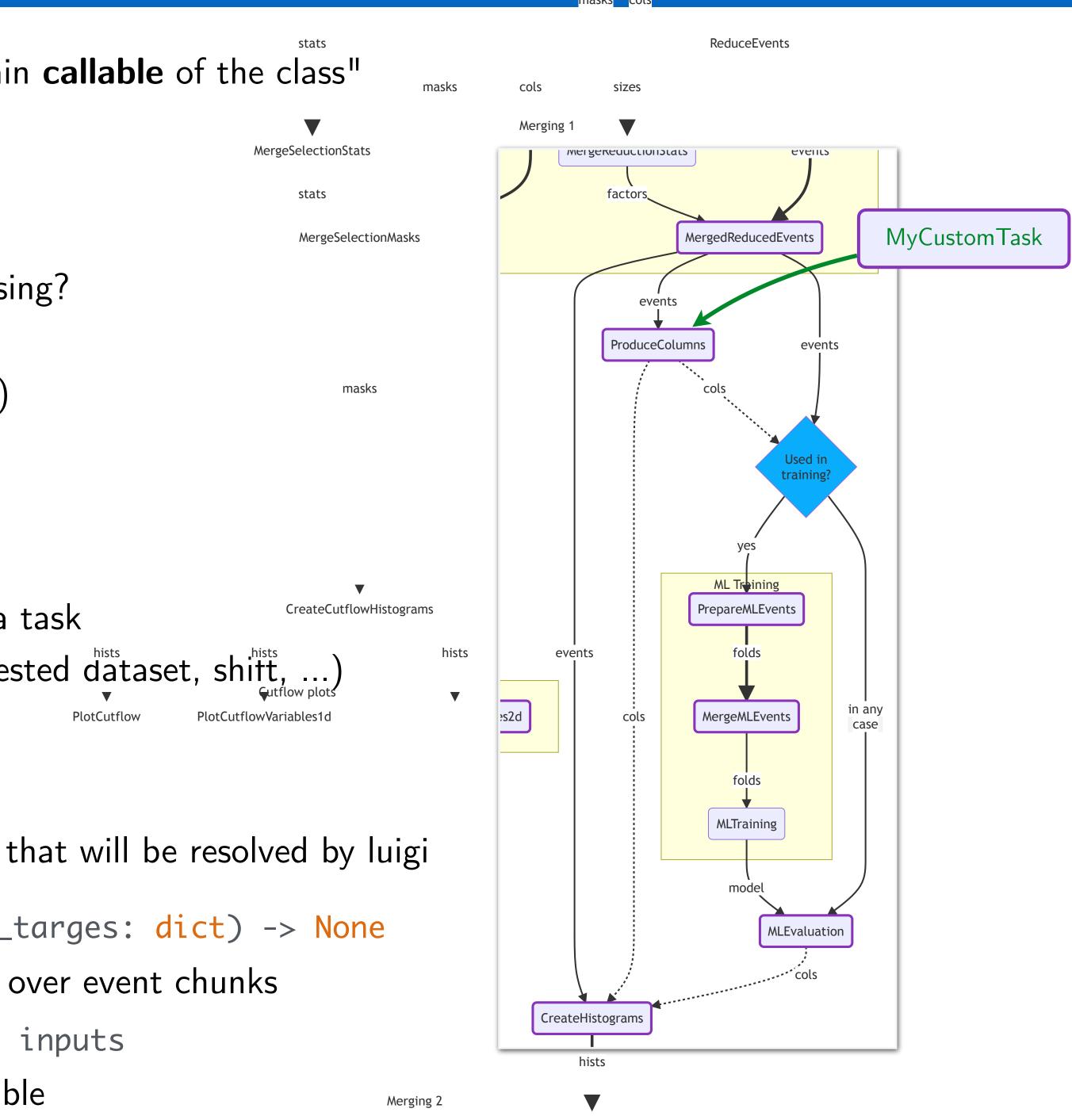
# • Three additional hooks

- init(self) -> None
  - ▷ Method called as soon as producer registered by a task
  - ▷ Receives important task variables via self (requested dataset, shift, ...)
- requires(self, reqs: dict) -> None
  - Method called when task declares its dependices
  - ▶ Allows injecting custom dependencies into reqs that will be resolved by luigi
- setup(self, reqs: dict, inputs: dict, reader\_targes: dict) -> None
   Method called in task's run() once before loop over event chunks
   Receives reqs defined before and corresponding inputs
   Allows setting up objects to be used in main callable

SelectEvents

columos

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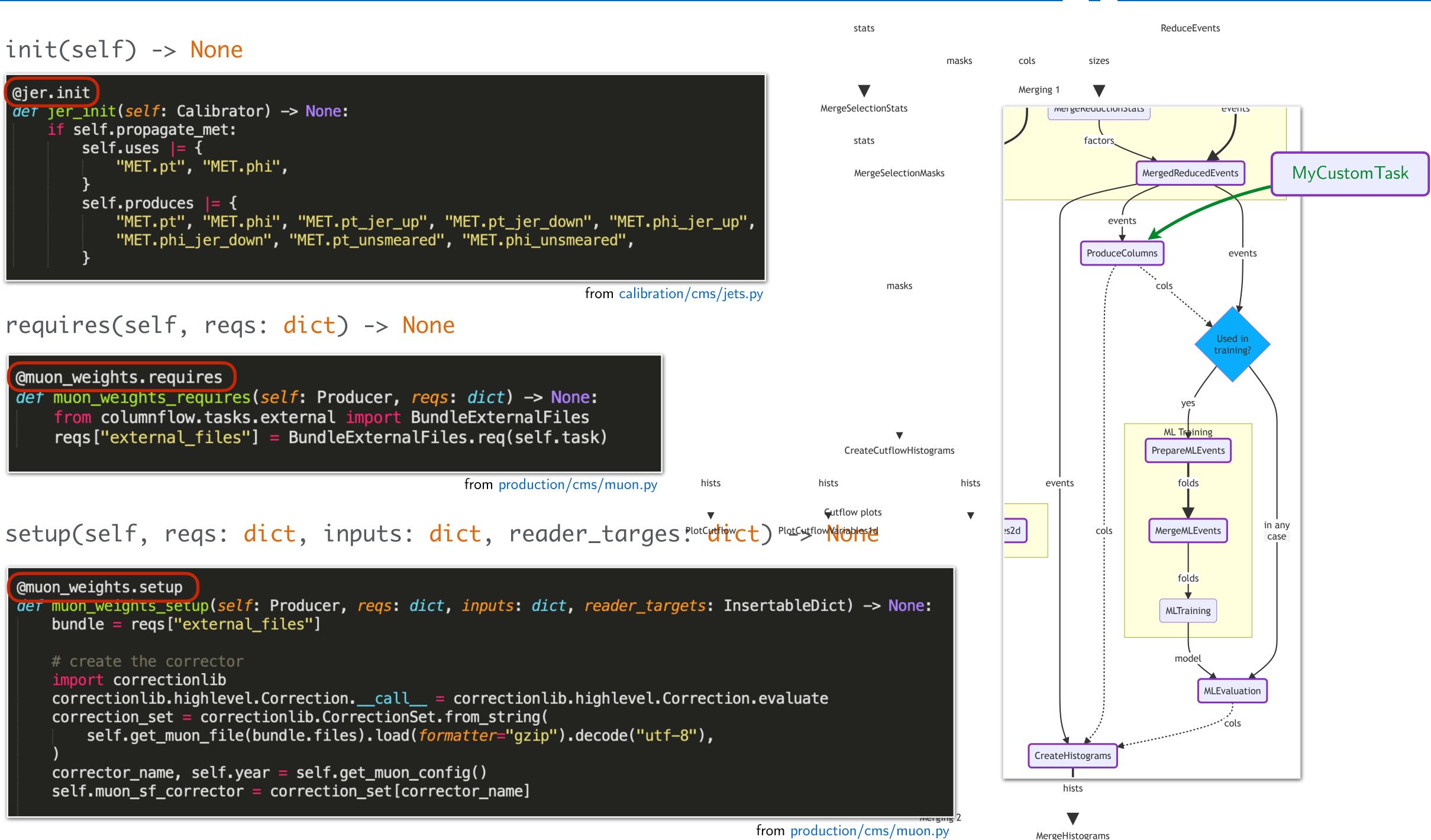


MergeHistograms



16 Writing your own producer (calibrator, selector, ...) (3)

### init(self) -> None



### requires(self, reqs: dict) -> None

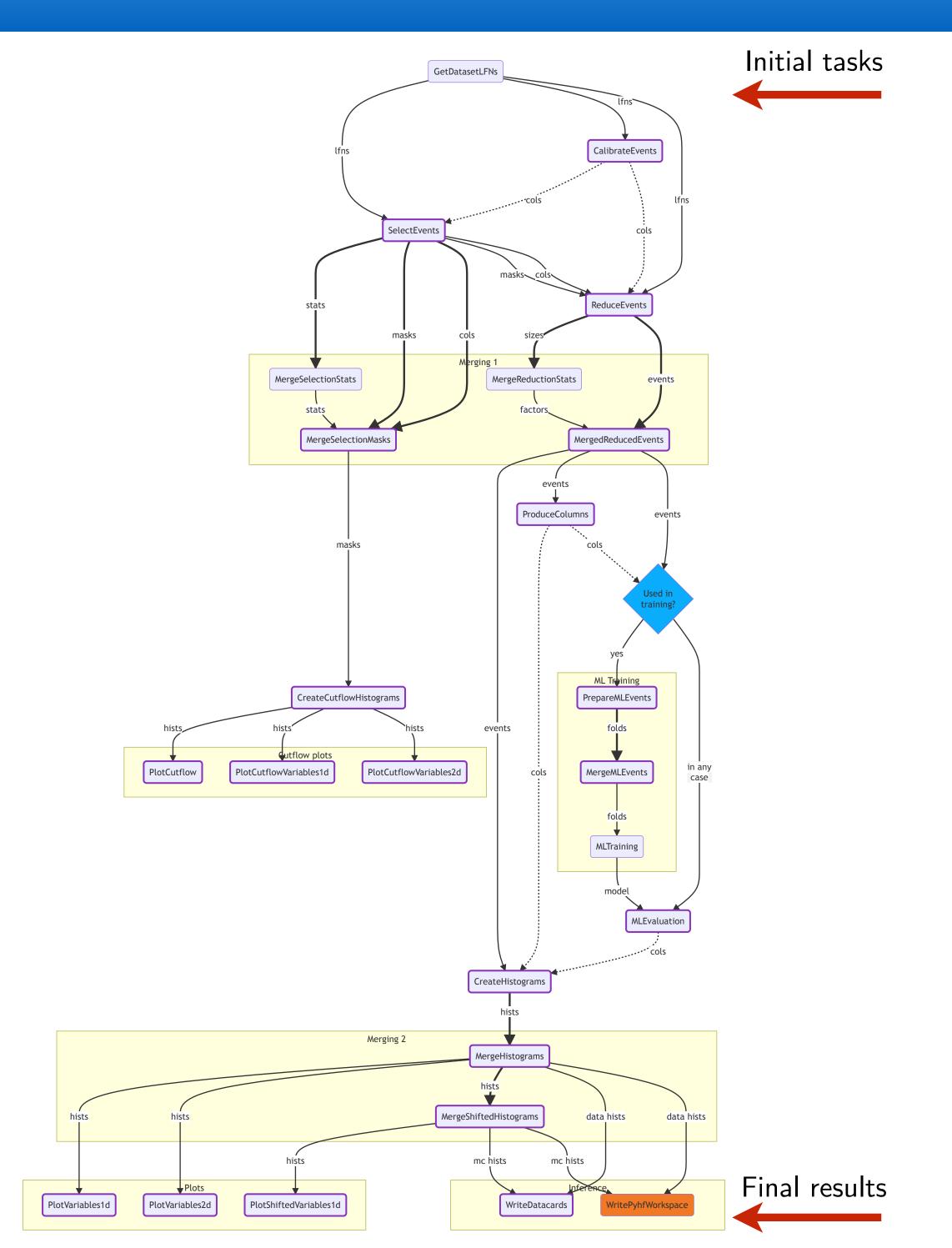
SelectEvents

coluncotsflow

### Marcel Rieger for the CF team

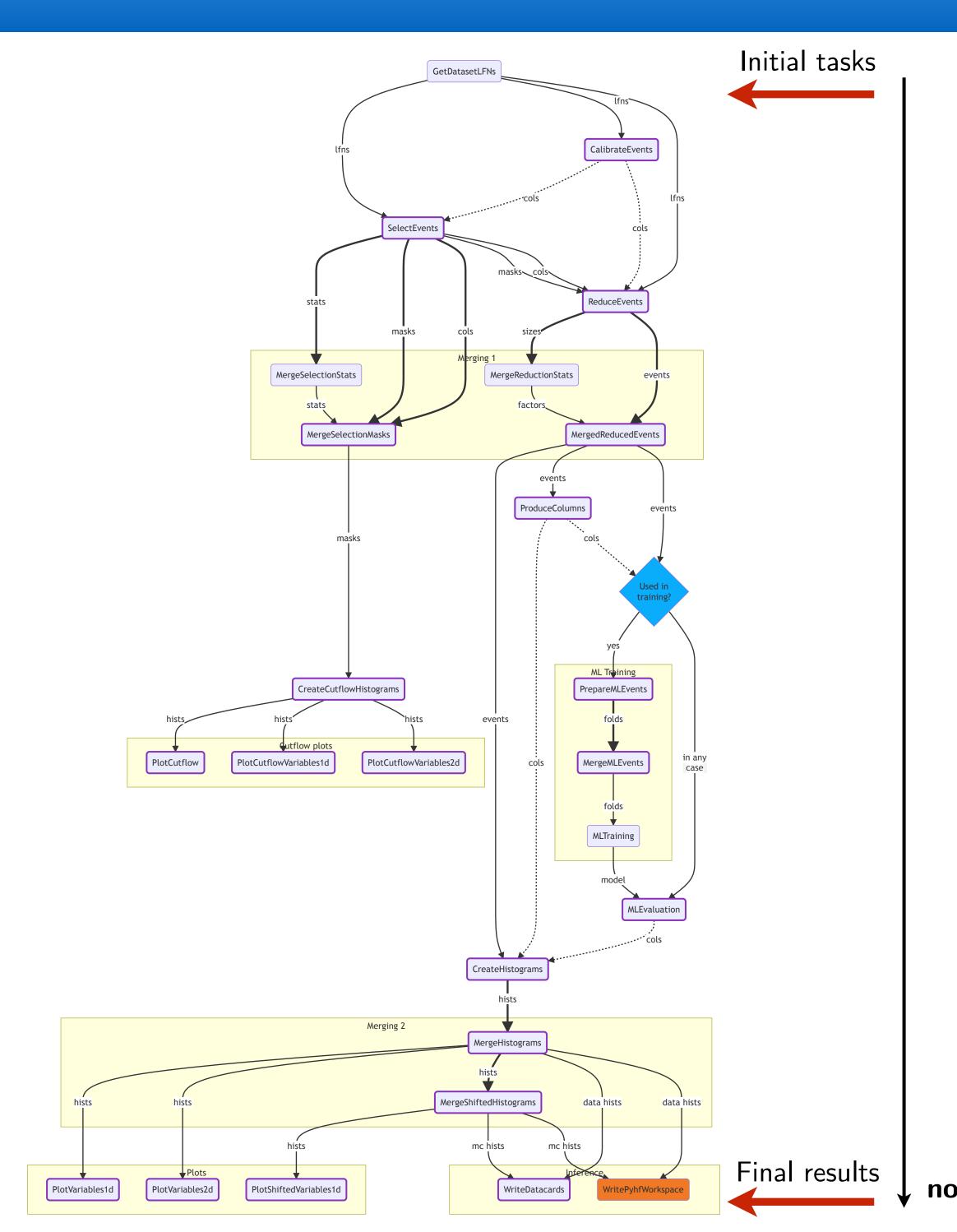


# 17 Conceptual handling of systematic uncertainties





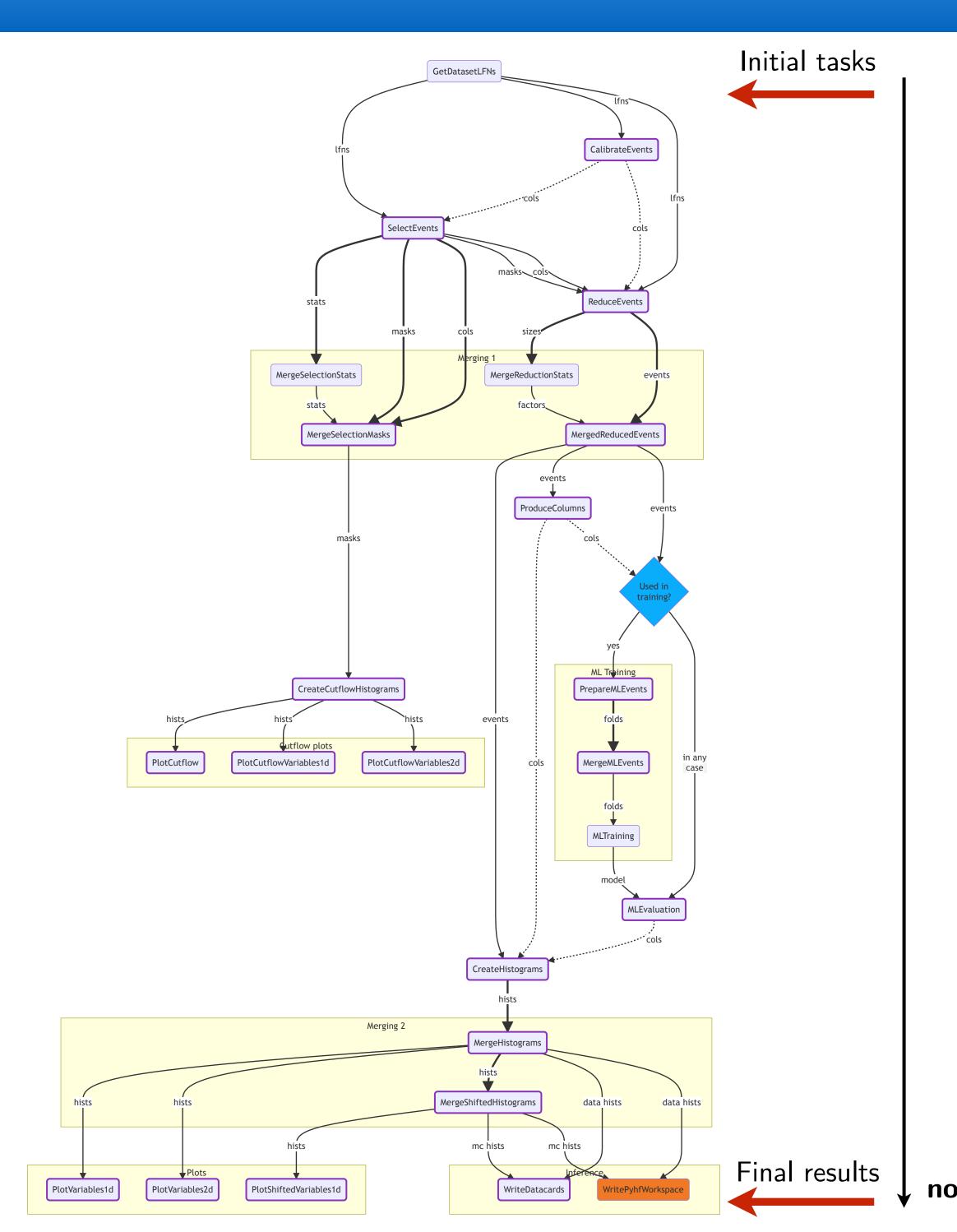
# 17 Conceptual handling of systematic uncertainties



nominal



# 17 Conceptual handling of systematic uncertainties



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# Key idea

Tasks *know* which uncertainties

- ▷ they implement
- they *depend on*  $\triangleright$ (through upstream tasks)

pileup(up|down)

