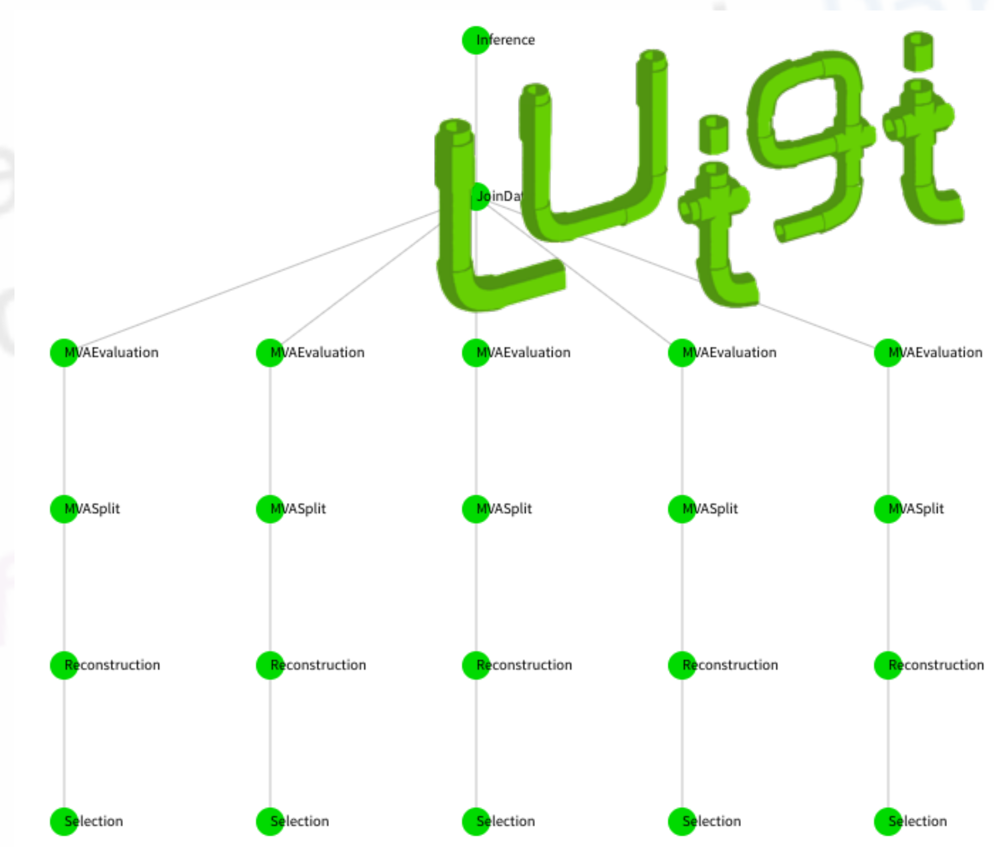


law
luigi analysis workflow

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE

FSP CMS
Erforschung von Universum und Materie

SPONSORED BY THE
Federal Ministry of Education and Research

luigi analysis workflow

— Large Scale End-to-End Analysis Automation over Distributed Resources —

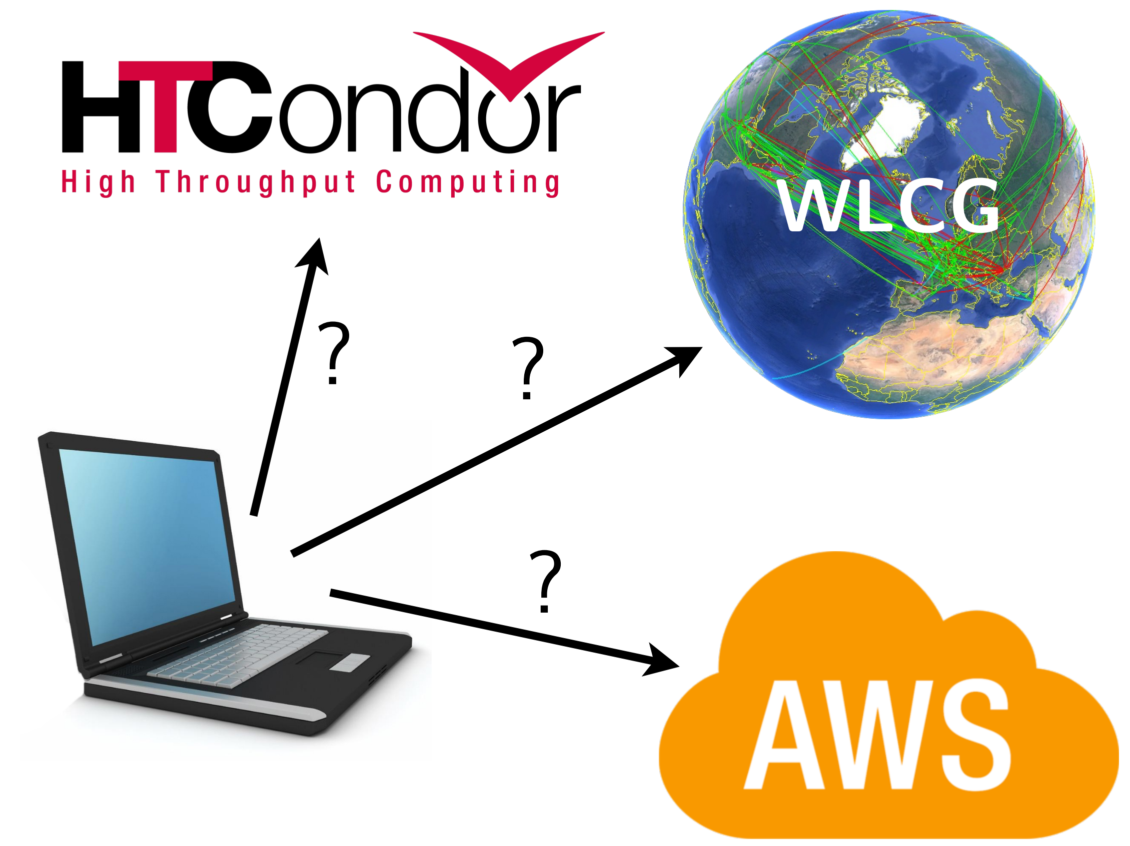
Marcel Rieger

CHEP 2023 - Norfolk

9.5.2023

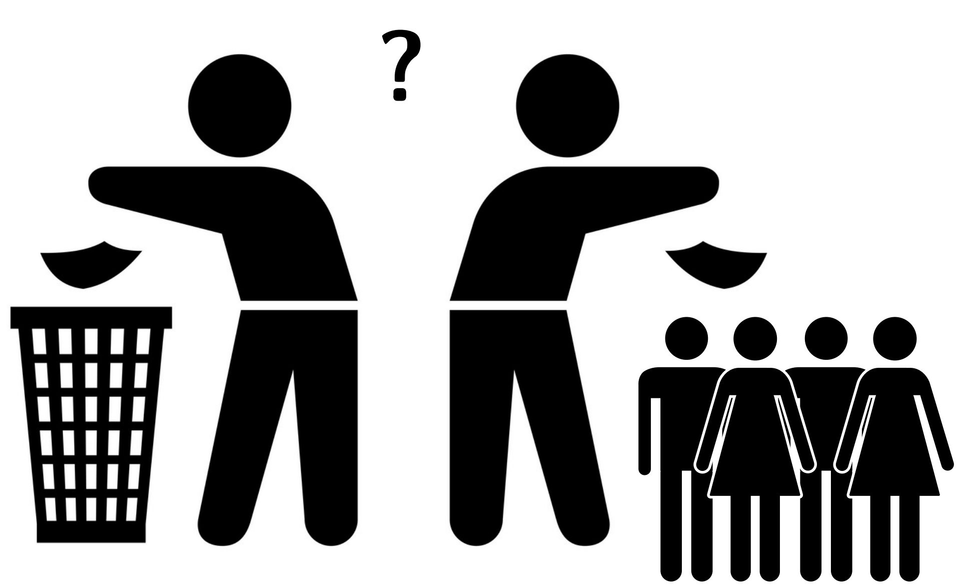
Motivational questions

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



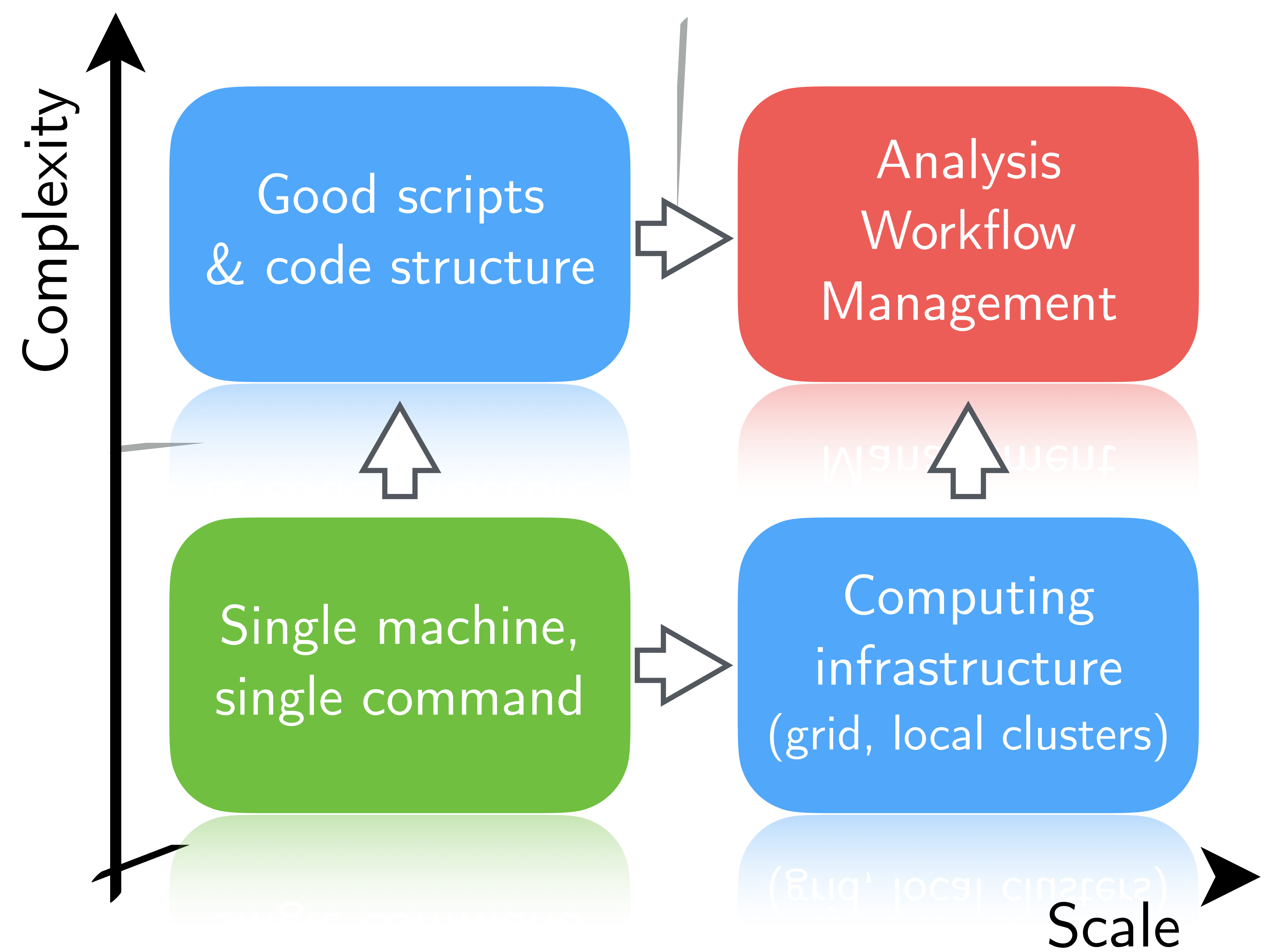
- **Reproducibility**: When a postdoc / PhD student leaves, ...
  - can someone else run the analysis?
  - is there a loss of information? Is a new *framework* required?
    - ▻ Dependencies often **only** exist in the physicists head!

- **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**!



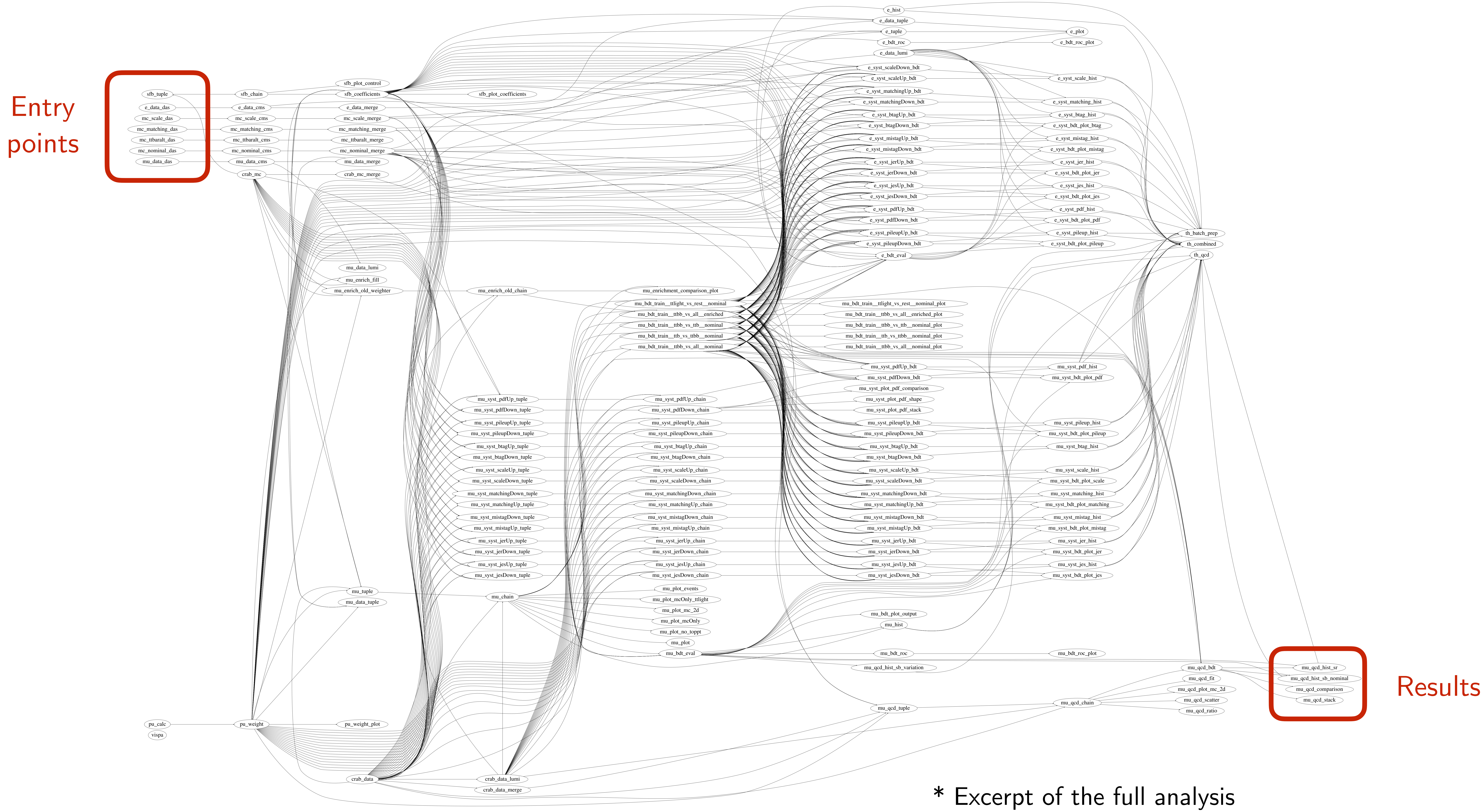
- Personal experience: ⅔ of "analysis" time for technicalities, ⅓ left for physics
  → **Physics output doubled if it were the other way round?**

- Most analyses are both **large and complex**
  - Structure & requirements between workloads mostly undocumented
  - Manual execution & steering of jobs, bookkeeping of data across storage elements, different data revisions, ...
  - → Time-consuming & error-prone



- **Workflow management must ...**
  - **provide full automation** → Execution through **a single command**
  - **cover all possible use cases** → Examples on next slides