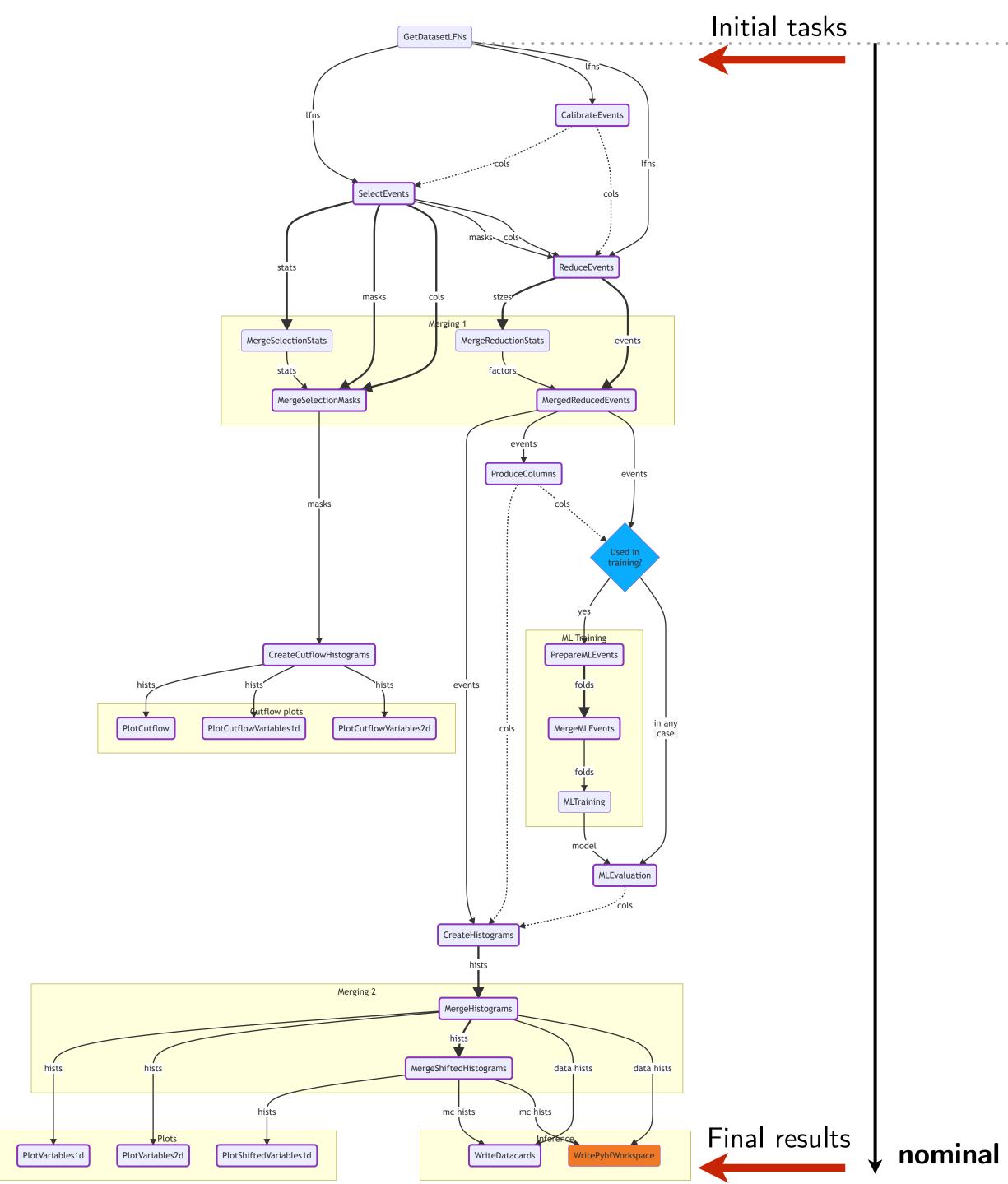
jec(up|down)

tune(up|down)

nominal



# 17 Conceptual handling of systematic uncertainties



### columnflow Marcel Rieger for the CF team

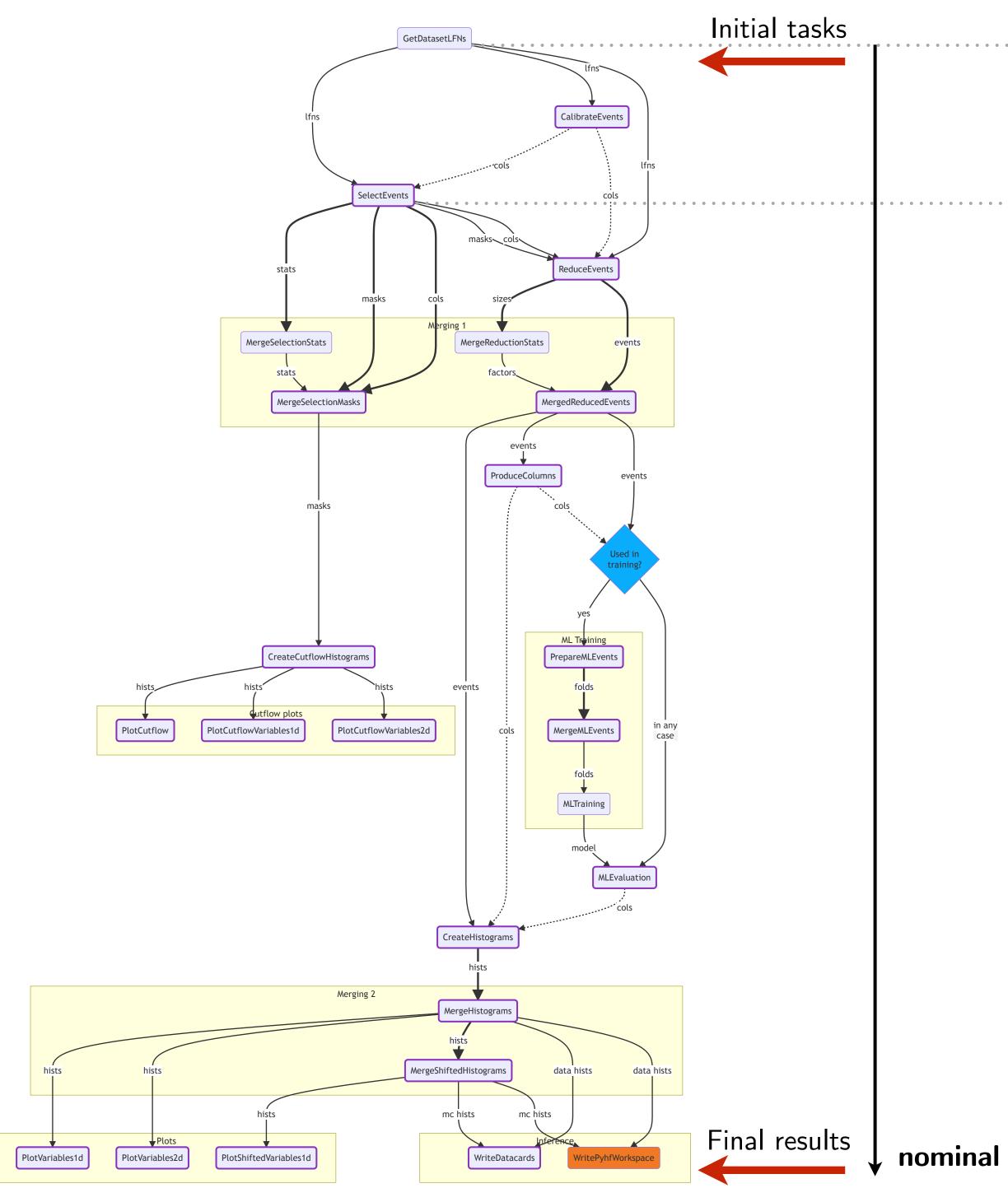
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# 17 Conceptual handling of systematic uncertainties



### columnflow Marcel Rieger for the CF team

## Key idea

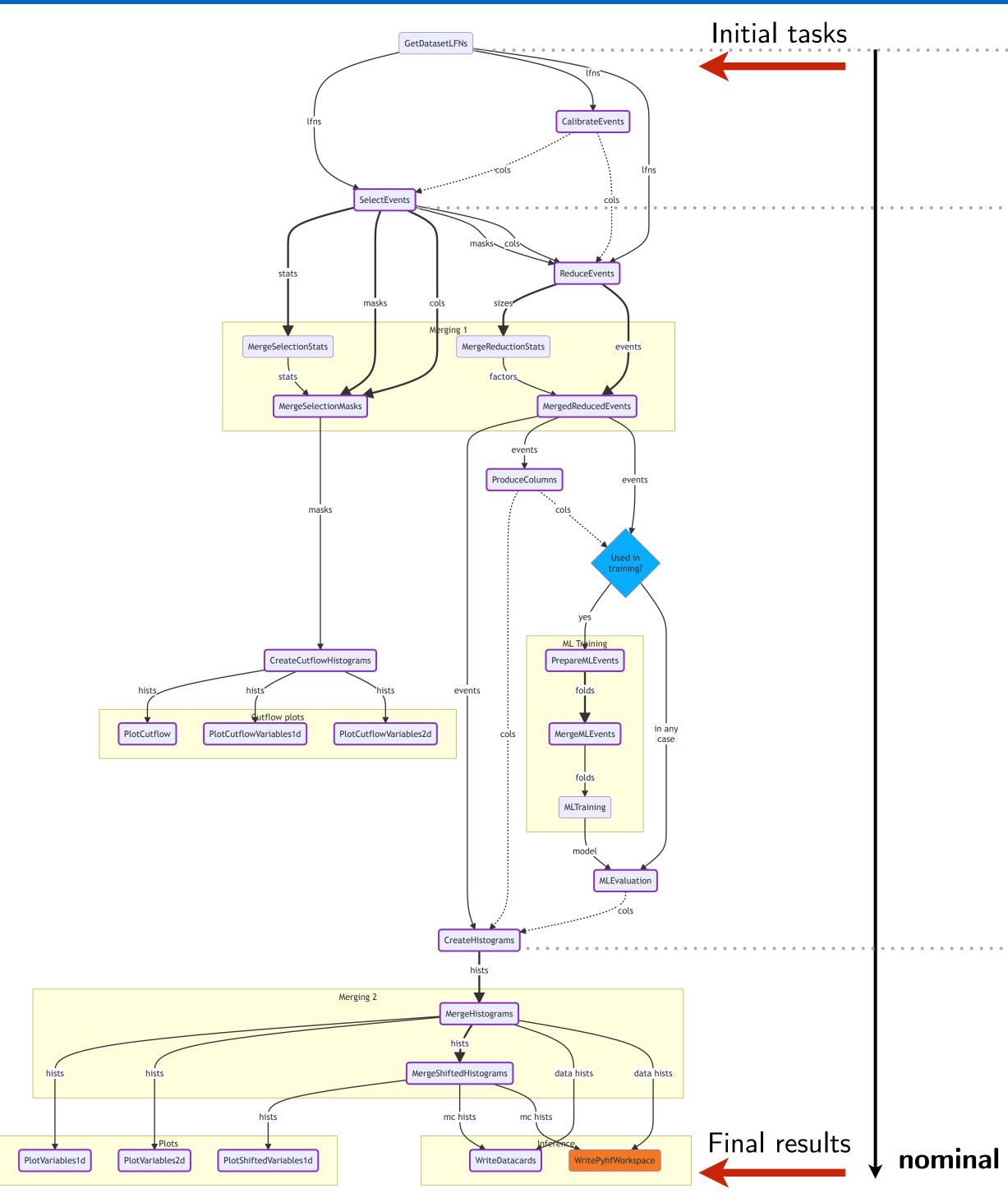
Tasks *know* which uncertainties

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reuses all nominal outputs above SelectEvents



# 17 Conceptual handling of systematic uncertainties



### columnflow Marcel Rieger for the CF team

## Key idea

Tasks *know* which uncertainties

- ▷ they implement
- they *depend on*  $\triangleright$ (through upstream tasks)

reuses all nominal outputs above SelectEvents

reuses all **nominal** outputs above

CreateHistograms

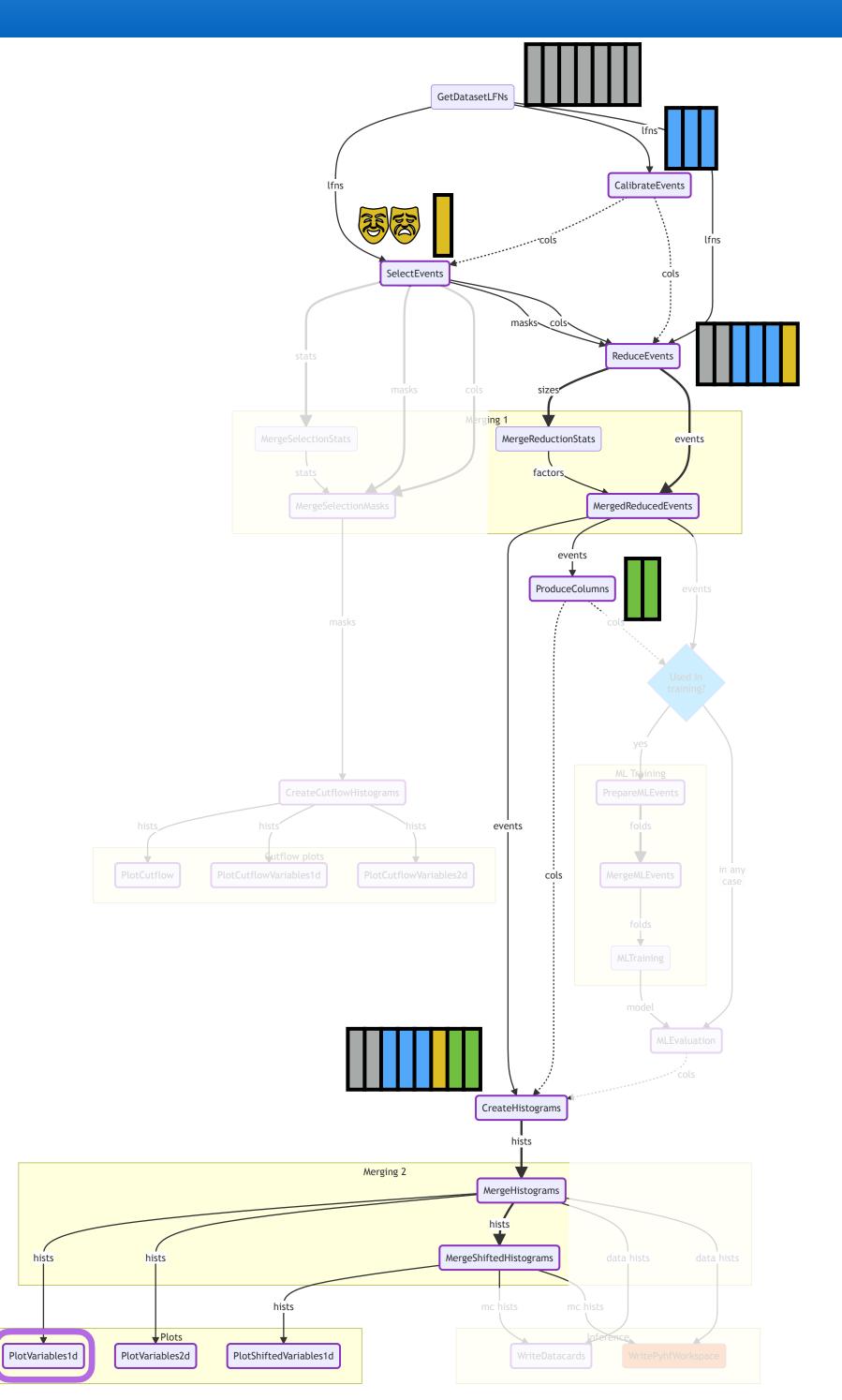
tune(up|down)

jec(up|down)

ileup(up|down)