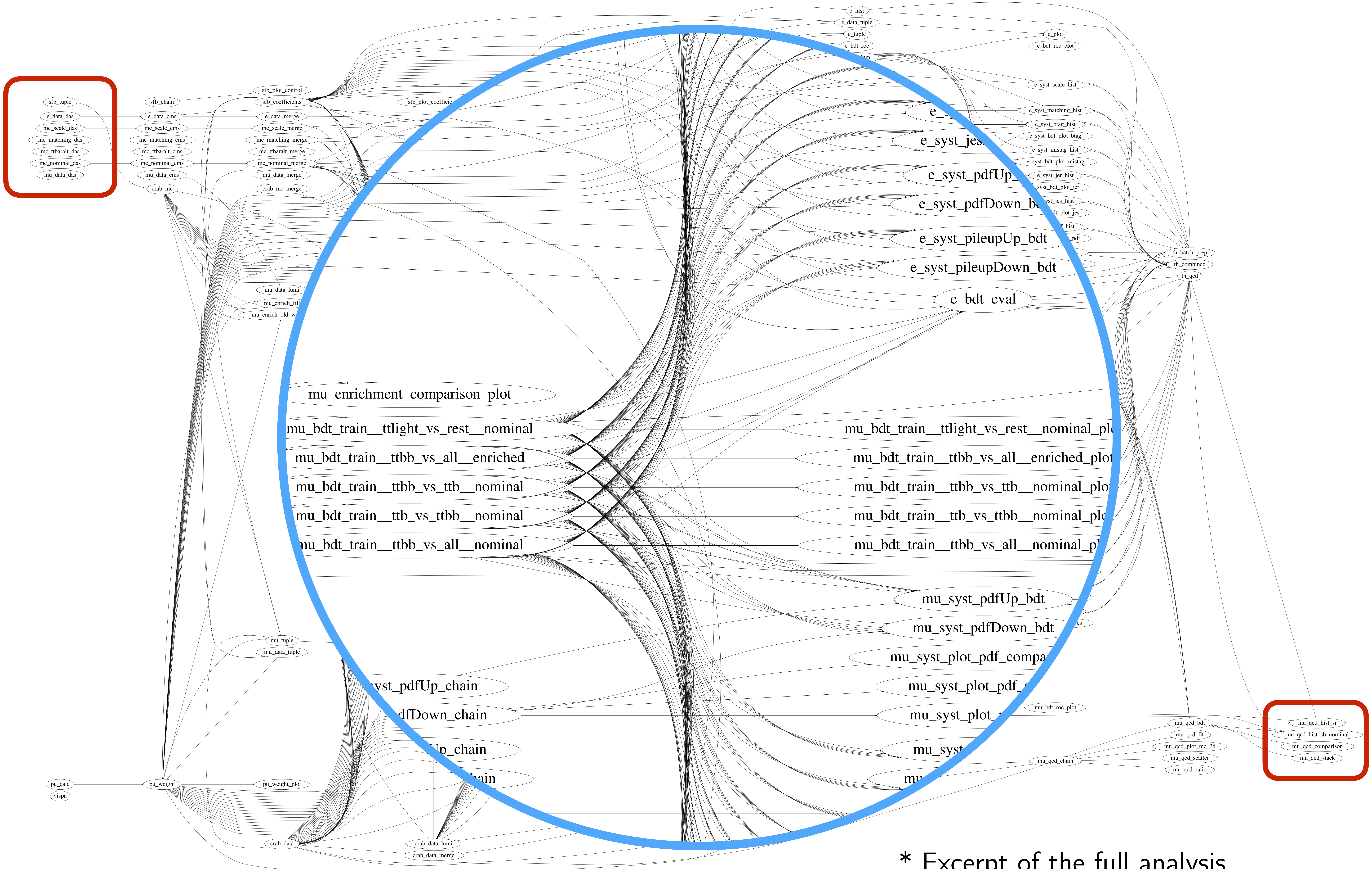
Example: ttbb measurement visualization



* Excerpt of the full analysis

Example: ttbb measurement visualization

Entry points



Results

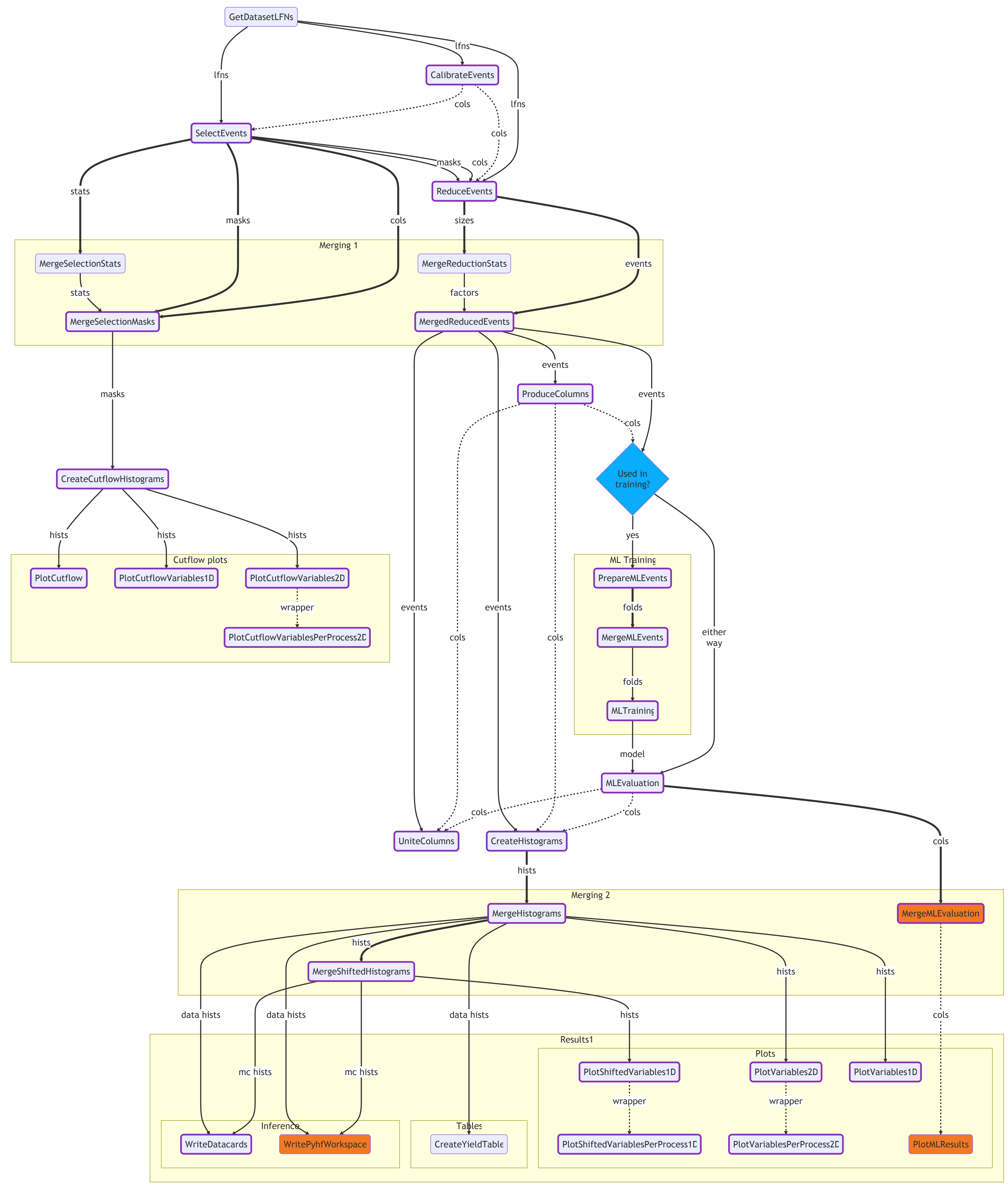
* Excerpt of the full analysis

Example: Fully orchestrated LHC Run 2 + 3 analysis with columnflow

Event processing

workflow

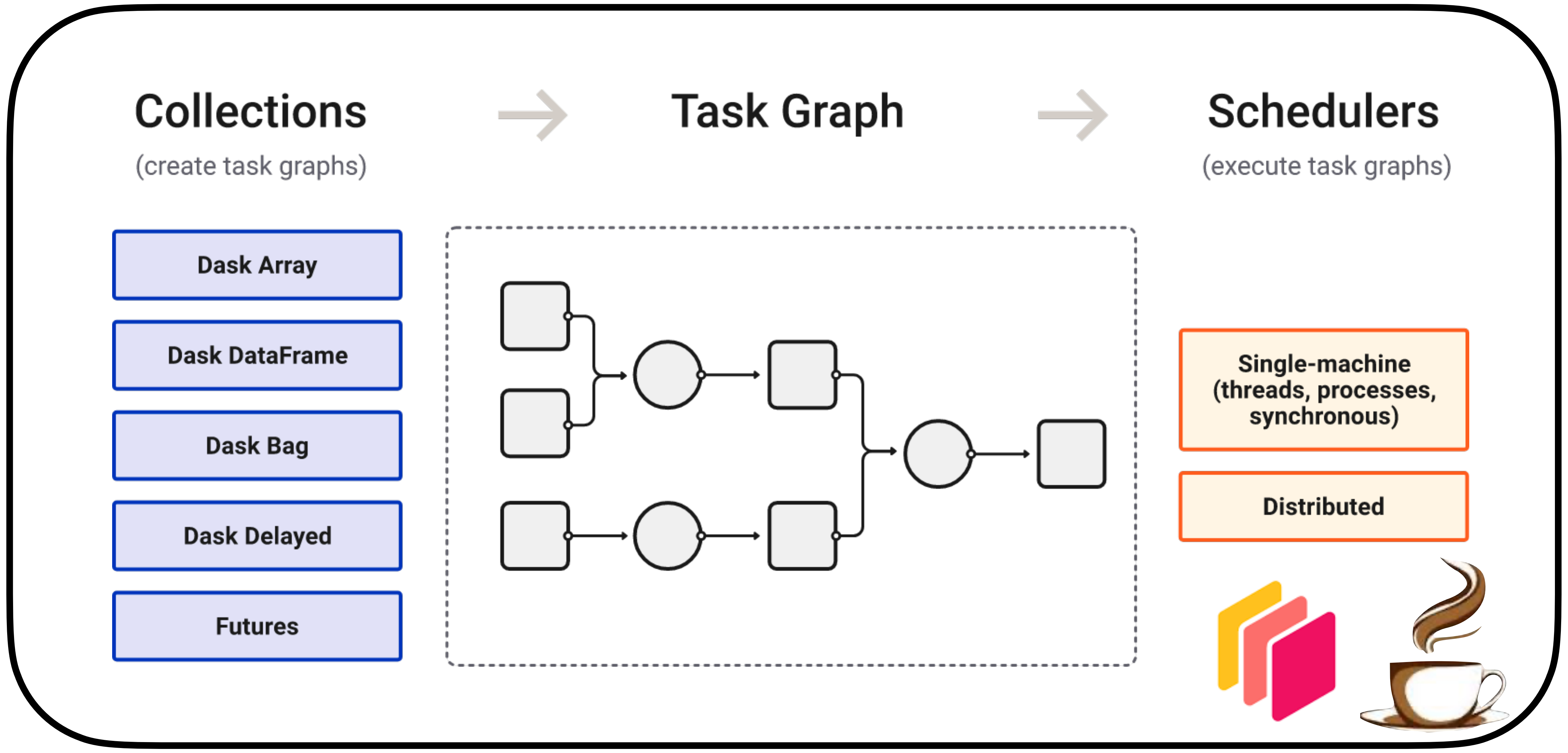
Plots & inference



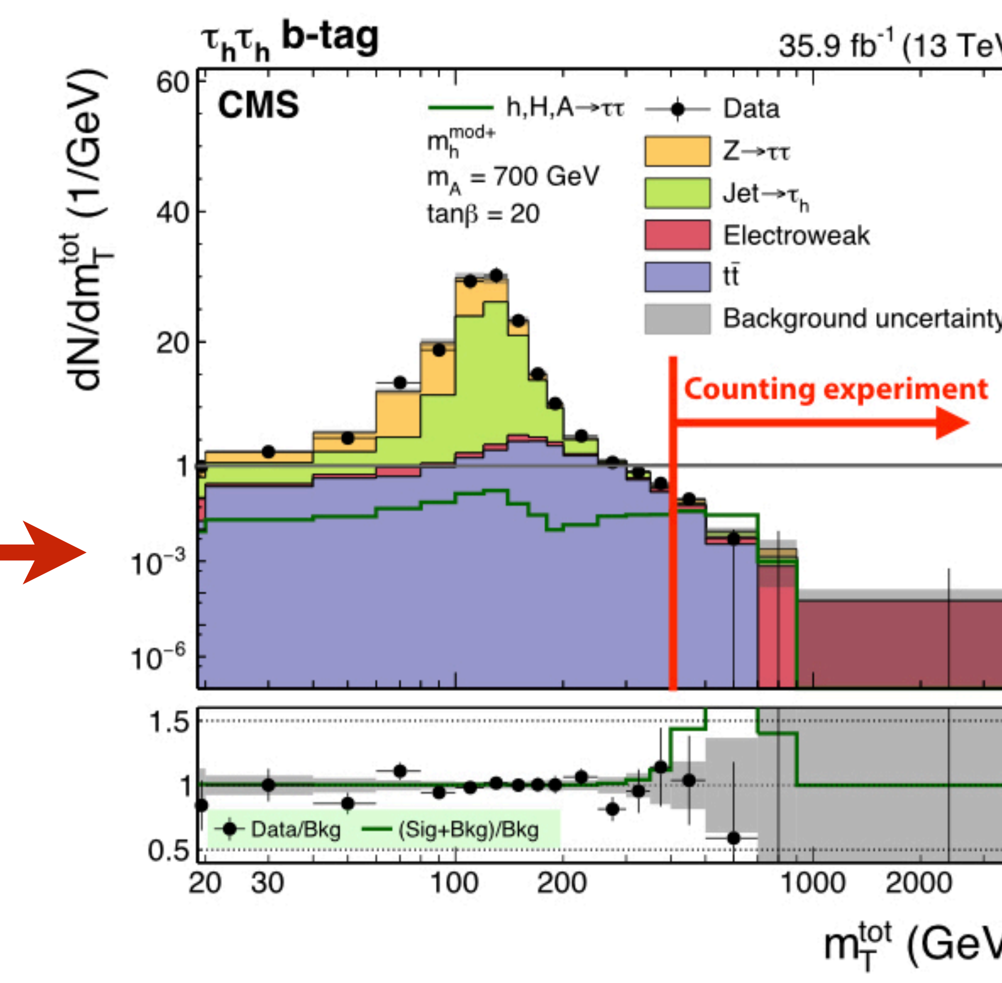
Source

From Elliott's talk

Entry point



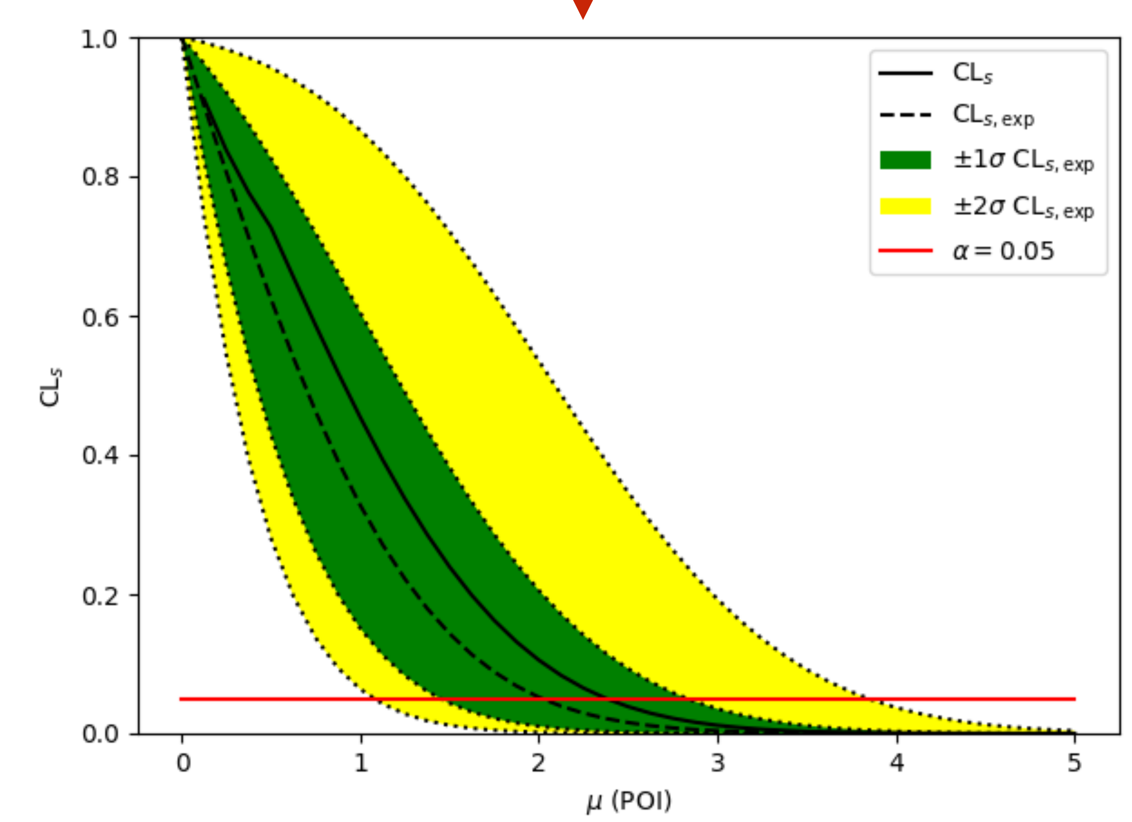
From Lindsey's talk



source

Result

pyhf
Combine
cabinetry