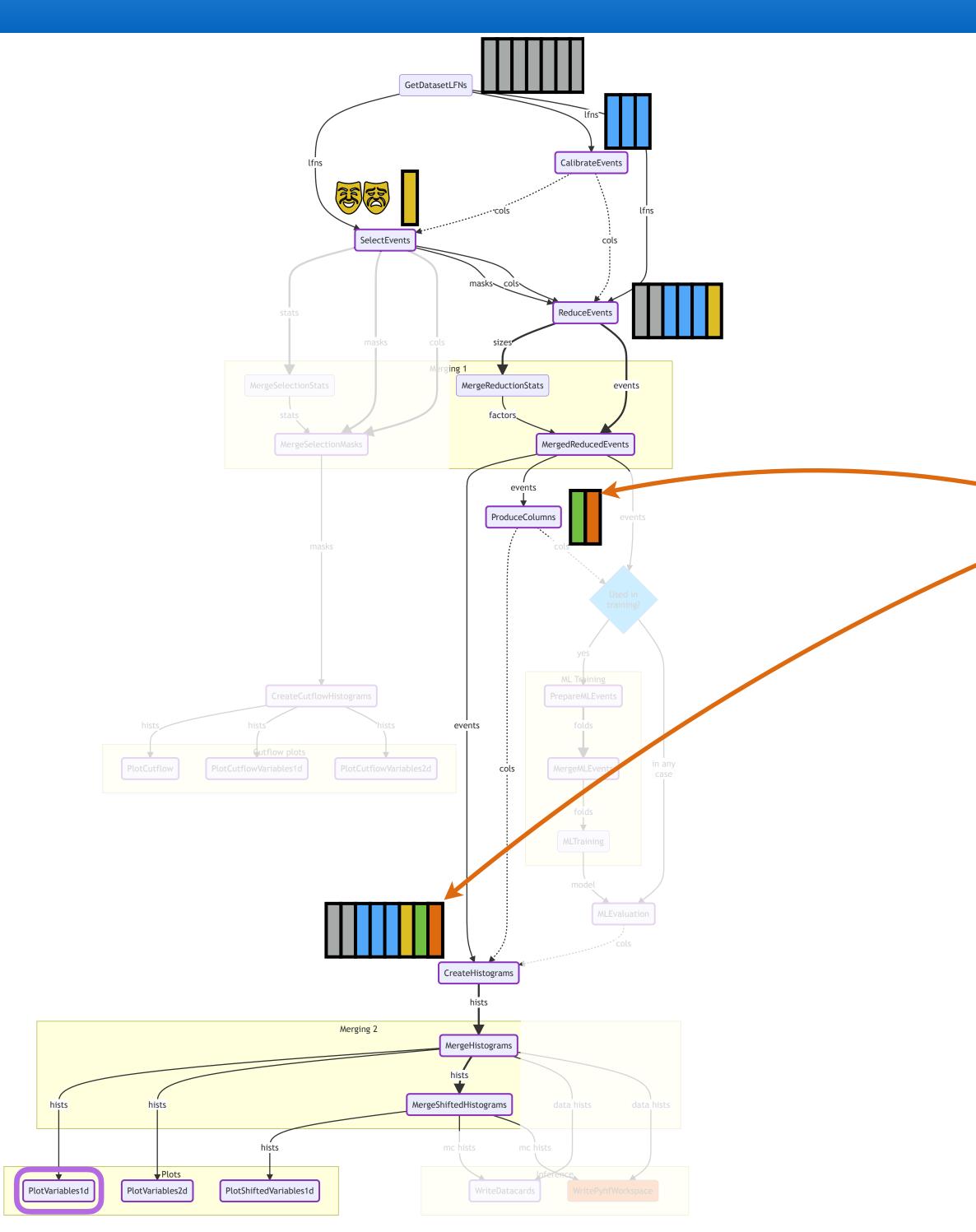
# 18 flow of columns: systematic uncertainties







# 18 flow of columns: systematic uncertainties

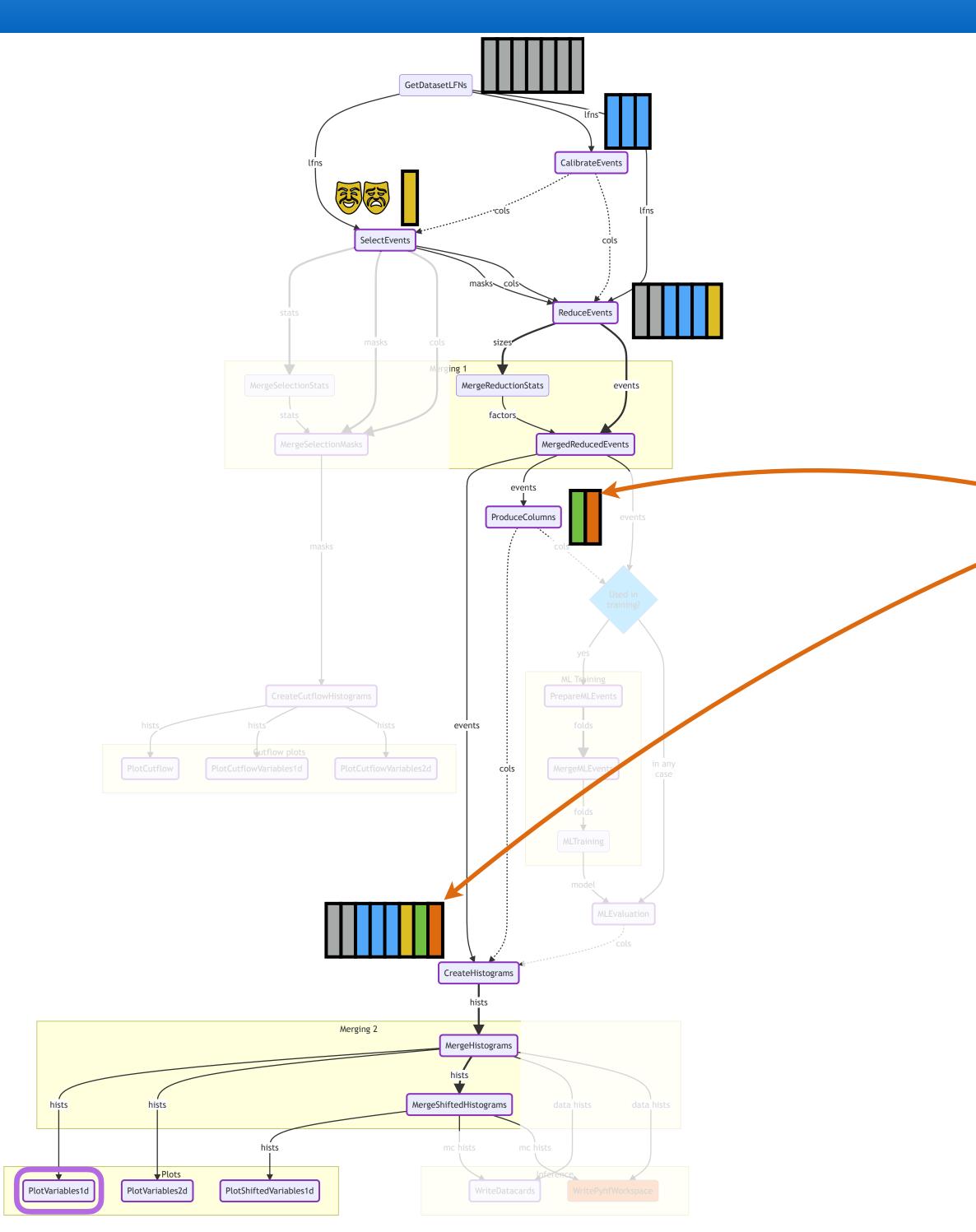




- Handling of systematics
  - fully outsourced to task dependency resolution
  - efficient, no unnecessary computations
  - executable with high parallelism



# 18 flow of columns: systematic uncertainties



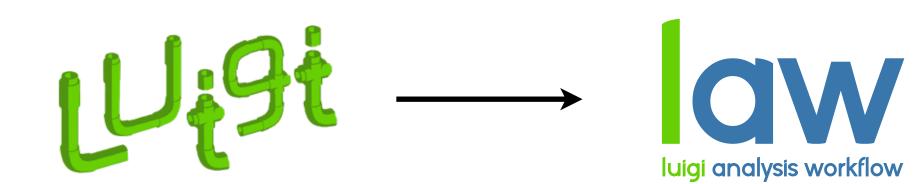


- Handling of systematics
  - fully outsourced to task dependency resolution
  - efficient, no unnecessary computations
  - executable with **high parallelism**
- It's the analyzer's choice
  - where varied columns
    are produced
  - if they are already part of *normal* columns
    - Computationally *trivial*: produce <u>right</u> away in
    - Computationally *demanding*: produce in parallel





# 19 Orchestration software stack



workflow engine (originally by Spotify) layer for HEP & scale-out (experiment independent) **columnflow** Marcel Rieger for the CF team



"framework" (experiment independent\*)



analysis



\* soon

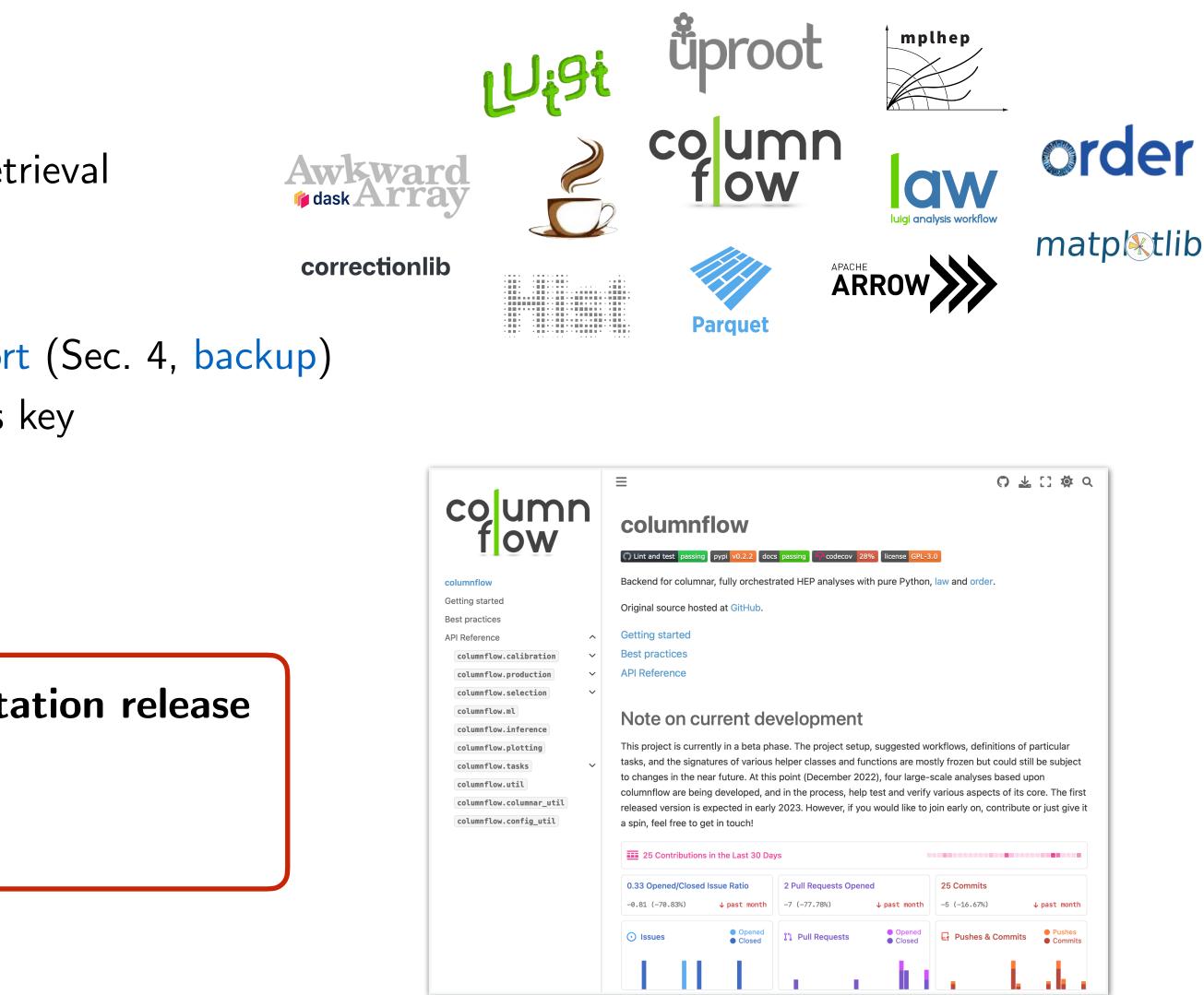
# 20 Summary

## Python framework for vectorized, columnar HEP analysis with nano-like inputs

- Mostly experiment agnostic core
- Fully orchestrated & automated
- Intermediate outputs
- Efficient through on-demand column production & retrieval
- Able to incorporate **any remote resource**
- Checks 15/17 "ideal workflow"items of CMS ATTF report (Sec. 4, backup)
  - Vast Python (HEP) community and tool landscape is key

### • Currently pushing for extensive documentation release

- Feedback still highly appreciated
- github.com/columnflow, columnflow.rtfd.io

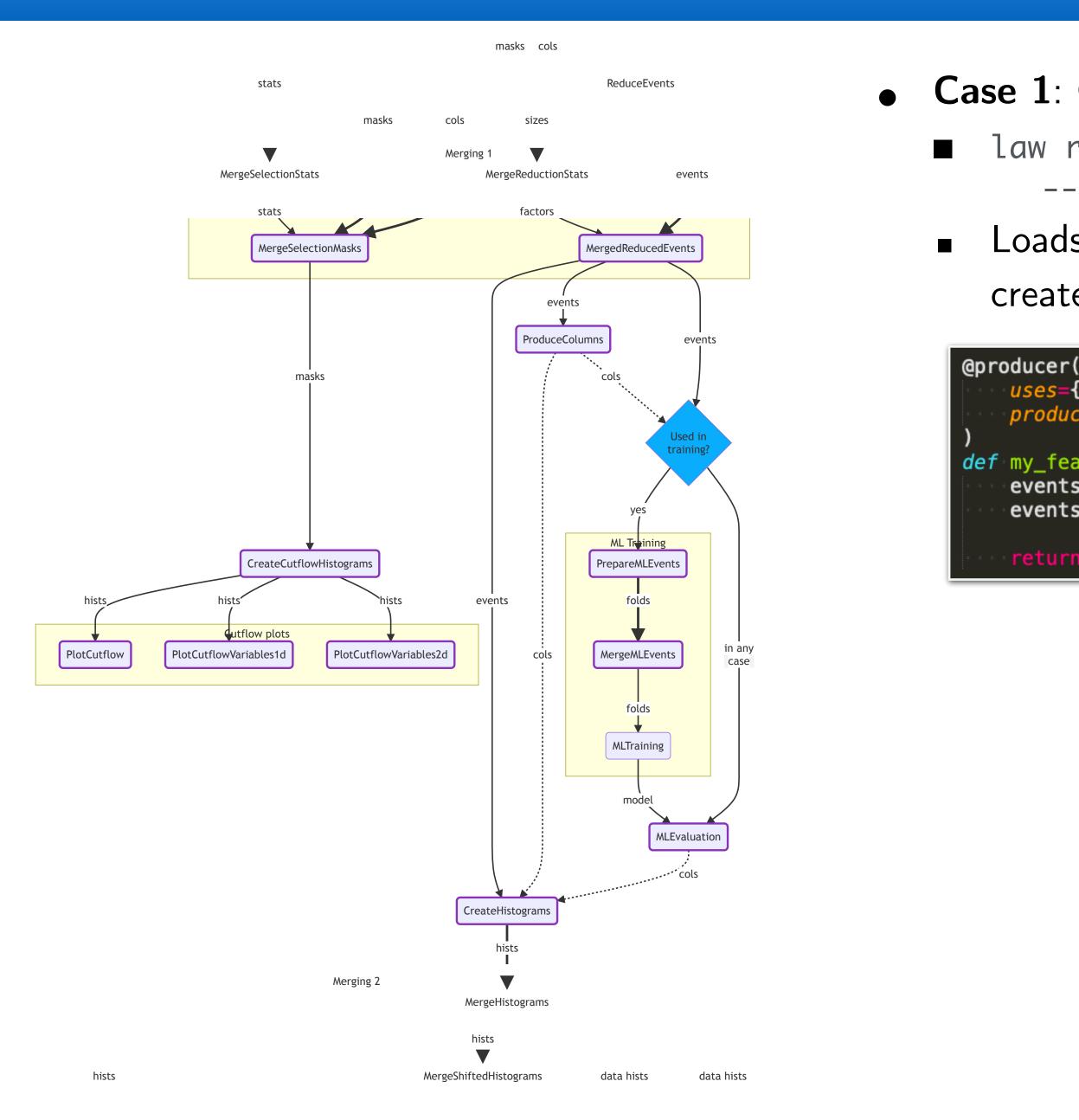




columnflow technicalities

# 22 Intermediate columns, on-demand production / retrieval

dep. deps. many



hists mc hists mc hists

les1d

Inference ▼Plots V WriteDatacards PlotVariables2d PlotShiftedVariables1d WritePyhfWorkspace



### • **Case 1**: Create histograms

law run cf.CreateHistograms --dataset tt \

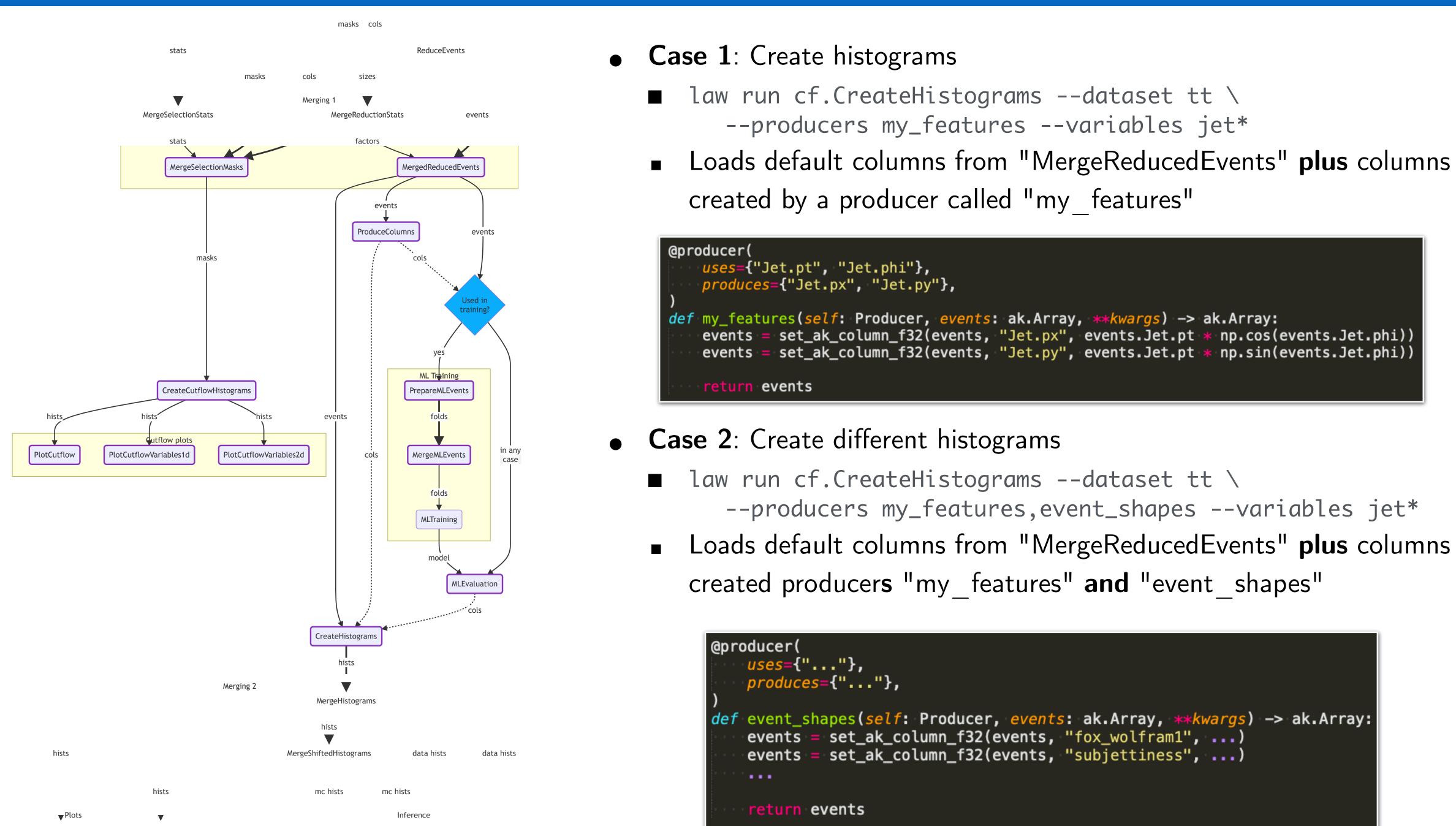
--producers my\_features --variables jet\*

Loads default columns from "MergeReducedEvents" plus columns created by a producer called "my features"

```
uses={"Jet.pt", "Jet.phi"},
   produces={"Jet.px", "Jet.py"},
def my_features(self: Producer, events: ak.Array, **kwargs) -> ak.Array:
    events = set_ak_column_f32(events, "Jet.px", events.Jet.pt * np.cos(events.Jet.phi))
   events = set_ak_column_f32(events, "Jet.py", events.Jet.pt * np.sin(events.Jet.phi))
```

return events

# 22 Intermediate columns, on-demand production / retrieval



PlotVariables2d PlotShiftedVariables1d WritePyhfWorkspace WriteDatacards

Only processes "event shapes", reuses columns from "my features"

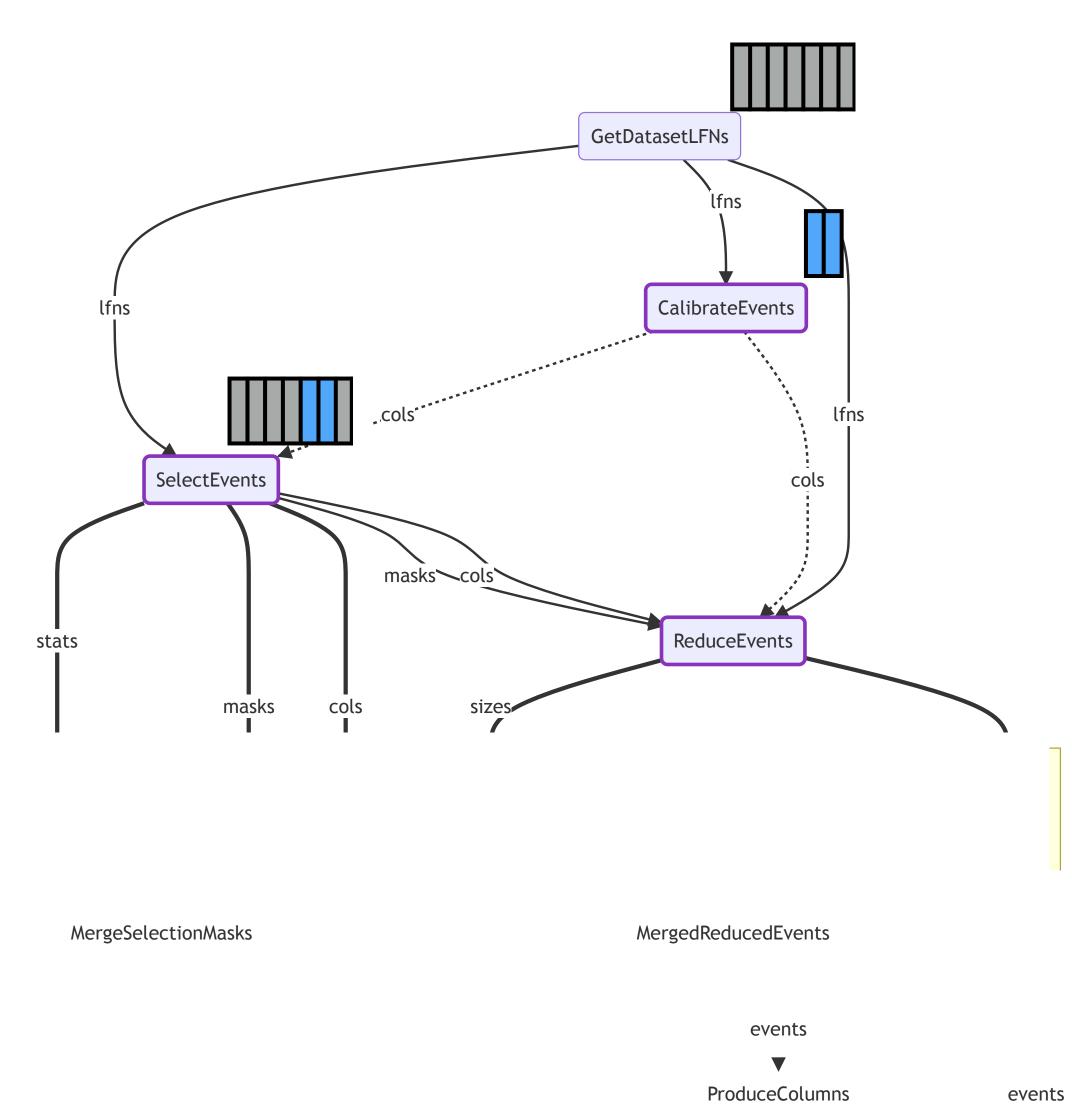


Loads default columns from "MergeReducedEvents" plus columns

```
events = set_ak_column_f32(events, "Jet.px", events.Jet.pt * np.cos(events.Jet.phi))
events = set_ak_column_f32(events, "Jet.py", events.Jet.pt * np.sin(events.Jet.phi))
```

```
--producers my_features, event_shapes --variables jet*
```

# 23 Layering of columns

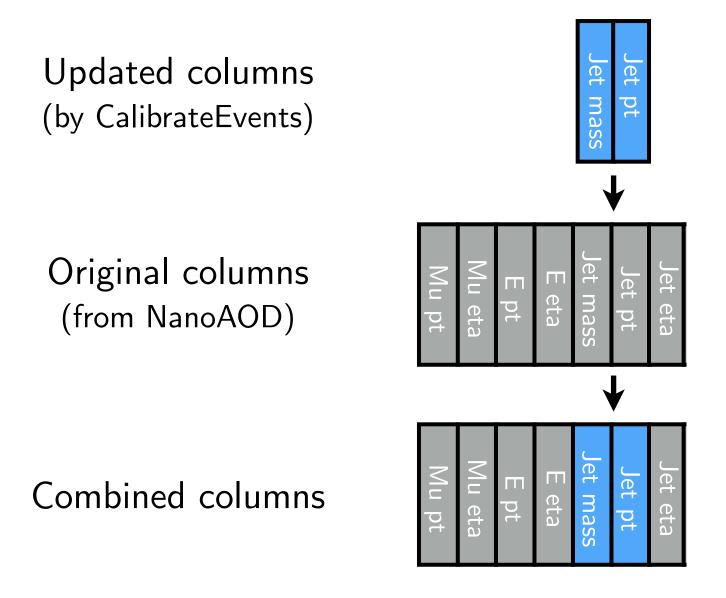


cols

events

### Layering of columns

e.g. in SelectEvents



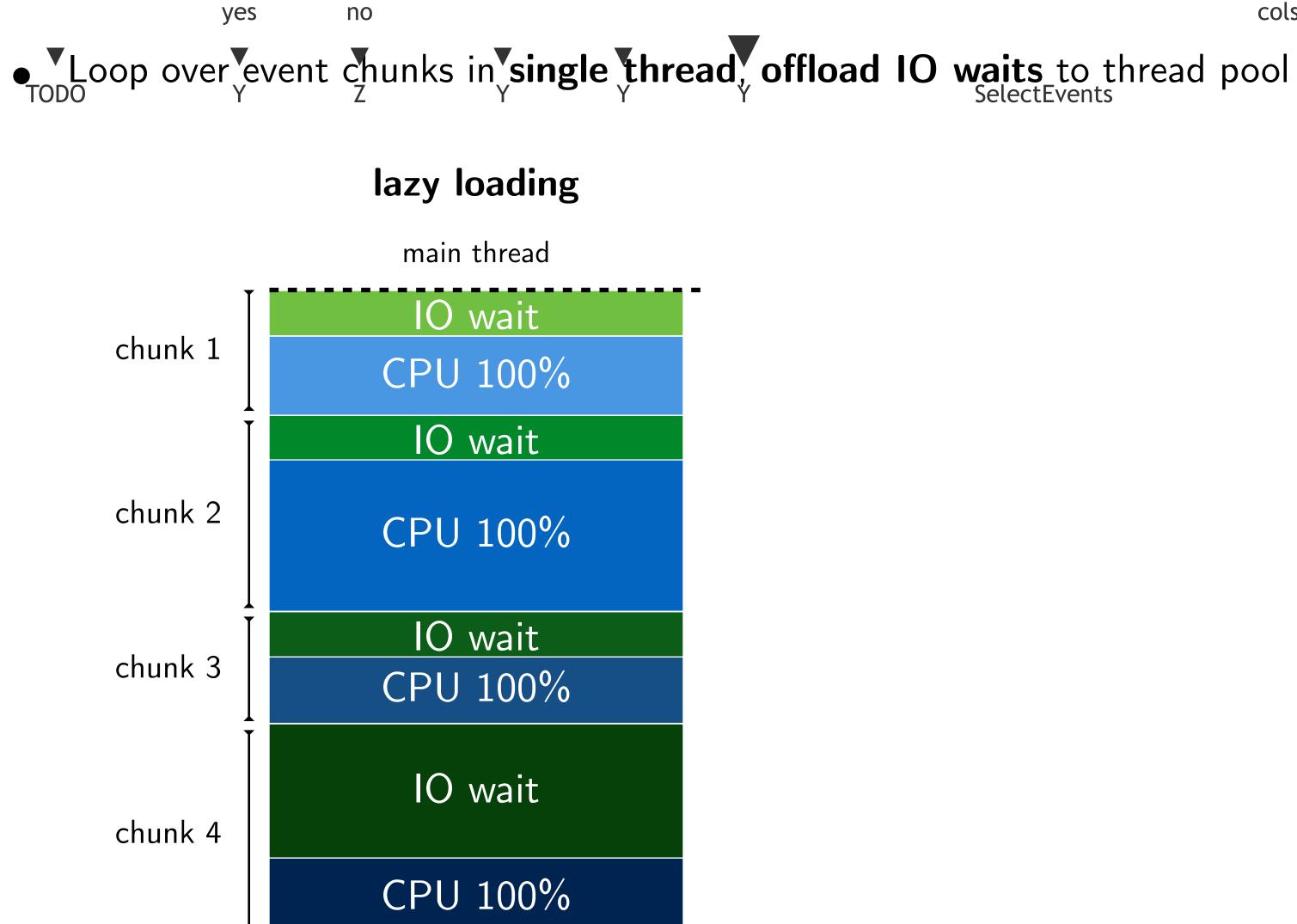


24 Parallelization and IQ

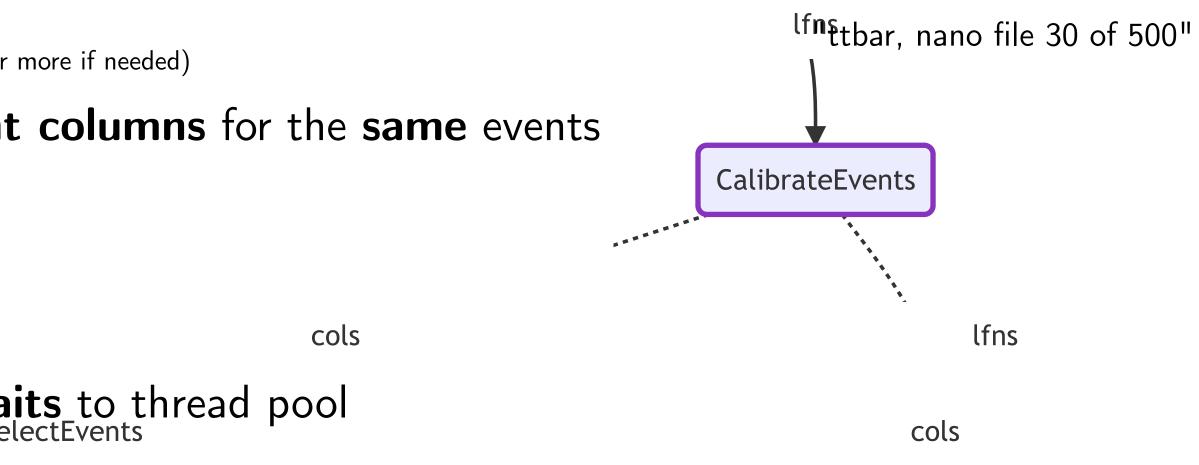
• Each task handles a single input in one\* process (\* or more if needed)