source

Result

NB: "Task graph" in the following is a higher-level concept

Luigi

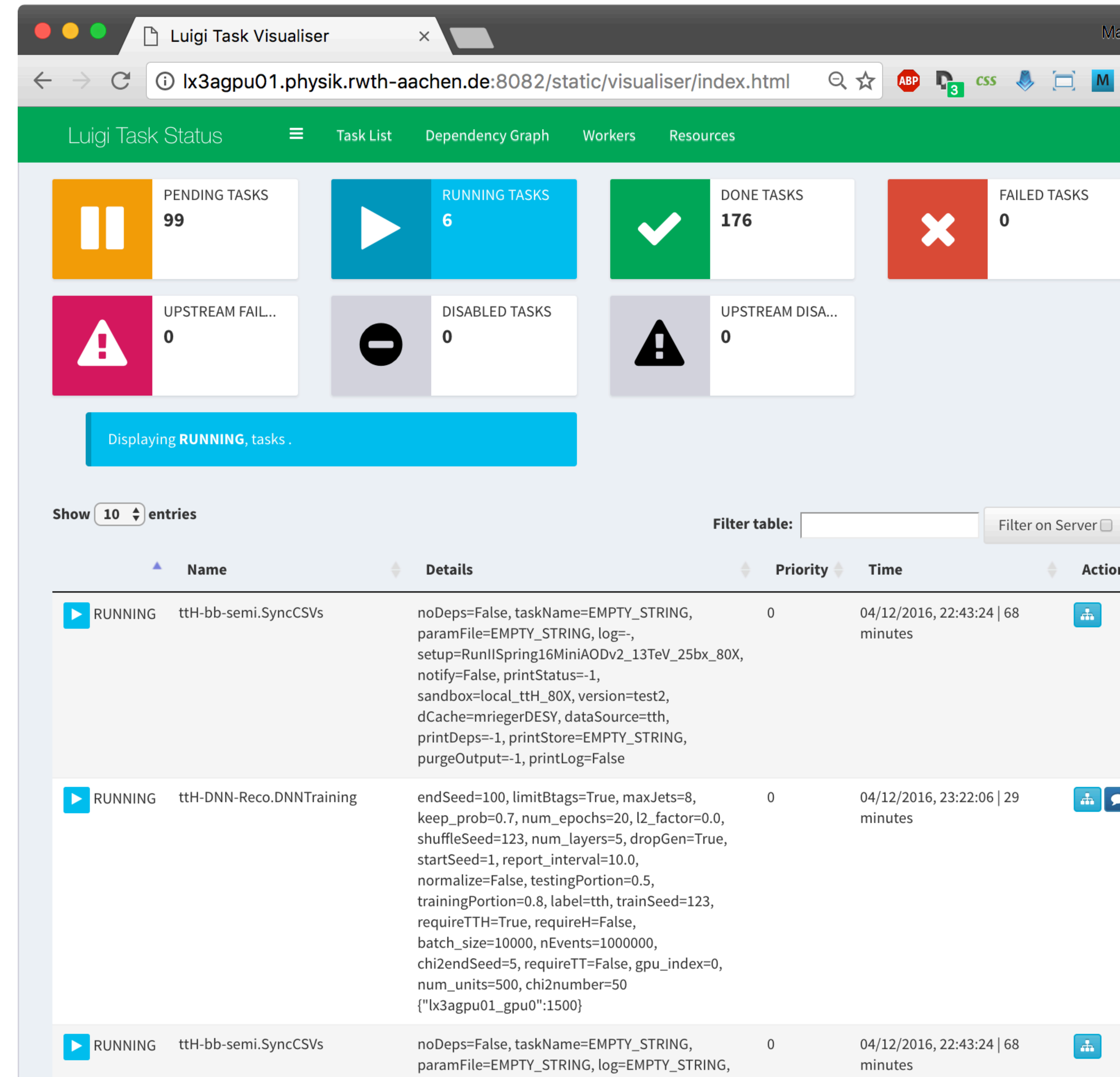
- Python package for building complex pipelines
- Development started at Spotify, now open-source and community-driven

Building blocks

1. Workloads defined as **Task** classes that can **require** other **Tasks**
2. Tasks produce output **Targets**
3. **Parameters** customize tasks & control runtime behavior

- Web UI with two-way messaging (task → UI, UI → task), automatic error handling, task history browser, collaborative features, command line interface, ...

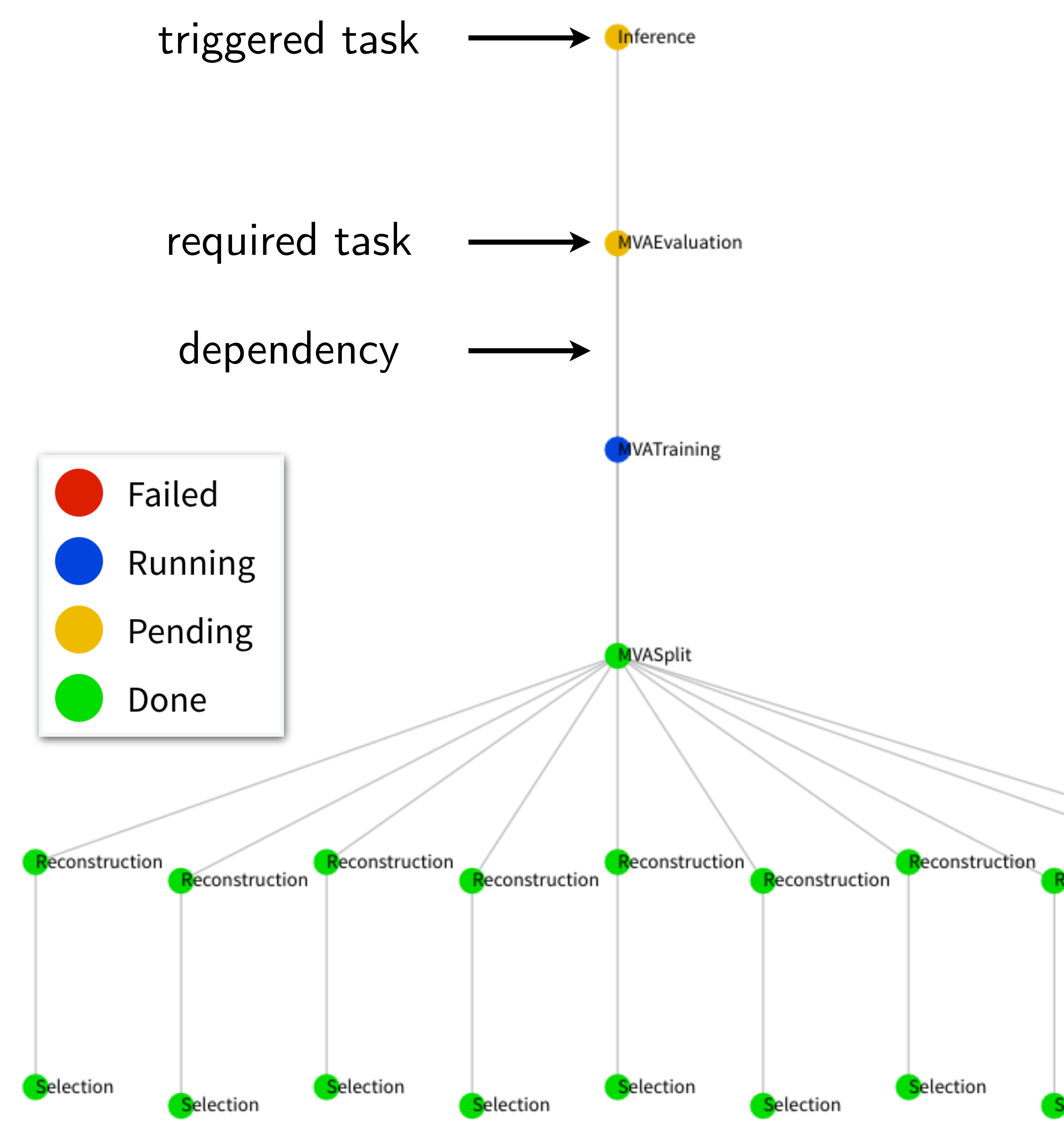
github.com/spotify/luigi



- Luigi's execution model is `make`-like

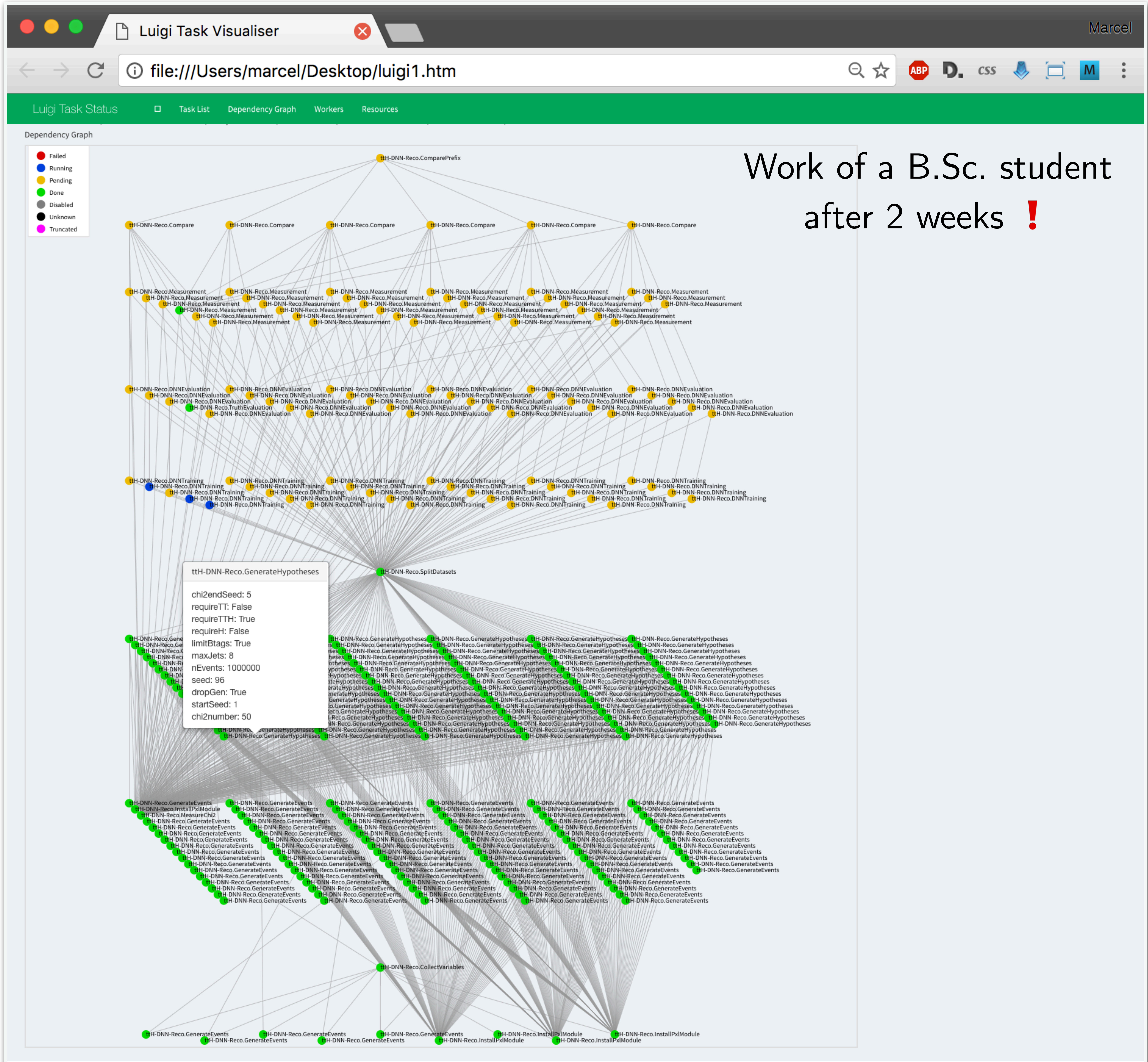
  1. Create dependency tree for triggered task
  2. Determine tasks to actually run:
     - Walk through tree (top-down)
     - For each path, stop if all output targets of a task exist*

- Only processes what is really necessary
- Scalable through simple structure
- Error handling & automatic re-scheduling



* in this case, the task is considered `complete`

Example dependency trees



Work of a B.Sc. student after 2 weeks !

```
# 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"
        ...
```

`Parameter` object on class-level

`string` on instance-level

luigi's local file target:

- `path: string`
- `exists(): bool`
- `remove()`
- `open(): fd`
- `...`

Encoding parameters into output target path

```
> python reco.py Reconstruction --dataset ttbar
```

law

luigi analysis workflow

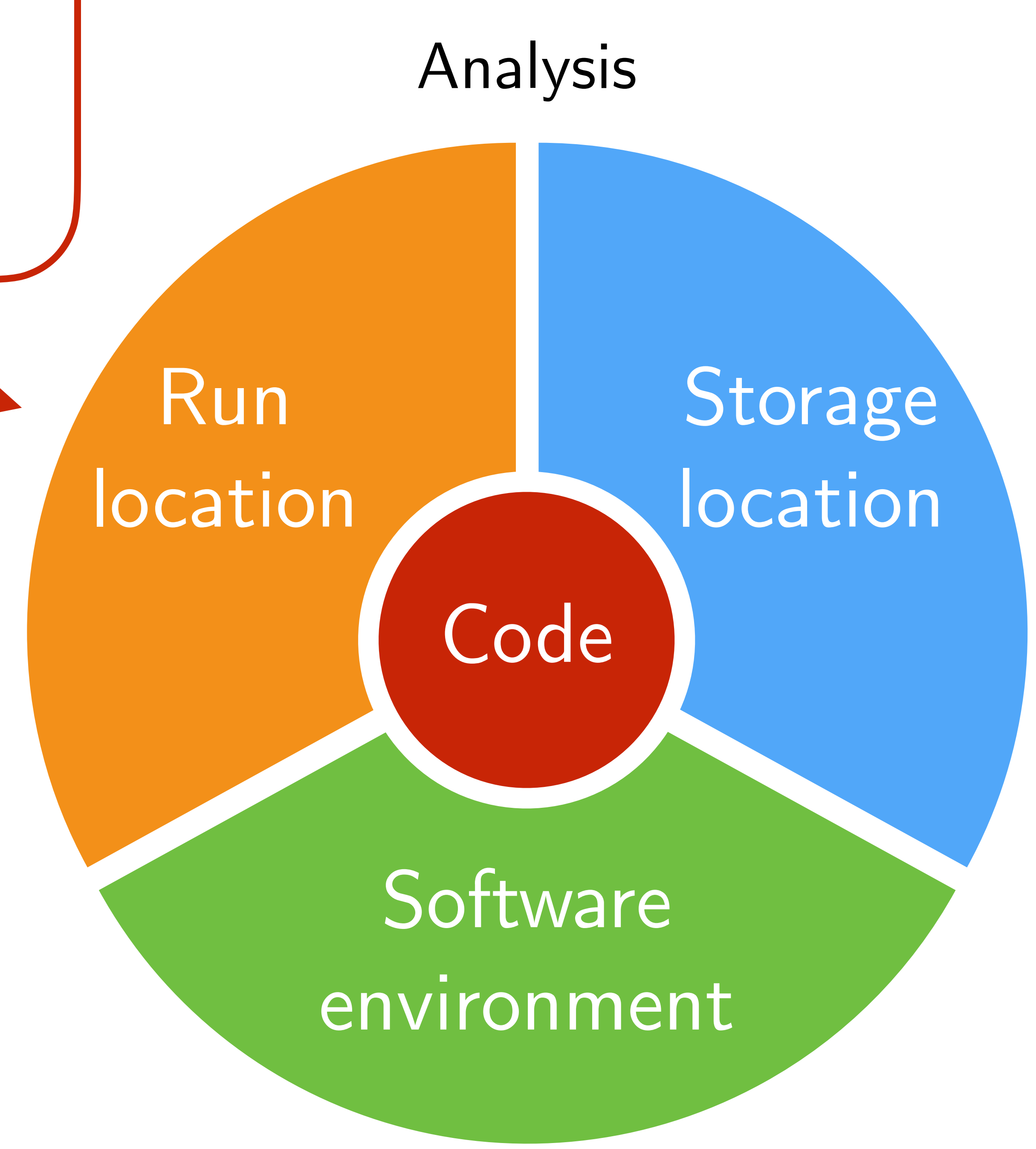
- law: extension **on top** of *luigi* (i.e. it does not replace *luigi*)

- 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*

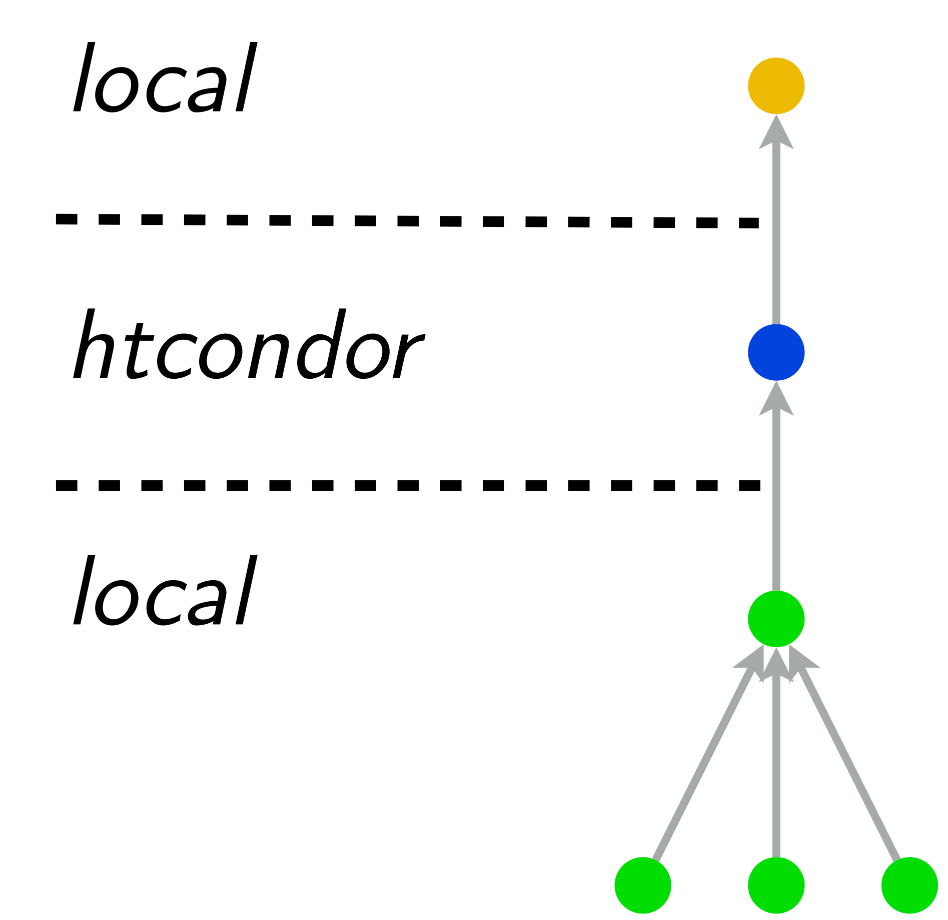
- **Most used** workflow system for analyses in CMS
  - O(20) analyses, O(60-80) people
  - Central groups, e.g. HIG, TAU, BTV, ...