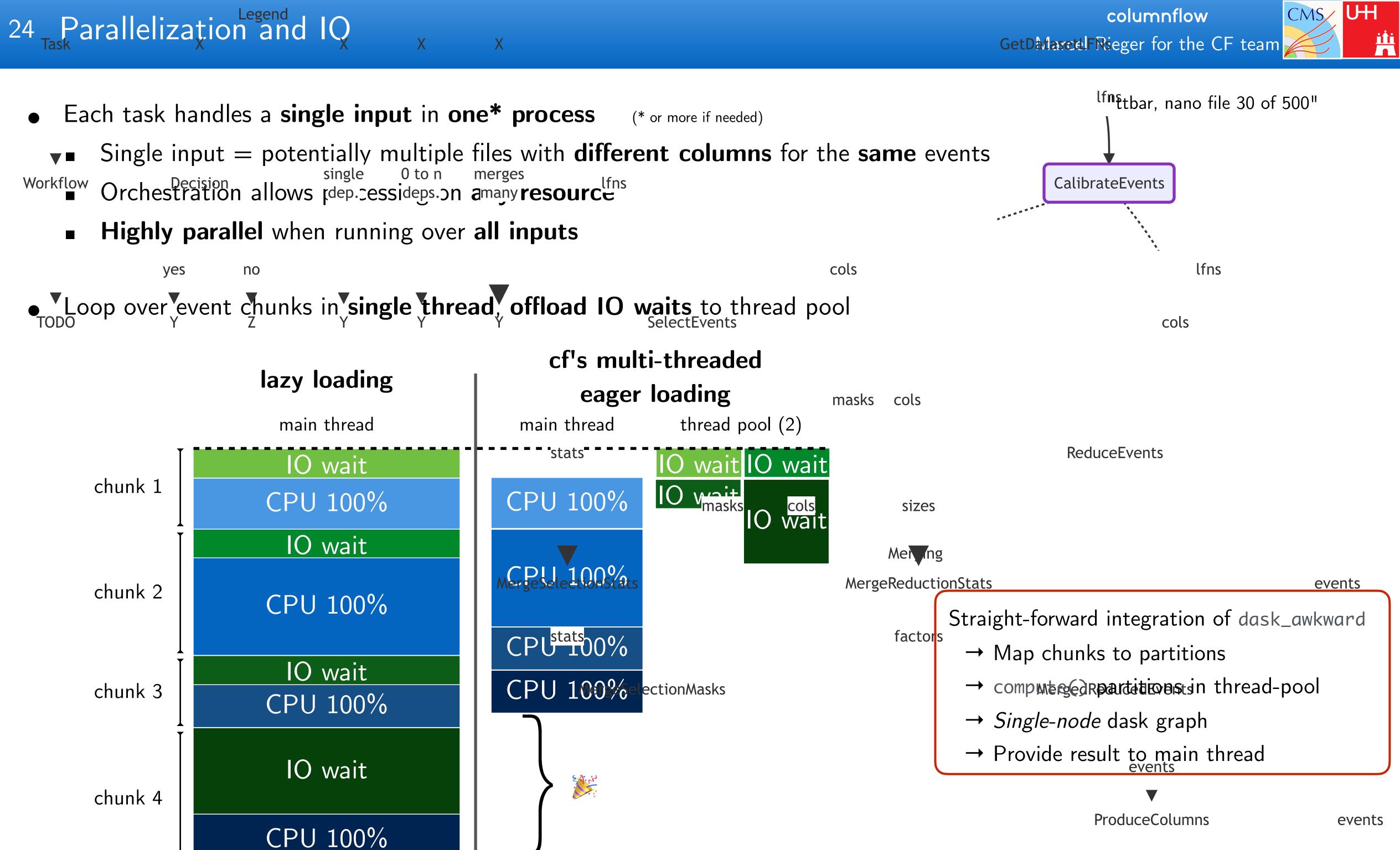
Χ

- Single input = potentially multiple files with different columns for the same events
   Workflow
   Orchestration allows rdep.cessideps.on
   amany resource
  - Highly parallel when running over all inputs









time



#### "Ideal workflow" in ATTF report 25

processing

lata

nalysis description

**r**ces-

esou

- **F1.1** Executable in "one go"  $\checkmark$
- **F1.2** Output intermediate results on demand  $\checkmark$
- **F1.3** Identify and rerun only necessary components  $\checkmark$
- **F1.4** Composition of columns to easy reuse / sharing  $\checkmark$
- **F1.5** Reproducibility via CI/CD  $\checkmark$
- **F1.6** Version checkpointing  $\checkmark$
- **F1.7** Support for custom NANO input  $\checkmark$
- **F2.1** Non-imperative paradigm ~
- **F2.2** Physics object representation for NANO objects  $\checkmark$
- **F2.3** Seamless handling of systematic uncertainties  $\checkmark$
- **F2.4** Automatic datacard writing  $\checkmark$
- **F2.5** Analysis results in different formats (datacards, pyhf workspace, HEPData, ...) ~
- **F2.6** Export to / import from dedicated, static workflow language
- **F2.7** Workflow configuration separated from analysis code  $\checkmark$
- **F2.8** Multidimensional histograms  $\checkmark$
- **F3.1** Resource agnosticism  $\checkmark$
- **F3.2** Easily scalable (local, multi-core, batch)  $\checkmark$



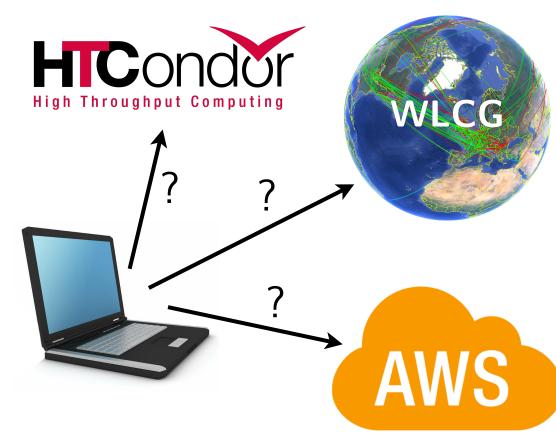
law & luigi

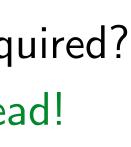
# 27 Motivational questions

- **Portability**: Does the analysis depend on ...
  - where it runs?
  - where it stores data?
    - Execution/storage should **not** dictate code design!

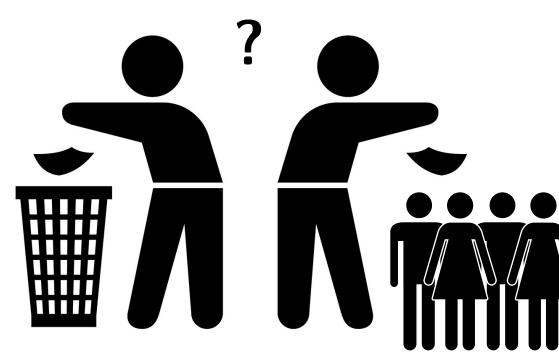
**Reproducibility**: When a postdoc / PhD student leaves, ...

- can someone else run the analysis?
- is there a loss of information? Is a new *framework* required?
  - ▷ Dependencies often only exist in the physicists head!
- **Preservation**: After an analysis is published ...
  - are people investing time to preserve their work?
  - can it be repeated after O(years)?
    - ▷ Daily working environment should provide preservation features **out-of-the-box**!
- Personal experience: <sup>2</sup>/<sub>3</sub> of "analysis" time for technicalities, <sup>1</sup>/<sub>3</sub> left for physics  $\rightarrow$  Physics output doubled if it were the other way round?





























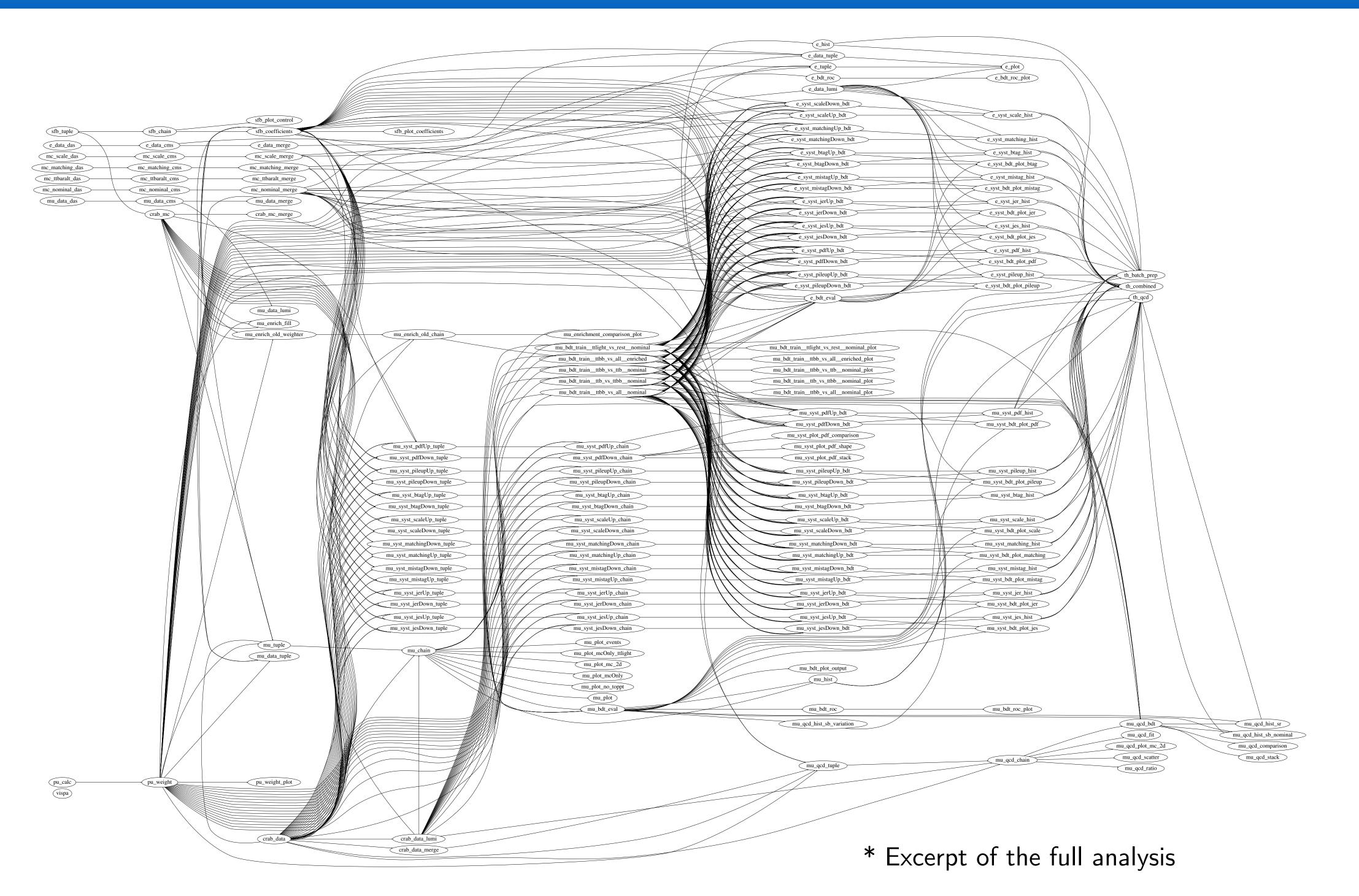






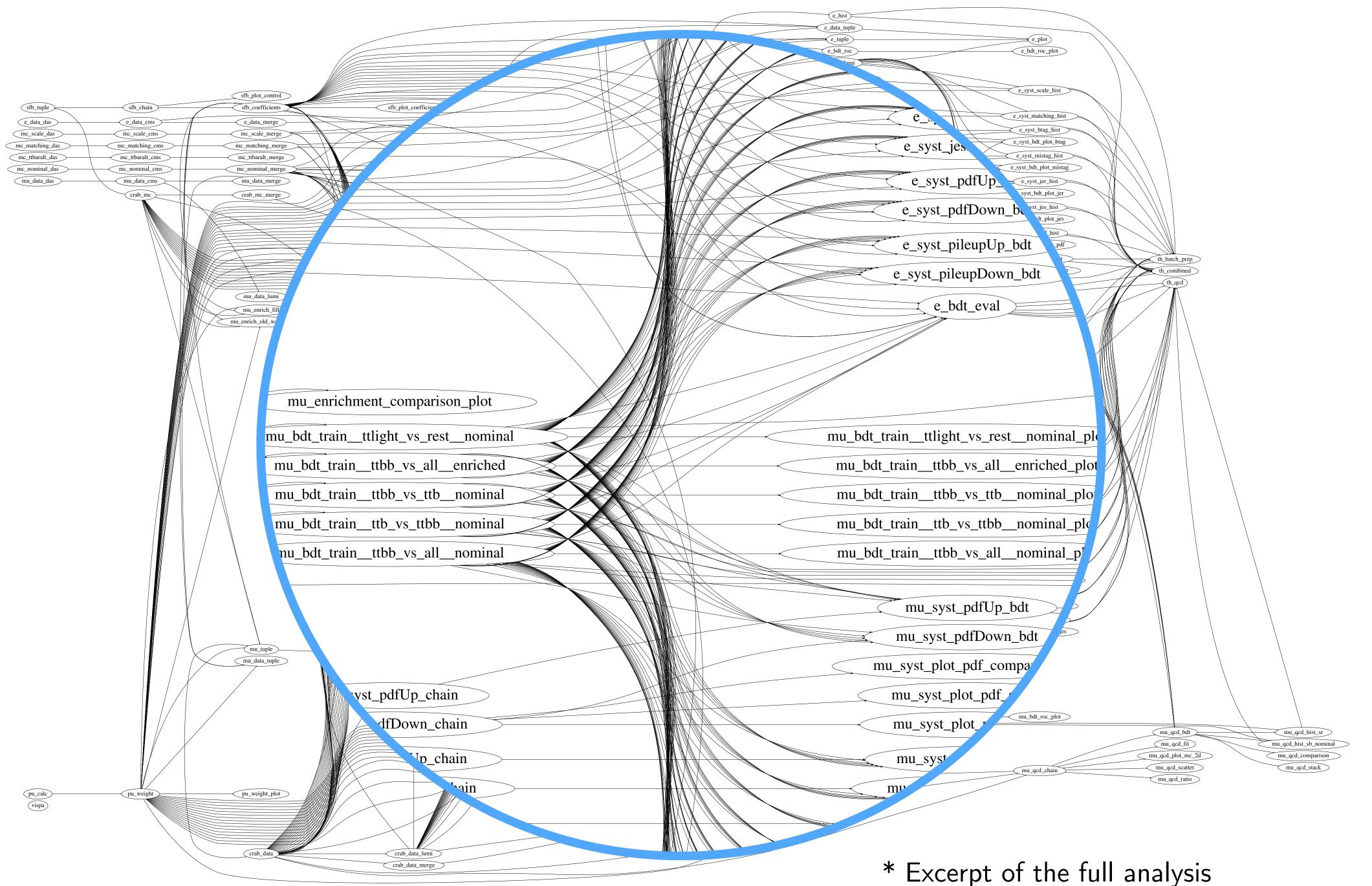


## 28 Example: ttbb cross section measurement





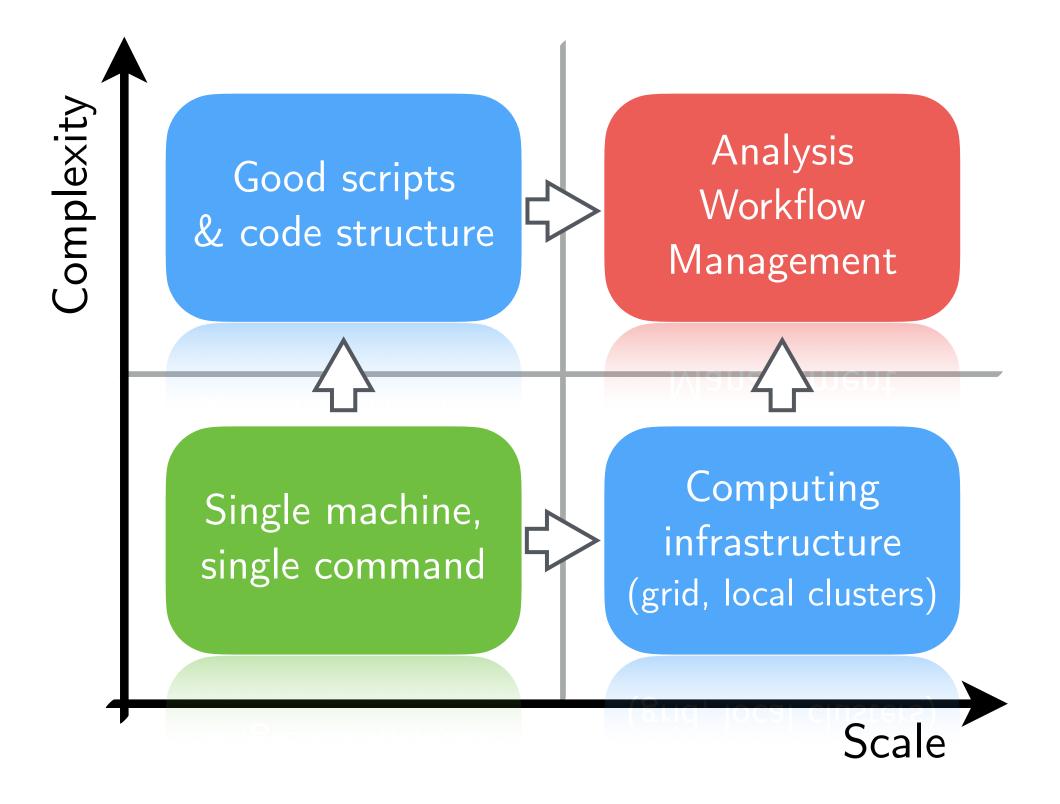
## 28 Example: ttbb cross section measurement





# 29 Landscape of HEP analyses

- Most analyses are both large and complex
  - Structure & requirements between workloads mostly undocumented
  - Manual execution & steering of jobs, bookkeeping of data across SEs, data revisions, ...
  - $\rightarrow$  Error-prone & time-consuming



## • In the following

- → Approach complexity with Ui9i
- → Enabling **large-scale** with

aw



#### Existing WMS: MC production 30



## Tailored systems

- Structure "iterative", a-priori unknown
- Dynamic workflows, fast R&D cycles
- DAG with arbitrary dependencies
- Incorporate *any* existing infrastructure
- Use custom software, everywhere

### Wishlist for end-user analyses

- Structure known in advance
- Workflows static & recurring
- One-dimensional design
- Special production infrastructure
- Homogeneous software requirements

→ Requirements for HEP analyses mostly orthogonal





- Python package for building complex pipelines
- Development started at Spotify, now open-source and cor

1. Workloads defined as **Task** classes that can **requ** Building blocks

- 2. Tasks produce output **Targets**
- 3. Parameters customize tasks & control

Web UI with two-way messaging (task  $\rightarrow$  UI, UI  $\rightarrow$  task), autocommand line interface, ...