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 ↔ job matching,
  job files fully configurable at submission time, internal job staging in case of saturated queues, ...
- 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)
INFO: [pid 30564] Worker Worker(host=lxplus129.cern.ch, username=mrieger) done!

lxplus129:law_test >
```



Job status polling from CMS HH combination

```
16:04:23: all: 3321, pending: 2821 (+2821), running: 426 (+426), finished: 74 (+74), retry: 0 (+0), failed: 0 (+0)
16:04:37: all: 3321, pending: 2829 (+2829), running: 5 (+5), finished: 487 (+487), retry: 0 (+0), failed: 0 (+0)
16:06:15: all: 3321, pending: 2827 (-2), running: 6 (+1), finished: 488 (+1), retry: 0 (+0), failed: 0 (+0)
16:06:17: all: 3321, pending: 2813 (-8), running: 424 (-2), finished: 84 (+10), retry: 0 (+0), failed: 0 (+0)
16:08:11: all: 3321, pending: 2820 (-7), running: 8 (+2), finished: 493 (+5), retry: 0 (+0), failed: 0 (+0)
16:08:26: all: 3321, pending: 2810 (-3), running: 422 (-2), finished: 89 (+5), retry: 0 (+0), failed: 0 (+0)
16:09:44: all: 3321, pending: 2819 (-1), running: 9 (+1), finished: 493 (+0), retry: 0 (+0), failed: 0 (+0)
16:10:03: all: 3321, pending: 2808 (-2), running: 420 (-2), finished: 93 (+4), retry: 0 (+0), failed: 0 (+0)
16:12:26: all: 3321, pending: 2817 (-2), running: 5 (-4), finished: 499 (+6), retry: 0 (+0), failed: 0 (+0)
16:12:46: all: 3321, pending: 2802 (-6), running: 422 (+2), finished: 97 (+4), retry: 0 (+0), failed: 0 (+0)
16:15:11: all: 3321, pending: 2811 (-6), running: 7 (+2), finished: 503 (+4), retry: 0 (+0), failed: 0 (+0)
16:15:39: all: 3321, pending: 2796 (-6), running: 420 (-2), finished: 105 (+8), retry: 0 (+0), failed: 0 (+0)
16:17:18: all: 3321, pending: 2806 (-5), running: 10 (+3), finished: 505 (+2), retry: 0 (+0), failed: 0 (+0)
16:17:49: all: 3321, pending: 2792 (-4), running: 415 (-5), finished: 114 (+9), retry: 0 (+0), failed: 0 (+0)
16:19:34: all: 3321, pending: 2800 (-6), running: 11 (+1), finished: 510 (+5), retry: 0 (+0), failed: 0 (+0)
16:20:15: all: 3321, pending: 2788 (-4), running: 413 (-2), finished: 120 (+6), retry: 0 (+0), failed: 0 (+0)
16:21:26: all: 3321, pending: 2795 (-5), running: 13 (+2), finished: 513 (+3), retry: 0 (+0), failed: 0 (+0)
16:21:53: all: 3321, pending: 2784 (-4), running: 411 (-2), finished: 126 (+6), retry: 0 (+0), failed: 0 (+0)
16:23:47: all: 3321, pending: 2791 (-4), running: 14 (+1), finished: 516 (+3), retry: 0 (+0), failed: 0 (+0)
16:24:10: all: 3321, pending: 2779 (-5), running: 411 (+0), finished: 131 (+5), retry: 0 (+0), failed: 0 (+0)
16:26:05: all: 3321, pending: 2705 (-86), running: 92 (+78), finished: 524 (+8), retry: 0 (+0), failed: 0 (+0)
16:26:33: all: 3321, pending: 2683 (-96), running: 502 (+91), finished: 136 (+5), retry: 0 (+0), failed: 0 (+0)
16:29:08: all: 3321, pending: 2690 (-15), running: 87 (-5), finished: 544 (+20), retry: 0 (+0), failed: 0 (+0)
16:29:21: all: 3321, pending: 2647 (-36), running: 530 (+28), finished: 144 (+8), retry: 0 (+0), failed: 0 (+0)
16:30:39: all: 3321, pending: 2651 (-39), running: 46 (-41), finished: 624 (+80), retry: 0 (+0), failed: 0 (+0)
16:30:54: all: 3321, pending: 2621 (-26), running: 550 (+20), finished: 150 (+6), retry: 0 (+0), failed: 0 (+0)
16:32:02: all: 3321, pending: 2634 (-17), running: 35 (-11), finished: 652 (+28), retry: 0 (+0), failed: 0 (+0)
16:32:26: all: 3321, pending: 2608 (-13), running: 555 (+5), finished: 158 (+8), retry: 0 (+0), failed: 0 (+0)
16:33:29: all: 3321, pending: 2630 (-4), running: 30 (-5), finished: 661 (+9), retry: 0 (+0), failed: 0 (+0)
16:34:18: all: 3321, pending: 2597 (-11), running: 561 (+6), finished: 163 (+5), retry: 0 (+0), failed: 0 (+0)
16:35:16: all: 3321, pending: 2621 (-9), running: 26 (-4), finished: 674 (+13), retry: 0 (+0), failed: 0 (+0)
16:36:06: all: 3321, pending: 2586 (-11), running: 560 (-1), finished: 175 (+12), retry: 0 (+0), failed: 0 (+0)
16:37:39: all: 3321, pending: 2612 (-9), running: 23 (-3), finished: 686 (+12), retry: 0 (+0), failed: 0 (+0)
16:39:19: all: 3321, pending: 2577 (-9), running: 559 (-1), finished: 185 (+10), retry: 0 (+0), failed: 0 (+0)
16:39:32: all: 3321, pending: 2603 (-9), running: 19 (-4), finished: 699 (+13), retry: 0 (+0), failed: 0 (+0)
16:41:04: all: 3321, pending: 2566 (-11), running: 556 (-3), finished: 199 (+14), retry: 0 (+0), failed: 0 (+0)
16:41:25: all: 3321, pending: 2593 (-10), running: 23 (+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
  - ! 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

- 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
  - ! 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, ...

Conveniently reading remote files

```python
# read a remote json file
target = law.WLCGFileTarget("/file.json", fs="wlcg_fs")

with target.open("r") as f:
    data = json.load(f)
```

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
  - ! 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, ...

Conveniently reading remote files

```
# read a remote json file
target = law.WLCGFileTarget("/file.json", fs="wlcg_fs")

# use convenience methods for common operations
data = target.load(formatter="json")
```

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
  - ! 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, ...

Conveniently reading remote files

```python
# same for root files with context guard
target = law.WLCGFileTarget("/file.root", fs="wlcg_fs")

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

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
  - ! 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, ...

Conveniently reading remote files

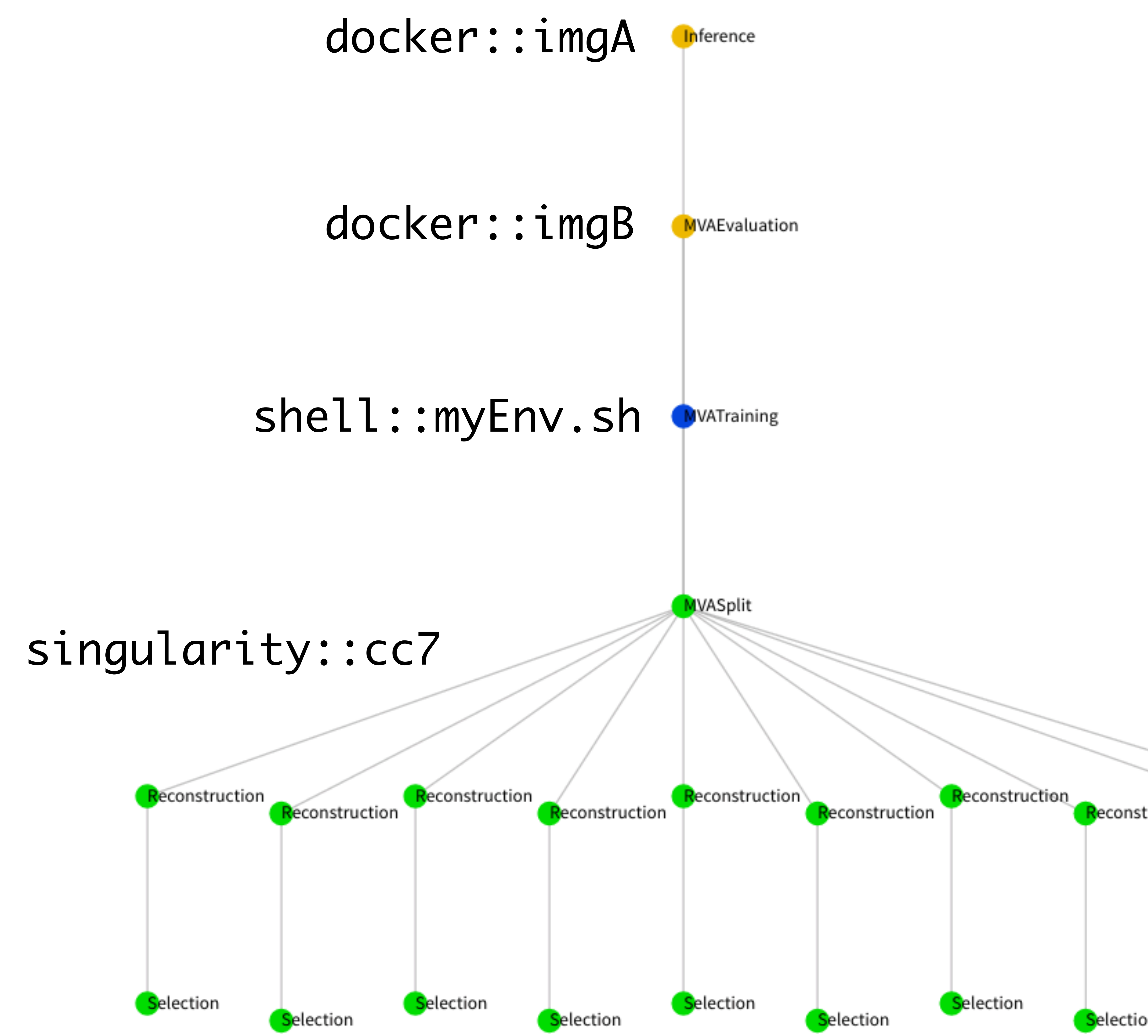
```
# multiple other "formatters" available
target = law.WLCGFileTarget("/model.pb", fs="wlcg_fs")

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

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
  - Docker images
  - Singularity images



- **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

```python
from analysis.tasks import Selection
import akward as ak

# create the task and ensure it's complete
task = Selection(dataset="ttH_bb", version="v3", shift="nominal")
task.law_run()

# read the selected events (a .parquet file)
events = task.output().load(formatter="awkward")

# get the number of jets per event
n_jets = ak.num(events.Jet, axis=1)
print(n_jets)
```

- **Notebooks**

```
In [5]: %law run ShowFrequencies --print-status -1

print task status with max_depth -1 and target_depth 0

0 > ShowFrequencies(slow=False)
│
└──1 > MergeCounts(slow=False)
       LocalFileTarget(fs=local_fs, path=$DATA_PATH/chars_merged.json)
         existent
   │
   ├──2 > CountChars(file_index=1, slow=False)
   │      LocalFileTarget(fs=local_fs, path=$DATA_PATH/chars_1.json)
   │        existent
   │  │
   │  └──3 > FetchLoremIpsum(file_index=1, slow=False)
   │         LocalFileTarget(fs=local_fs, path=$DATA_PATH/loremipsum_1.txt)
   │           existent
```

launch binder

```python
# 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"
        ...
```