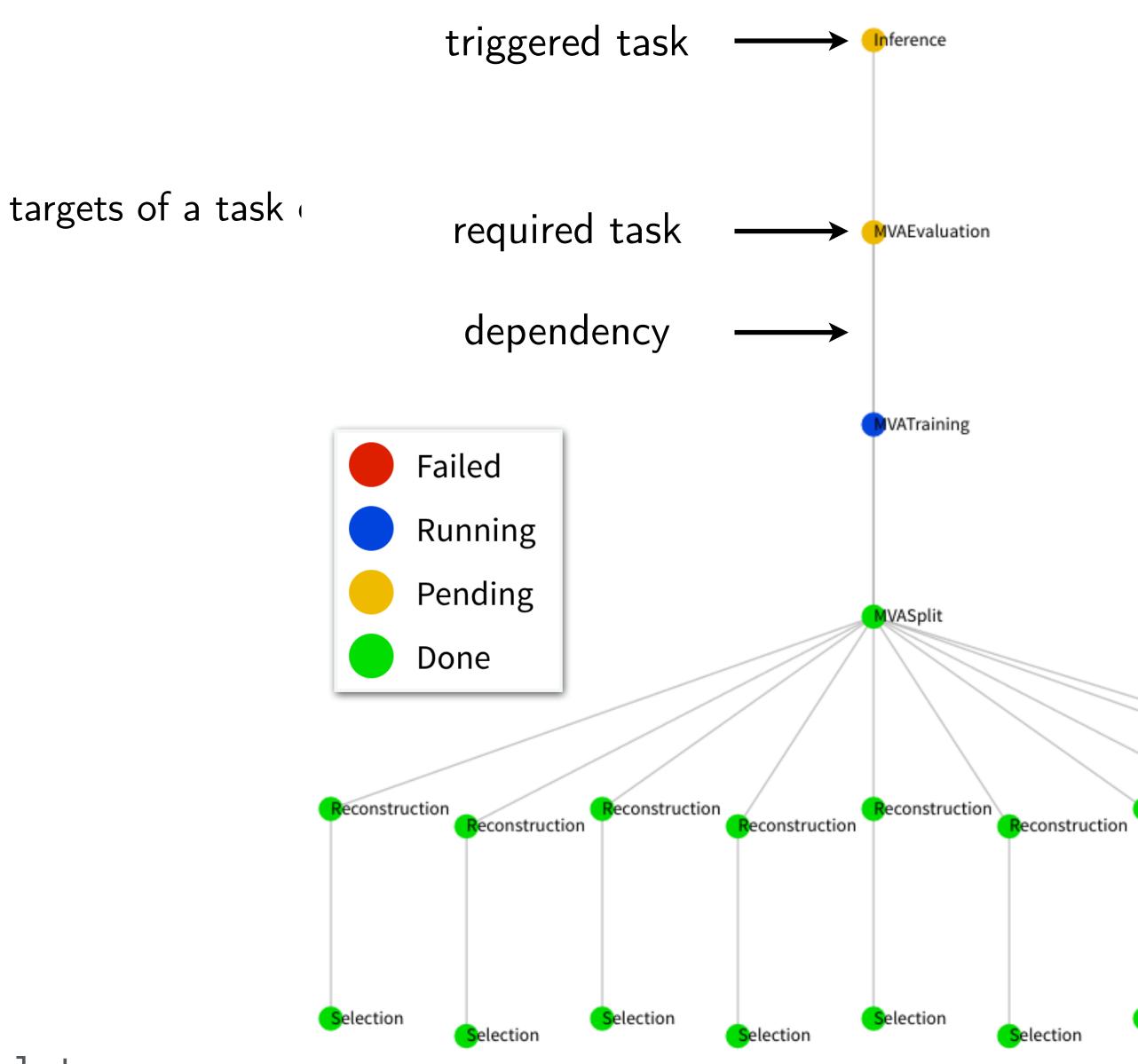
ommunity-drive	github.c	com/spotify/ 493	luigi Unstar	15.2k	ះ Fork	2.3k	
<b>uire</b> other <b>Tasl</b>		Luigi Task Visualiser ) lx3agpu01.physik.rwt Status ≡ Task L			ualiser/index.h Resources	tml Q	AP 📭
runtime behavi		99 UPSTREAM FAIL	RUNNING     6       DISABLEI		DONE     176     UPSTR     0	TASKS EAM DISA	×
comatic error ha	Displayin Show 10 🔷 ent	g RUNNING, tasks . tries			Filter ta	ble:	
		Name	🔶 Details		¢	Priority 🔶	Time
	RUNNING	ttH-bb-semi.SyncCSVs	paramFile=E setup=RunIIS notify=False, sandbox=loc dCache=mrie printDeps=-1	e, taskName=EMPTY_ MPTY_STRING, log=-, Spring16MiniAODv2_1 printStatus=-1, al_ttH_80X, version=to egerDESY, dataSources , printStore=EMPTY_S =-1, printLog=False	3TeV_25bx_80X, est2, =tth,	0	04/12/2016, 22:43 minutes
	RUNNING	ttH-DNN-Reco.DNNTraining	keep_prob=0 shuffleSeed= startSeed=1, normalize=Fa trainingPorti requireTTH= batch_size=1 chi2endSeed	0, limitBtags=True, ma 0.7, num_epochs=20, l 123, num_layers=5, d report_interval=10.0, alse, testingPortion=0 on=0.8, label=tth, train True, requireH=False, 10000, nEvents=100000 l=5, requireTT=False, g 500, chi2number=50 _gpu0":1500}	2_factor=0.0, ropGen=True, .5, nSeed=123, 00,	0	04/12/2016, 23:22 minutes
	RUNNING	ttH-bb-semi.SyncCSVs	paramFile=E	e, taskName=EMPTY_ MPTY_STRING, log=EN Spring16MiniAODv2_1	MPTY_STRING,	0	04/12/2016, 22:43 minutes



# <sup>32</sup> make-like execution system

- Luigi's execution model is make-like
  - 1. Create dependency tree for triggered task
  - 2. Determine tasks to actually run:
    - Walk through tree (top-down)
    - For each path, stop if all output
- Only processes what is really necessary
- Scalable through simple structure
- Error handling & automatic re-scheduling

### \* in this case, the task is considered complete









# 33 Luigi in a nutshell

.

# reco.py

import luigi

from my\_analysis.tasks import Selection

class Reconstruction(luigi.Task):

dataset = luigi.Parameter(default="ttH")

def requires(self): return Selection(dataset=self.dataset)

def output(self): return luigi.LocalTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

. . .

> python reco.py Reconstruction --dataset ttbar

# perform reco on file described by "inp" and produce "outp"



# 33 Luigi in a nutshell

# reco.py

import luigi

from my\_analysis.tasks import Selection

class Reconstruction(luigi.Task):

dataset = luigi.Parameter(default="ttH")

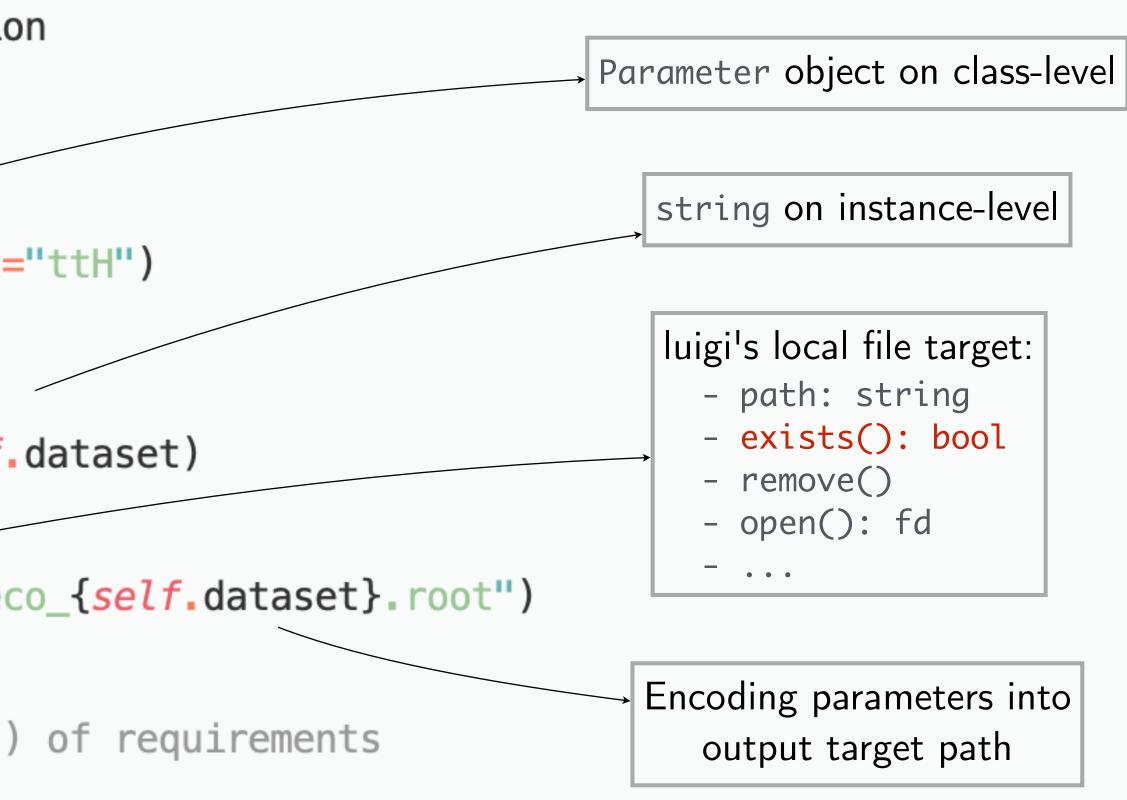
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def output(self): return luigi.LocalTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

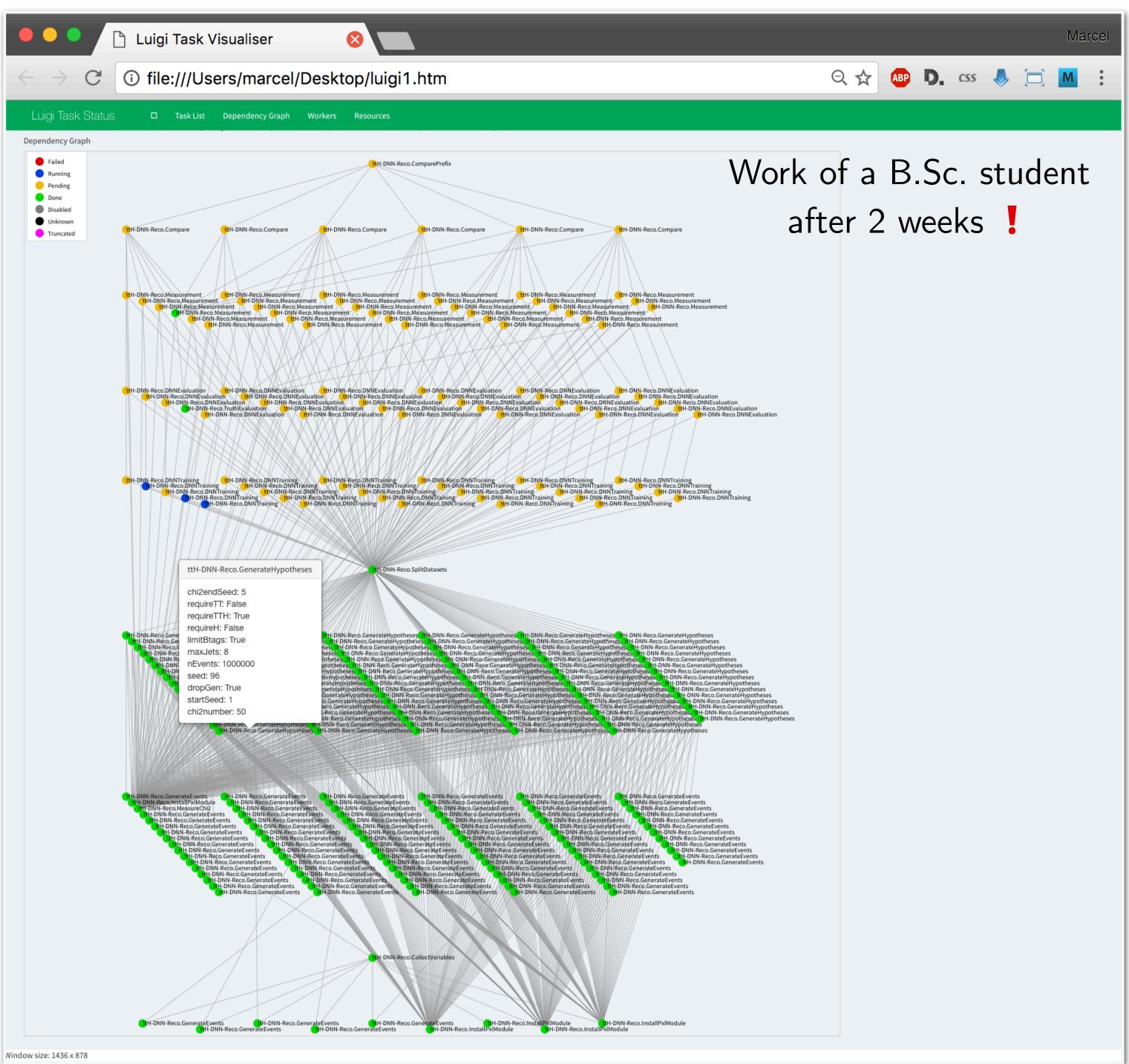
# perform reco on file described by "inp" and produce "outp" . . .

> python reco.py Reconstruction --dataset ttbar





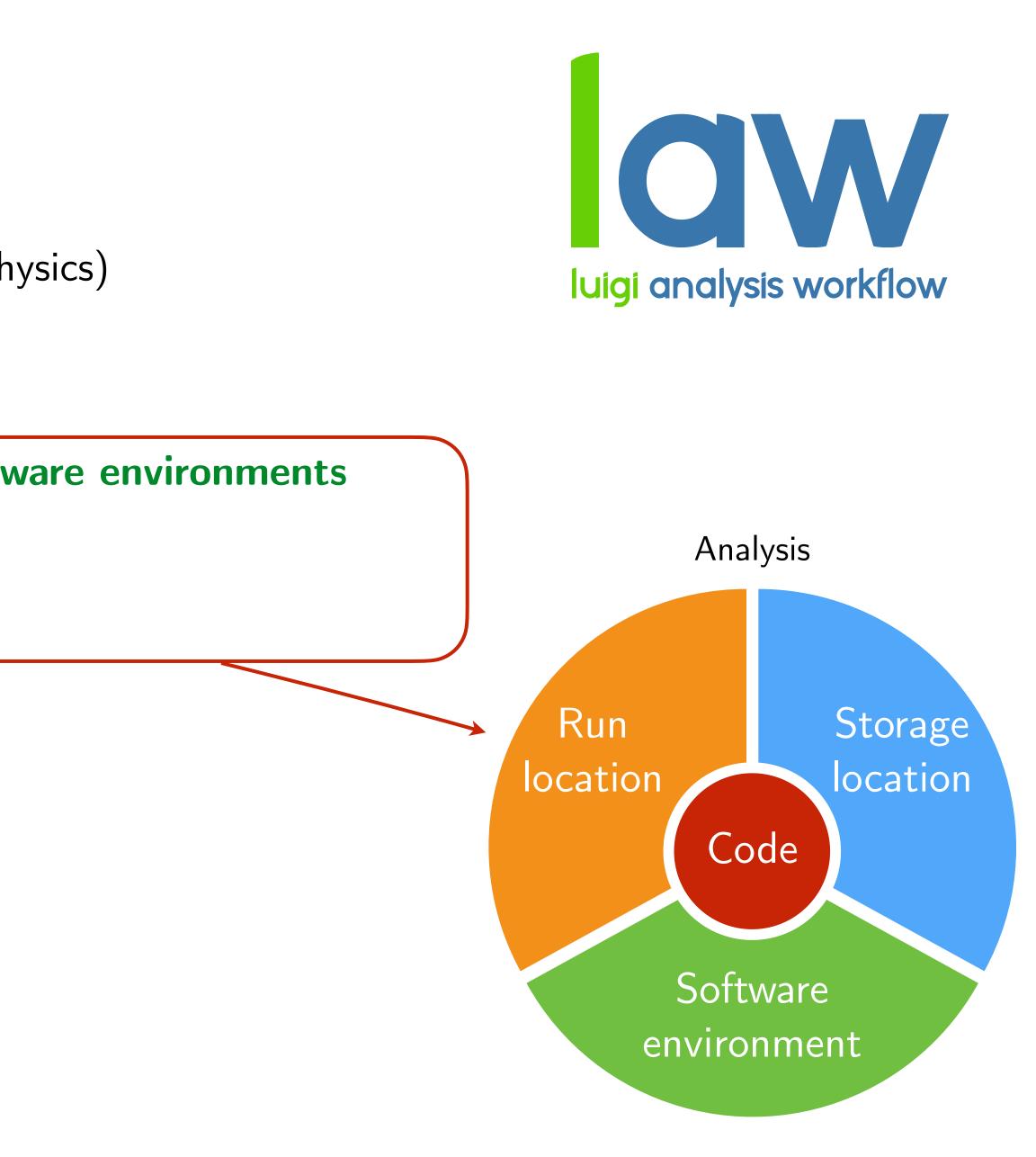
# 34 Example dependency trees





## 35 Law

- law: extension **on top** of *luigi* (i.e. it does not replace *luigi*)
- Software design follows 3 primary goals:
  - 1. Experiment-agnostic core (in fact, not even related to physics)
  - 2. Scalability on HEP infrastructure (but not limited to it)
  - 3. Decoupling of run locations, storage locations & software environments
    - ▷ Not constrained to specific resources
    - ▷ All components interchangeable
- Toolbox to follow an **analysis design pattern** 
  - No constraint on language or data structures
  - → Not a *framework*
- Most used workflow system for analyses in CMS
  - O(20) analyses, O(60-80) people
  - Central groups, e.g. HIG, TAU, BTV





## 1. Job submission

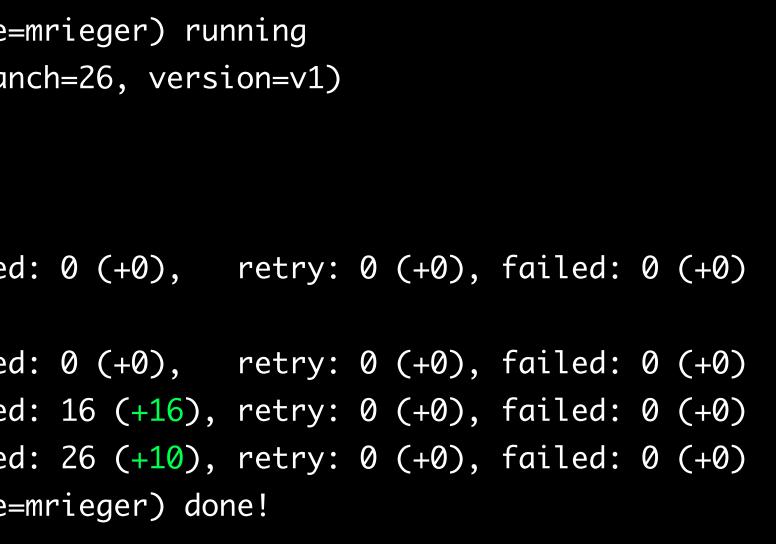


- Idea: submission built into tasks, **no need to write extra code**
- Currently supported job systems: HTCondor, LSF, gLite, ARC, Slurm, CMS-CRAB
- Mandatory features such as automatic resubmission, flexible task  $\leftrightarrow$  job matching, job files fully configurable at submission time, internal job staging when queues are saturated, ...
- From the htcondor at cern example:

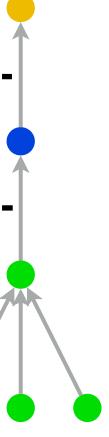
```
lxplus129:law_test > law run CreateChars --workflow htcondor
INFO: [pid 30564] Worker Worker(host=lxplus129.cern.ch, username=mrieger) running
                 CreateChars(branch=-1, start_branch=0, end_branch=26, version=v1)
going to submit 26 htcondor job(s)
submitted 1/26 job(s)
submitted 26/26 job(s)
14:35:40: all: 26, pending: 26 (+26), running: 0 (+0), finished: 0 (+0), retry: 0 (+0), failed: 0 (+0)
14:37:10: all: 26, pending: 0 (+0), running: 26 (+26), finished: 0 (+0), retry: 0 (+0), failed: 0 (+0)
14:37:40: all: 26, pending: 0 (+0), running: 10 (-16), finished: 16 (+16), retry: 0 (+0), failed: 0 (+0)
14:38:10: all: 26, pending: 0 (+0), running: 0 (+0), finished: 26 (+10), retry: 0 (+0), failed: 0 (+0)
INF0: [pid 30564] Worker Worker(host=lxplus129.cern.ch, username=mrieger) done!
```

lxplus129:law\_test >





local htcondor local



# 37 Scaling

### Job status polling example from CMS HH combination

16:04:23:	all:	3321,	pending:	2821	(+2821)	, runnir	ng: 4
16:04:37:	all:	3321,	pending:	2829	(+2829)	, runnir	ng: 5
16:06:15:	all:	3321,	pending:	2827	(-2), r	unning:	6 (+
16:06:17:	all:	3321,	pending:	2813	(-8), r	unning:	424
16:08:11:	all:	3321,	pending:	2820	(-7), r	unning:	8 (+
16:08:26:	all:	3321,	pending:	2810	(-3), r	unning:	422
16:09:44:	all:	3321,	pending:	2819	(-1), r	unning:	9 (+
16:10:03:	all:	3321,	pending:	2808	(-2), r	unning:	420
16:12:26:	all:	3321,	pending:	2817	(-2), r	unning:	5 (-
16:12:46:	all:	3321,	pending:	2802	(-6), r	unning:	422
16:15:11:	all:	3321,	pending:	2811	(-6), r	unning:	7 (+
16:15:39:	all:	3321,	pending:	2796	(-6), r	unning:	420
16:17:18:		-				)	
16:17:49:		-				)	
16:19:34:		F				0	
16:20:15:			•			<u> </u>	
16:21:26:		-				)	
16:21:53:			•			-	
16:23:47:		-	. )			)	
16:24:10:		-				•	
16:26:05:		-	)			)	
16:26:33:		-				•	
16:29:08:		F	•			•	
16:29:21:			•			-	
16:30:39:		F				•	
16:30:54:						<u> </u>	
16:32:02:						<u> </u>	
16:32:26:		-			- P P	•	
16:33:29:						•	
16:34:18:		-				•	
16:35:16:		-				•	
16:36:06:		-				•	
16:37:39:		-				•	
16:39:19:							
16:39:32:						0	
16:41:04:			-			-	
16:41:25:	all:	3321,	pending:	2593	(-10),	running:	23

**426** (+426), finished: **74** (+74), retry: **0** (+0), failed: **0** (+0) **5** (+5), finished: **487** (+487), retry: **0** (+0), failed: **0** (+0) -1), finished: **488** (+1), retry: **0** (+0), failed: **0** (+0) (-2), finished: **84** (+10), retry: **0** (+0), failed: **0** (+0) -2), finished: **493** (+5), retry: **0** (+0), failed: **0** (+0) (-2), finished: **89** (+5), retry: **0** (+0), failed: **0** (+0) -1), finished: **493** (+0), retry: **0** (+0), failed: **0** (+0) (-2), finished: **93** (+4), retry: **0** (+0), failed: **0** (+0) -4), finished: **499** (+6), retry: **0** (+0), failed: **0** (+0) (+2), finished: **97** (+4), retry: **0** (+0), failed: **0** (+0) 2), finished: **503** (+4), retry: **0** (+0), failed: **0** (+0) (-2), finished: **105** (+8), retry: **0** (+0), failed: **0** (+0) (+3), finished: **505** (+2), retry: **0** (+0), failed: **0** (+0) (-5), finished: **114** (+9), retry: **0** (+0), failed: **0** (+0) (+1), finished: **510** (+5), retry: **0** (+0), failed: **0** (+0) (-2), finished: **120** (+6), retry: **0** (+0), failed: **0** (+0) (+2), finished: **513** (+3), retry: **0** (+0), failed: **0** (+0) (-2), finished: **126** (+6), retry: **0** (+0), failed: **0** (+0) (+1), finished: **516** (+3), retry: **0** (+0), failed: **0** (+0) (+0), finished: **131** (+5), retry: **0** (+0), failed: **0** (+0) (+78), finished: **524** (+8), retry: **0** (+0), failed: **0** (+0) 2 (+91), finished: **136** (+5), retry: **0** (+0), failed: **0** (+0) (-5), finished: **544** (+20), retry: **0** (+0), failed: **0** (+0) **0** (+28), finished: **144** (+8), retry: **0** (+0), failed: **0** (+0) (-41), finished: **624** (+80), retry: **0** (+0), failed: **0** (+0) 0 (+20), finished: 150 (+6), retry: 0 (+0), failed: 0 (+0) (-11), finished: **652** (+28), retry: **0** (+0), failed: **0** (+0) **5** (+5), finished: **158** (+8), retry: **0** (+0), failed: **0** (+0) (-5), finished: **661** (+9), retry: **0** (+0), failed: **0** (+0) **1** (+6), finished: **163** (+5), retry: **0** (+0), failed: **0** (+0) (-4), finished: **674** (+13), retry: **0** (+0), failed: **0** (+0) 0 (-1), finished: 175 (+12), retry: 0 (+0), failed: 0 (+0) (-3), finished: **686** (+12), retry: **0** (+0), failed: **0** (+0) (-1), finished: **185** (+10), retry: **0** (+0), failed: **0** (+0) (-4), finished: **699** (+13), retry: **0** (+0), failed: **0** (+0) 6 (-3), finished: **199** (+14), retry: **0** (+0), failed: **0** (+0) (+4), finished: **705** (+6), retry: **0** (+0), failed: **0** (+0)



### **2.** Remote targets



- Idea: work with remote files as if they were local
- Remote targets built on top of GFAL2 Python bindings
  - ▷ Supports all WLCG protocols (XRootD, WebDAV, GridFTP, dCache, SRM, ...) + DropBox
  - API **identical** to local targets  $\triangleright$
  - Actual remote interface **interchangeable** (GFAL2 is just a good default, fsspec integration easily possible)
- Mandatory features: automatic retries, **local caching** (backup), configurable protocols, round-robin, ...

```
"FileSystem" configuration
```

```
# law.cfg
[wlcg_fs]
base: root://eosuser.cern.ch/eos/user/m/mrieger
. . .
```



- Base path prefixed to all paths using this "fs"
- Configurable per file operation (stat, listdir, ...)
- Protected against removal of parent directories

### **2.** Remote targets



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- Mandatory features: automatic retries, **local caching** (backup), configurable protocols, round-robin, ...

*# read a remote json file* with target.open("r") as f: data = json.load(f)



```
Conveniently reading remote files
```

```
target = law.WLCGFileTarget("/file.json", fs="wlcg_fs")
```

### **2.** Remote targets



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- Mandatory features: automatic retries, **local caching** (backup), configurable protocols, round-robin, ...

*# read a remote json file* 

data = target.load(formatter="json")



```
Conveniently reading remote files
```

```
target = law.WLCGFileTarget("/file.json", fs="wlcg_fs")
# use convenience methods for common operations
```

### **2.** Remote targets



- Idea: work with remote files as if they were local
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  - API **identical** to local targets  $\triangleright$
  - Actual remote interface **interchangeable** (GFAL2 is just a good default, fsspec integration easily possible)
- Mandatory features: automatic retries, **local caching** (backup), configurable protocols, round-robin, ...

*# same for root files with context guard* 

with target.load(formatter="root") as tfile: tfile.ls()



```
Conveniently reading remote files
```

```
target = law.WLCGFileTarget("/file.root", fs="wlcg_fs")
```

### **2.** Remote targets



- Idea: work with remote files as if they were local
- Remote targets built on top of GFAL2 Python bindings
  - ▷ Supports all WLCG protocols (XRootD, WebDAV, GridFTP, dCache, SRM, ...) + DropBox
  - API **identical** to local targets  $\triangleright$
  - Actual remote interface **interchangeable** (GFAL2 is just a good default, fsspec integration easily possible)
- Mandatory features: automatic retries, **local caching** (backup), configurable protocols, round-robin, ...

*# multiple other "formatters" available* 

graph = target.load(formatter="tensorflow") session = tf.Session(graph=graph)



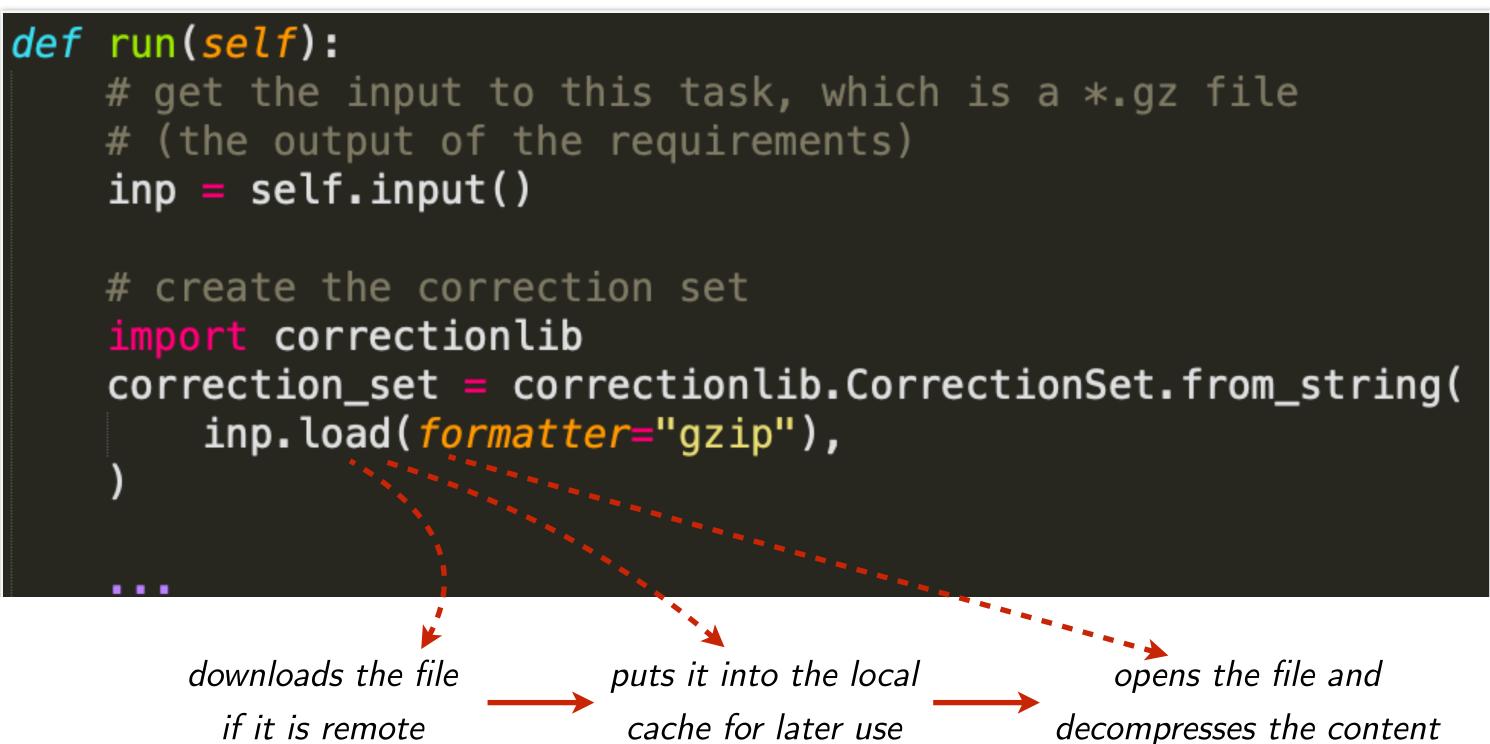
```
Conveniently reading remote files
```

```
target = law.WLCGFileTarget("/model.pb", fs="wlcg_fs")
```

### **2.** Remote targets



- Idea: work with remote files as if they were local
- Remote targets built on top of GFAL2 Python bindings
  - ▷ Supports all WLCG protocols (XRootD, WebDAV, GridFTP, dCache, SRM, ...) + DropBox
  - API **identical** to local targets  $\triangleright$
  - Actual remote interface **interchangeable** (GFAL2 is just a good default, fsspec integration easily possible)
- Mandatory features: automatic retries, local caching (backup), configurable protocols, round-robin, ...