- ☑ luigi task
- ☐ law task
- ☐ Run on HTCondor
- ☐ Store on EOS
- ☐ Run in docker

Example ☞

```
> python reco.py Reconstruction --dataset ttbar
```

```python
# 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"
        ...
```

- ☑ luigi task
- ☑ law task
- ☐ Run on HTCondor
- ☐ Store on EOS
- ☐ Run in docker

Example ☞

```
> law run Reconstruction --dataset ttbar
```

```python
# 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"
        ...
```

- [x] luigi task
- [x] law task
- [x] Run on HTCondor
- [ ] Store on EOS
- [ ] Run in docker

Example ☞

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

```python
# 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"
        ...
```

- [x] luigi task
- [x] law task
- [x] Run on HTCondor
- [x] Store on EOS
- [ ] Run in docker

Example ☞

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

```python
# 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"
        ...
```

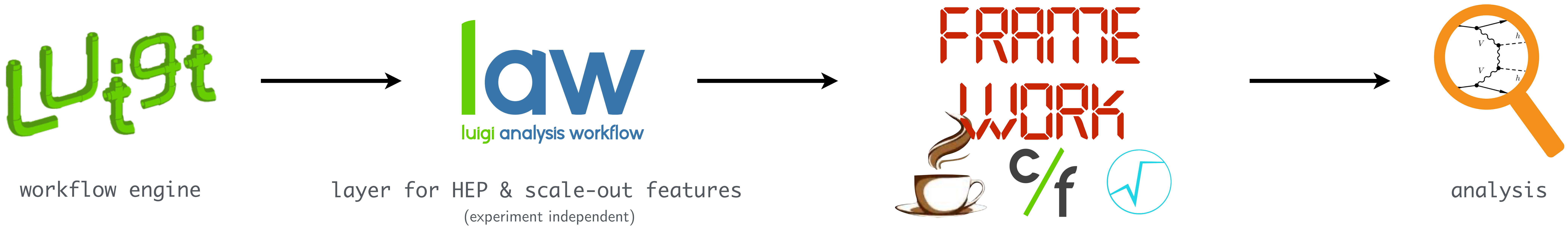
- ✔ luigi task
- ✔ law task
- ✔ Run on HTCondor
- ✔ Store on EOS
- ✔ Run in docker

Example ☞

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

Summary

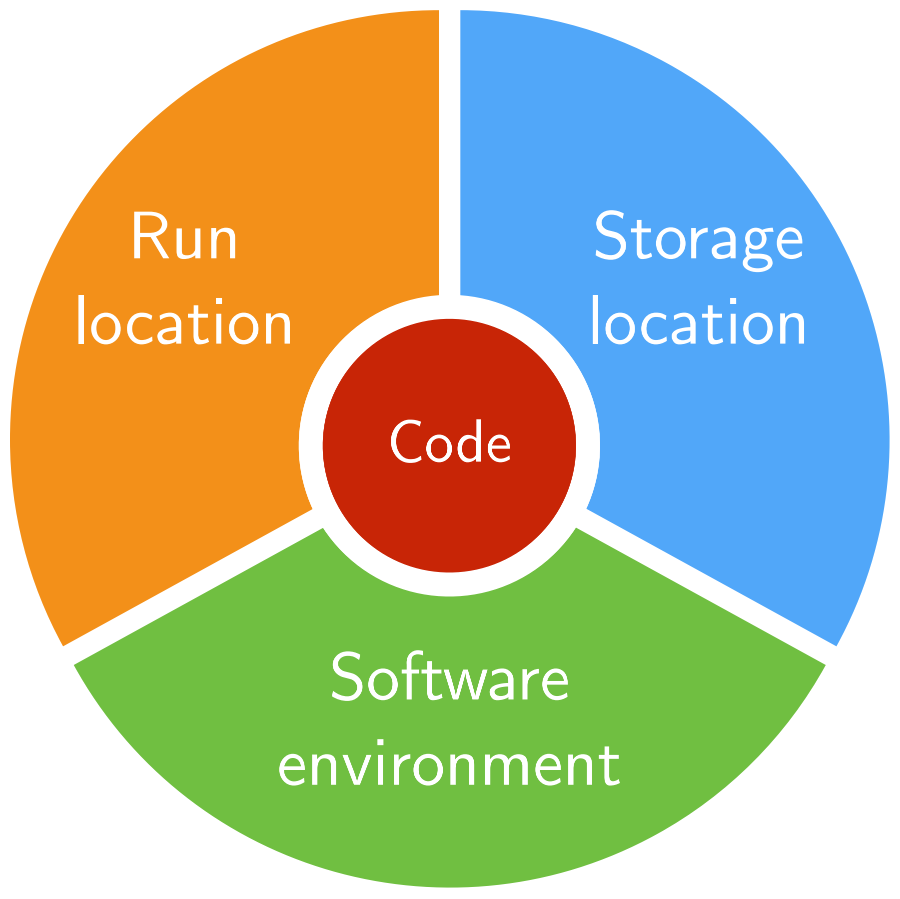
- Resource-agnostic workflow management **essential** for large & complex analyses
  → Need for a flexible **design pattern** to automate arbitrary workloads



→ **All** information transparently encoded through **tasks**, **targets** & **requirements**
→ **End-to-end automation** of analyses over distributed resources
→ Full decoupling of **run locations**, **storage locations** & **software environments**
→ Allows to build frameworks that check every point in the CMS analysis wishlist (mostly exp. agnostic)

→ github.com/riga/law, law.readthedocs.io
→ github.com/spotify/luigi, luigi.readthedocs.io

Collaboration & contributions welcome!



Backup

Other "workflow" engines

- **Metrics for comparison**
  - Low-level array processing vs. high-level embedding
  - Pythonic usage
  - Usage Overhead (requires a DB, server, custom hardware, ...)
  - Built-in features
  - Configurability
  - ...

Existing WMS: MC production

Tailored systems

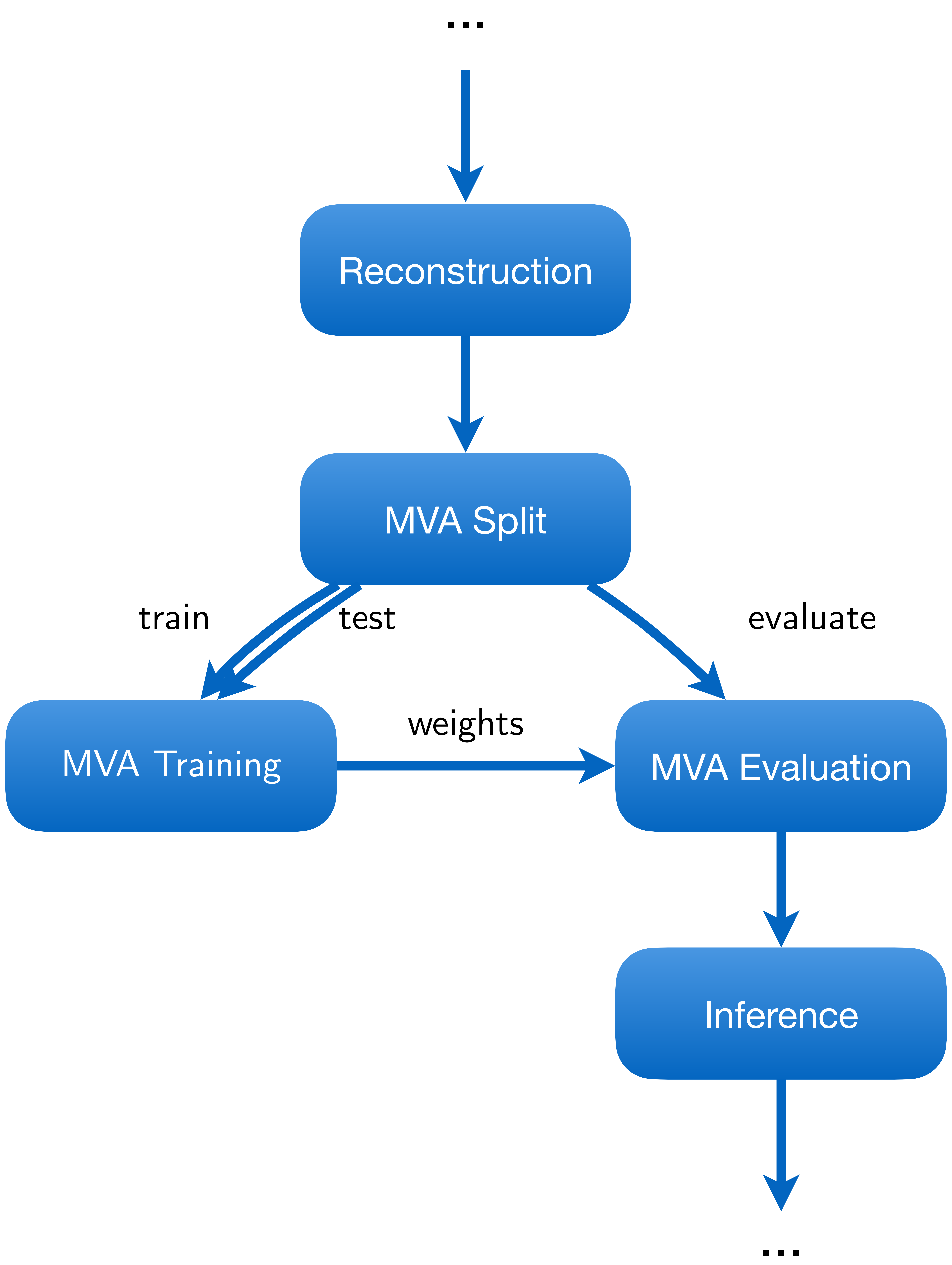
- Structure known in advance
- Workflows static & recurring
- One-dimensional design
- Special production infrastructure
- Homogeneous software requirements