if it is remote



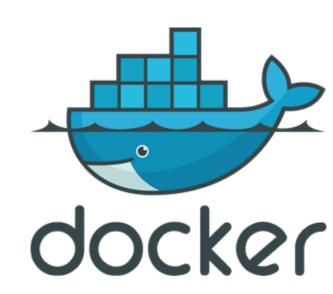
## 3. Environment sandboxing



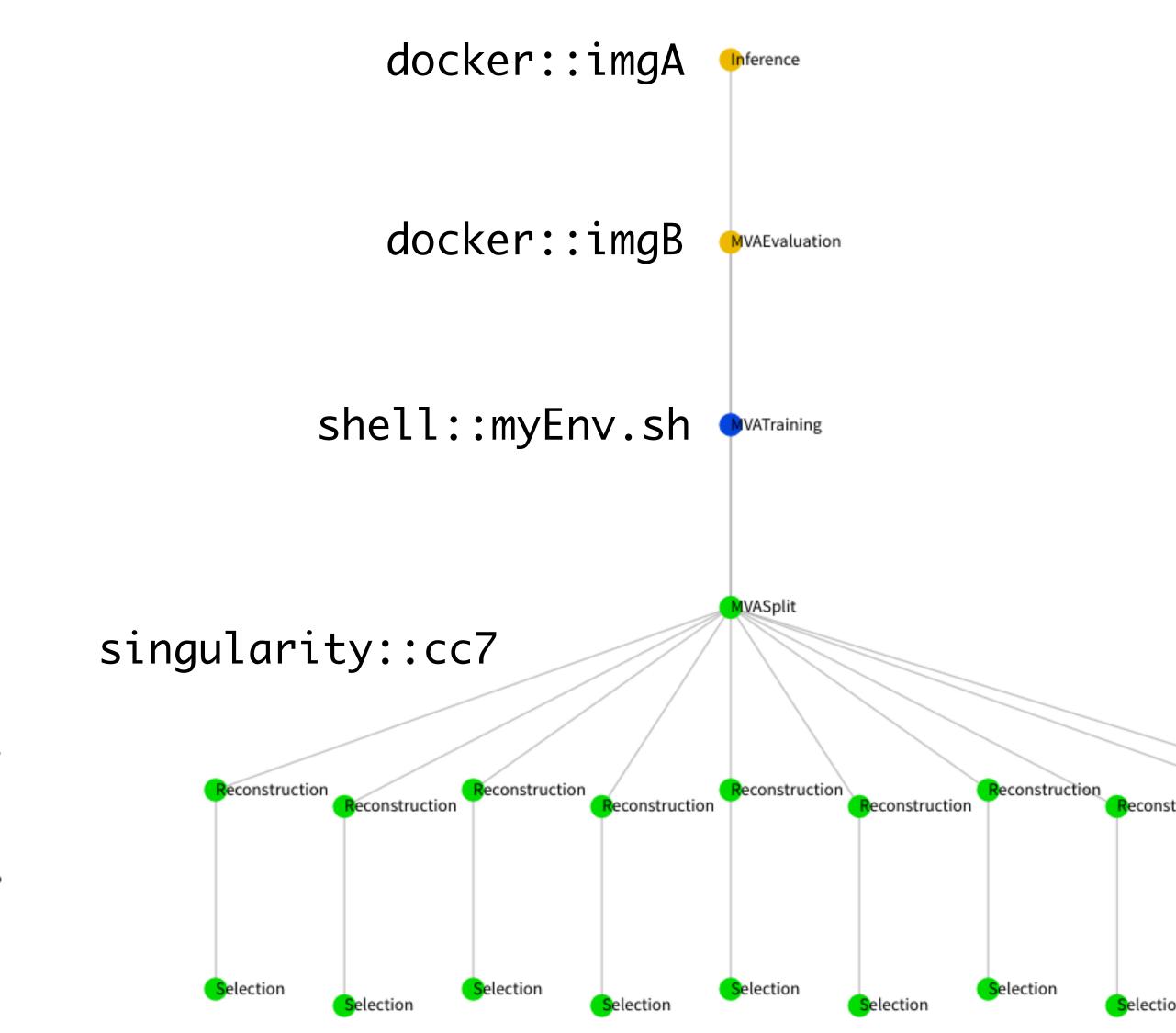
- Diverging software requirements between typical workloads is a great feature / challenge / problem
- Introduce sandboxing:
  - ▶ Run entire task in **different environment**
- Existing sandbox implementations:
  - ▷ Sub-shell with init file (e.g. for CMSSW)
  - Virtual envs  $\triangleright$
  - Docker images  $\triangleright$
  - Singularity images  $\triangleright$











.

# reco.py

import luigi

from my\_analysis.tasks import Selection

class Reconstruction(luigi.Task):

dataset = luigi.Parameter(default="ttH")

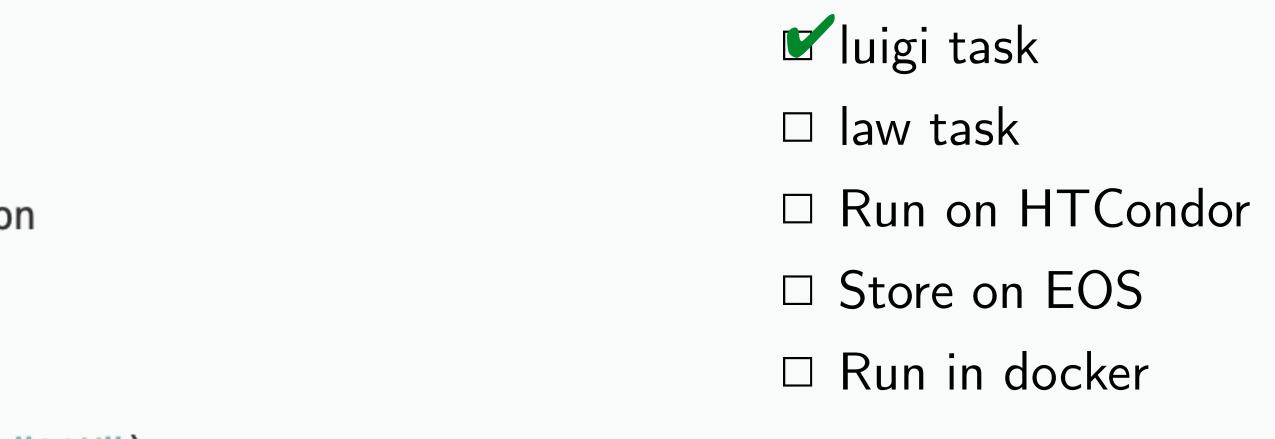
def requires(self): return Selection(dataset=self.dataset)

def output(self): return luigi.LocalTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

# perform reco on file described by "inp" and produce "outp" . . .

> python reco.py Reconstruction --dataset ttbar









# reco.py

import luigi import law from my\_analysis.tasks import Selection

class Reconstruction(law\_Task):

dataset = luigi.Parameter(default="ttH")

def requires(self): return Selection(dataset=self.dataset)

def output(self): return law.LocalFileTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

# perform reco on file described by "inp" and produce "outp" . . .

> law run Reconstruction --dataset ttbar

✓ luigi task Value law task □ Run on HTCondor  $\Box$  Store on EOS □ Run in docker







# reco.py

import luigi import law from my\_analysis.tasks import Selection

class Reconstruction(law.Task, law.HTCondorWorkflow):

dataset = luigi.Parameter(default="ttH")

def requires(self): return Selection(dataset=self.dataset)

def output(self): return law.LocalFileTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

# perform reco on file described by "inp" and produce "outp" . . .

> law run Reconstruction --dataset ttbar --workflow htcondor

✓ luigi task V law task **Run on HTCondor**  $\Box$  Store on EOS

□ Run in docker









# reco.py

import luigi import law from my\_analysis.tasks import Selection

class Reconstruction(law.Task, law.HTCondorWorkflow):

dataset = luigi.Parameter(default="ttH")

def requires(self): return Selection(dataset=self.dataset)

def output(self): return law.WLCGFileTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

# perform reco on file described by "inp" and produce "outp" . . .

> law run Reconstruction --dataset ttbar --workflow htcondor

✓ luigi task Value law task Run on HTCondor Store on EOS □ Run in docker









```
# reco.py
```

import luigi import law from my\_analysis.tasks import Selection

#### class Reconstruction(law.SandboxTask, law.HTCondorWorkflow):

dataset = luigi.Parameter(default="ttH") sandbox = "docker::cern/cc7-base"

def requires(self): return Selection(dataset=self.dataset)

def output(self): return law.WLCGFileTarget(f"reco\_{self.dataset}.root")

def run(self): inp = self.input() # output() of requirements outp = self.output()

# perform reco on file described by "inp" and produce "outp" . . .

> law run Reconstruction --dataset ttbar --workflow htcondor

✓ luigi task Value law task **Run on HTCondor** Store on EOS Run in docker









# 41 Triggers: CLI, scripting and notebooks

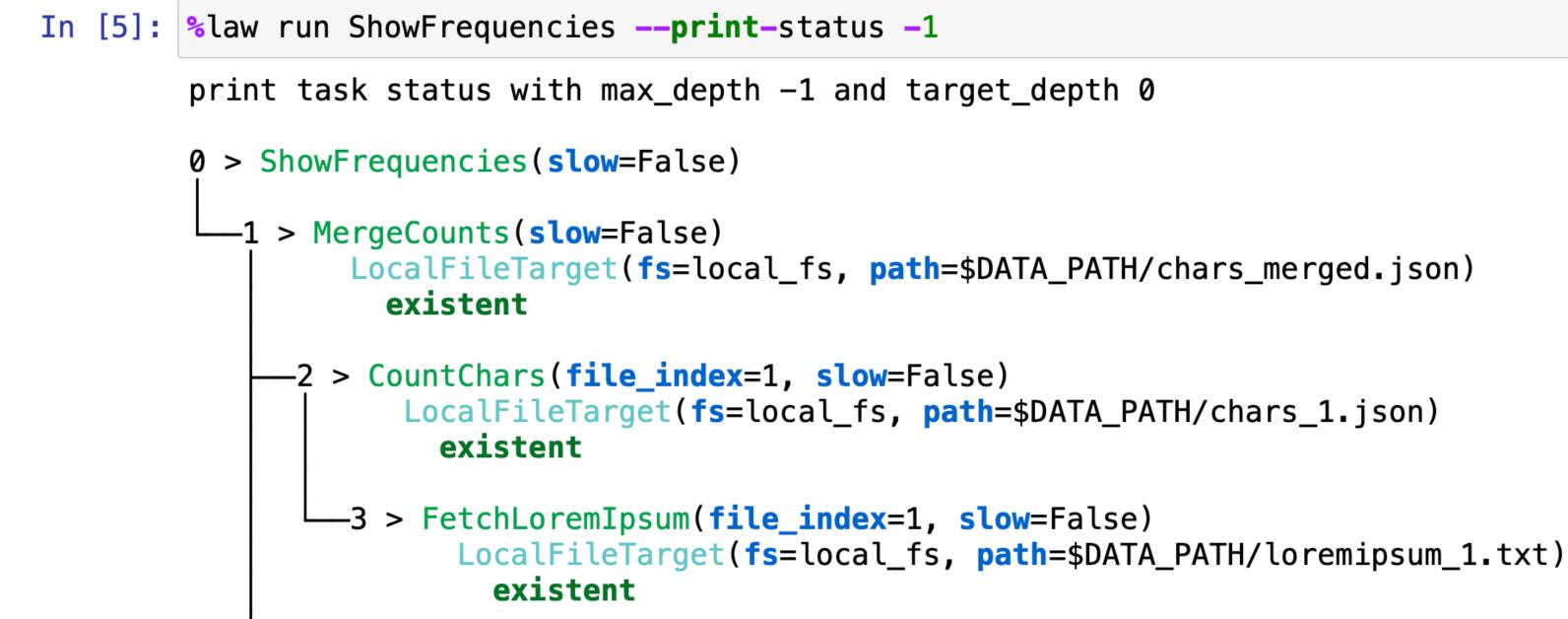
# CLI

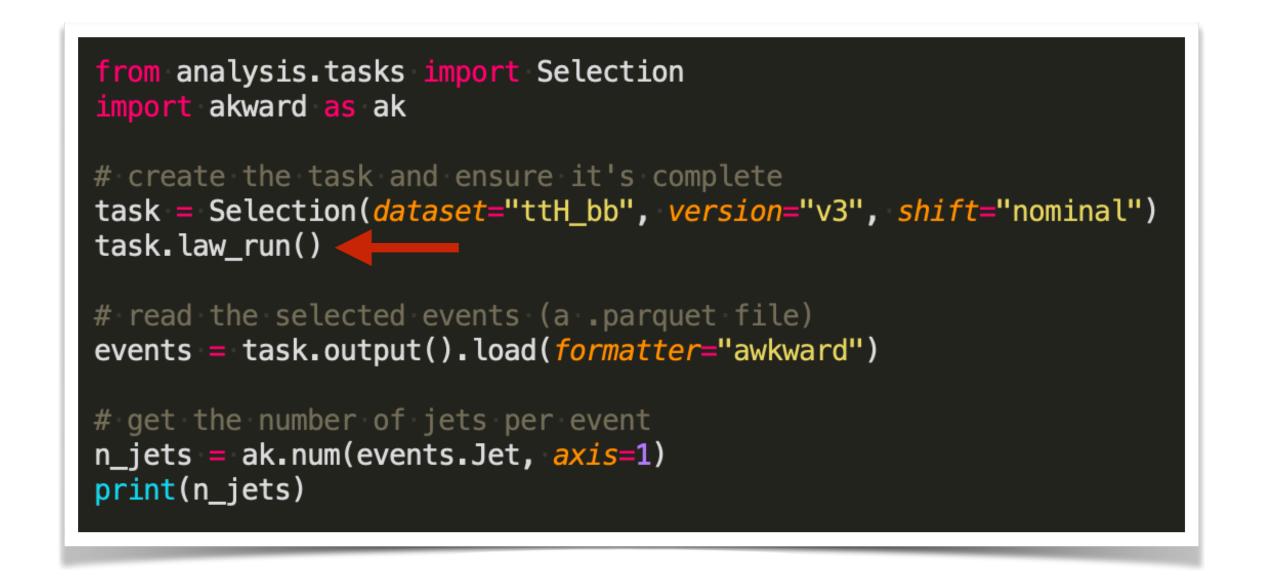
- > law run Reconstruction --dataset ttbar --workflow htcondor
- Full auto-completion of tasks and parameters

## Scripting

- Mix task completeness checks, job execution & input/output retrieval with custom scripts
- Easy interface to existing tasks for prototyping

## **Notebooks**



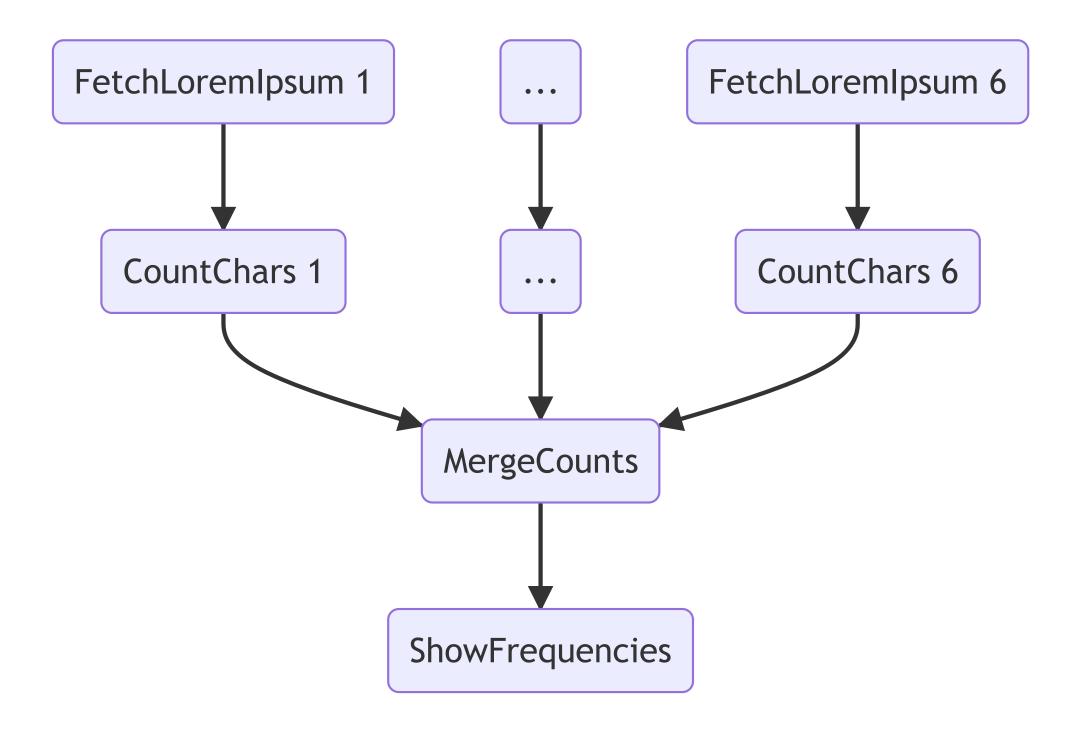






# 42 Demo

- Print character frequencies in the "loremipsum" placeholder text (from examples/loremipsum)
  - Fetch 6 paragraphs as txt files from some server  $\triangleright$
  - Count character frequencies and save them in json  $\triangleright$
  - Merge into a single json file  $\triangleright$
  - Print frequencies  $\triangleright$
- Sowing CLI usage in the following, but 😵 launch binder for the notebook version









# 44 order: Structuring CMS metadata

- Pythonic class collection to help structuring CMS metadata
- Provides programmatic access to and relations between various entities

Name	Purpose
<u>Analysis</u>	Represents the central object of a physics analysis.
<u>Campaign</u>	Provides data of a well-defined range of data-taking, detector alignment, MC settings, datasets, etc.
<u>Config</u>	Holds analysis information related to a campaign instance (most configuration happens here!).
Dataset	Definition of a dataset, produced for / measured in a campaign.
Process	Phyiscs process with cross sections for multiple center-of-mass energies, labels, etc.
<u>Channel</u>	Analysis channel, often defined by a particular decay resulting in distinct final state objects.
<u>Category</u>	Category definition, (optionally) within the phase-space of an analysis channel.
<u>Variable</u>	Generic variable description providing expression and selection statements, titles, binning, etc.
<u>Shift</u>	Represents a systematic shift with a name, direction and type.

### Examples

In [3]: dataset\_ttH.get\_process("ttH").get\_xsec(ecm= **Out[3]:**  $0.5071 \stackrel{+0.0294118}{_{-0.0466532}}$  (scale)

### columnflow Marcel Rieger for the CF team

=13)	In [12]:	<pre>cfg.get_variable("jet1_px").get_full_title(root=True)</pre>
	Out[12]:	'jet1_px;Leading jet p_{x} / GeV;Entries / 20.0 GeV'

Heavily used throughout columnflow, common objects (datasets and cross-sections) centralized in () /uhh-cms/cmsdb

Note: Moving code-base to CMS-wide project via CAT group, datasets & cross-sections to be managed centrally 🎉