Wishlist for end-user analyses

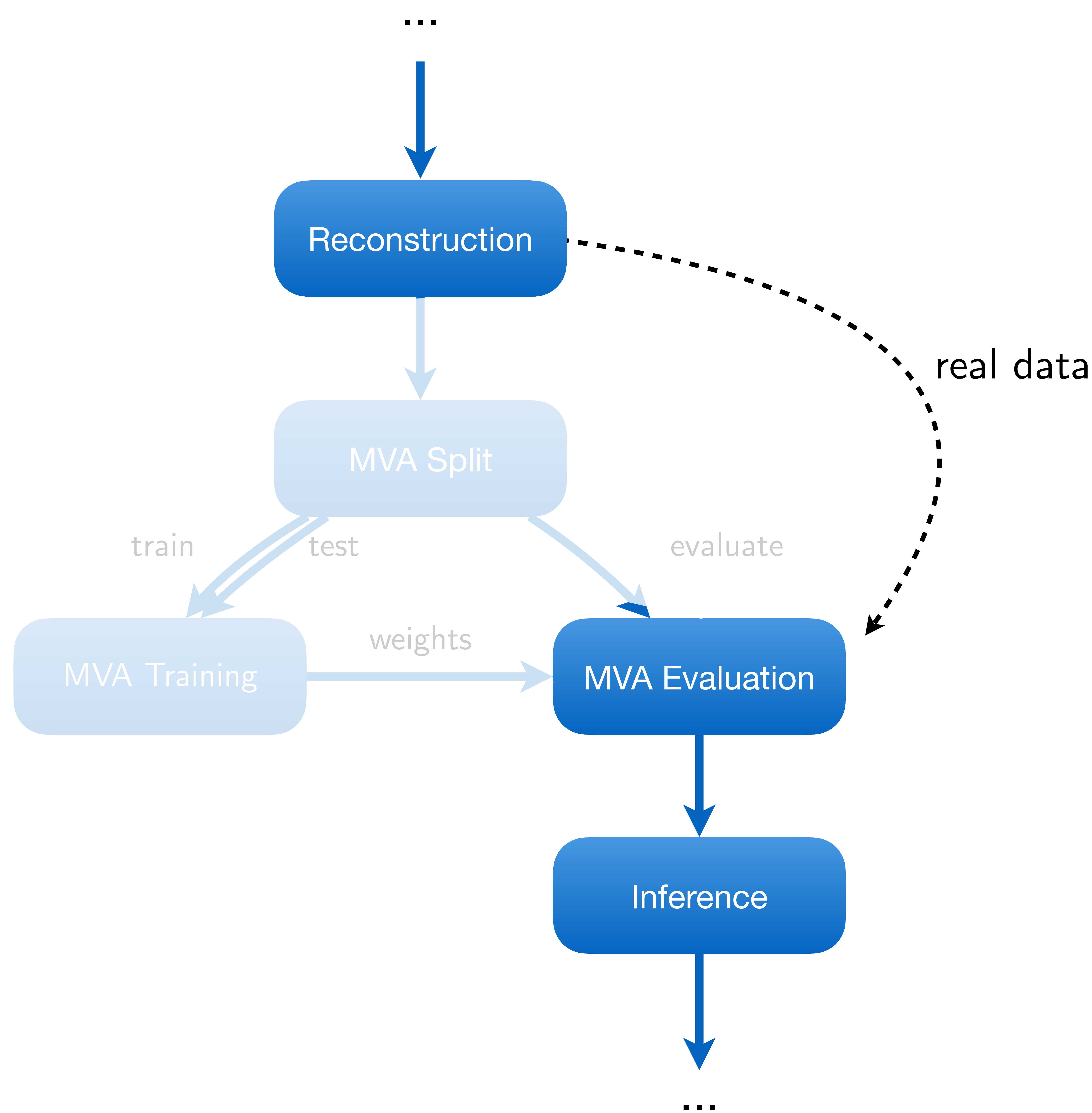
- Structure "iterative", a-priori unknown
- Dynamic workflows, fast R&D cycles
- DAG with arbitrary dependencies
- Incorporate *any* existing infrastructure
- Use custom software, everywhere

→ Requirements for HEP analyses mostly orthogonal

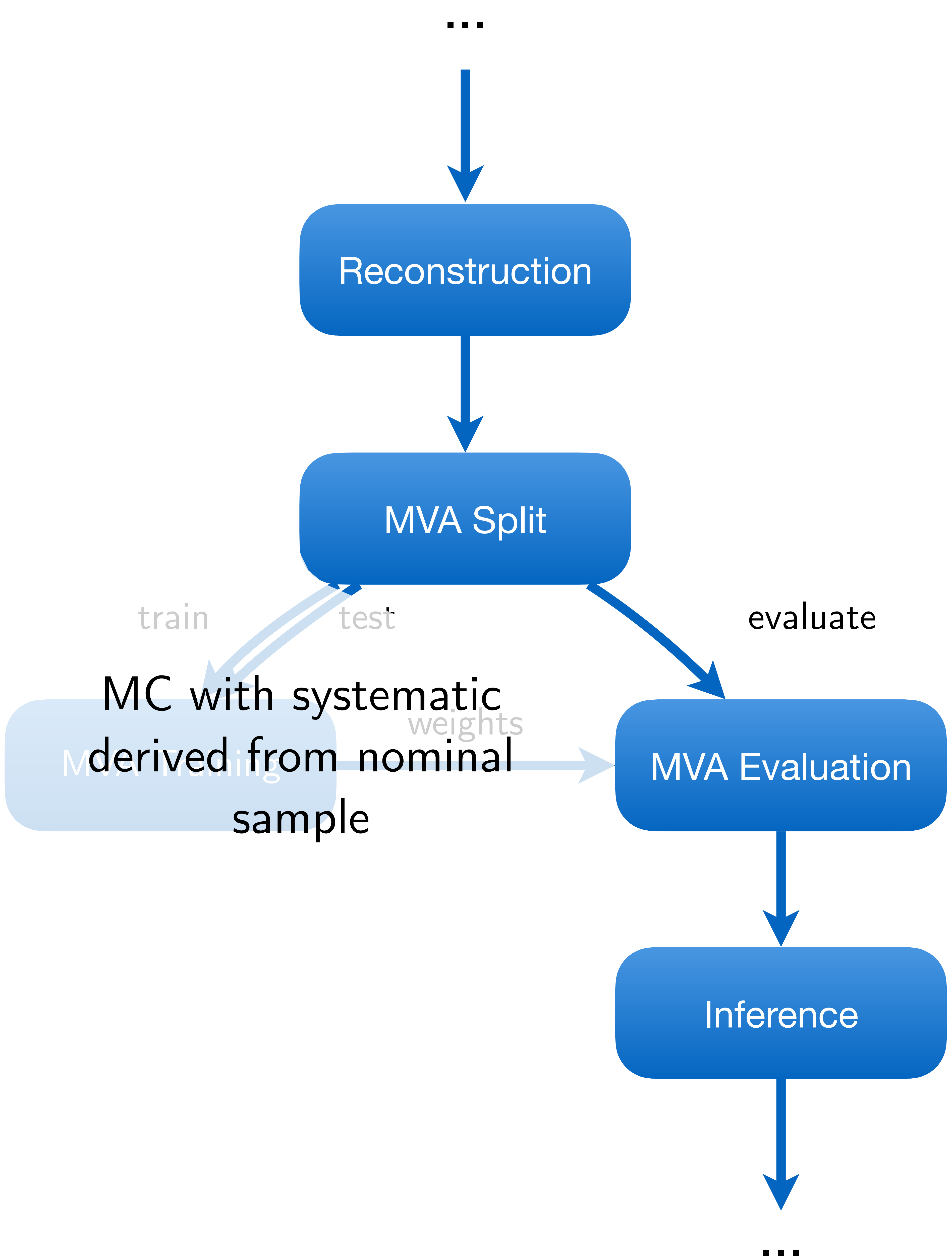
Nominal MC


...
Reconstruction
MVA Split
train
test
evaluate
weights
MVA Training
MVA Evaluation
Inference
...

Data

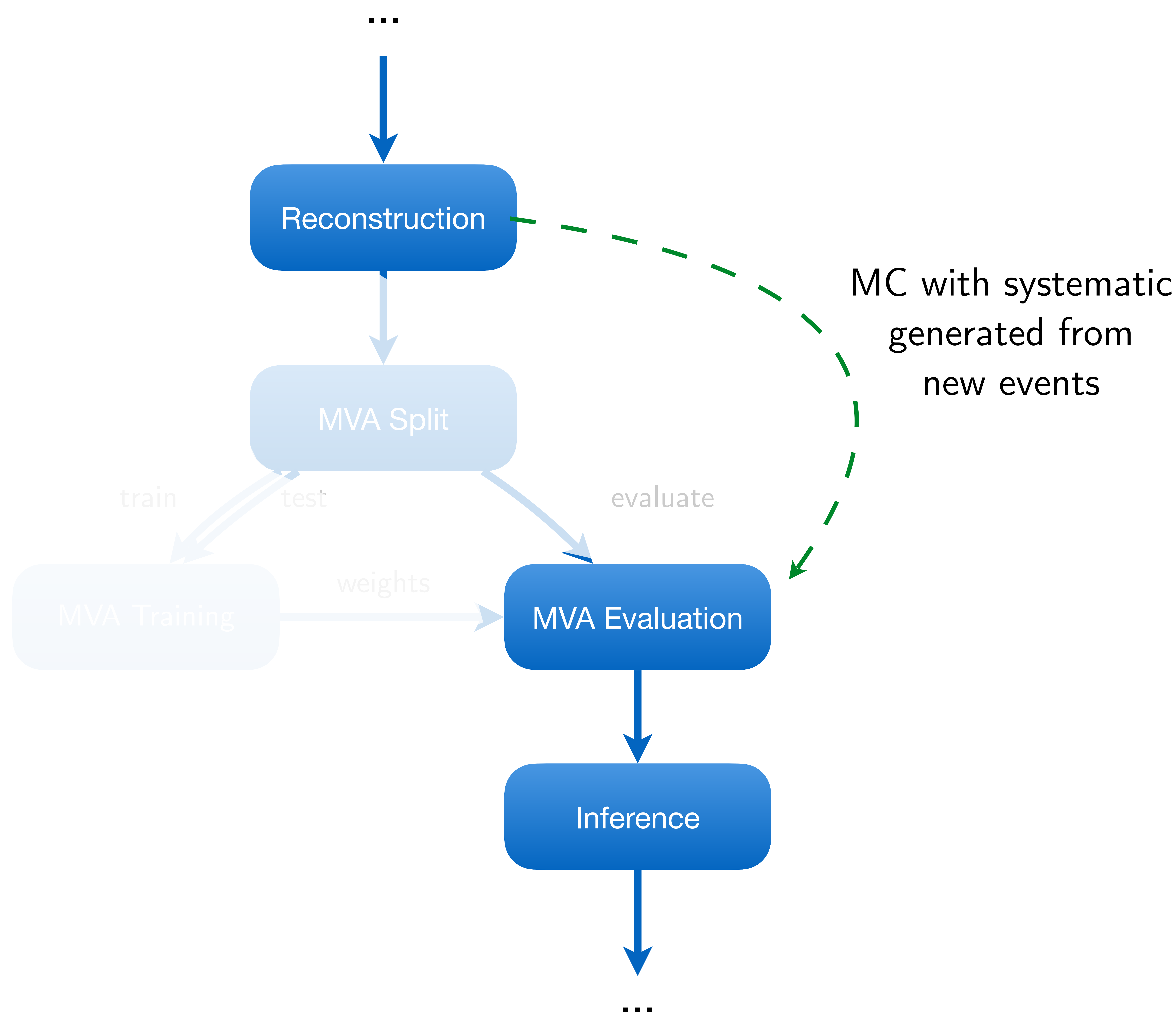

...
Reconstruction
real data
MVA Split
train
test
evaluate
weights
MVA Training
MVA Evaluation
Inference
...

MC, Syst. I



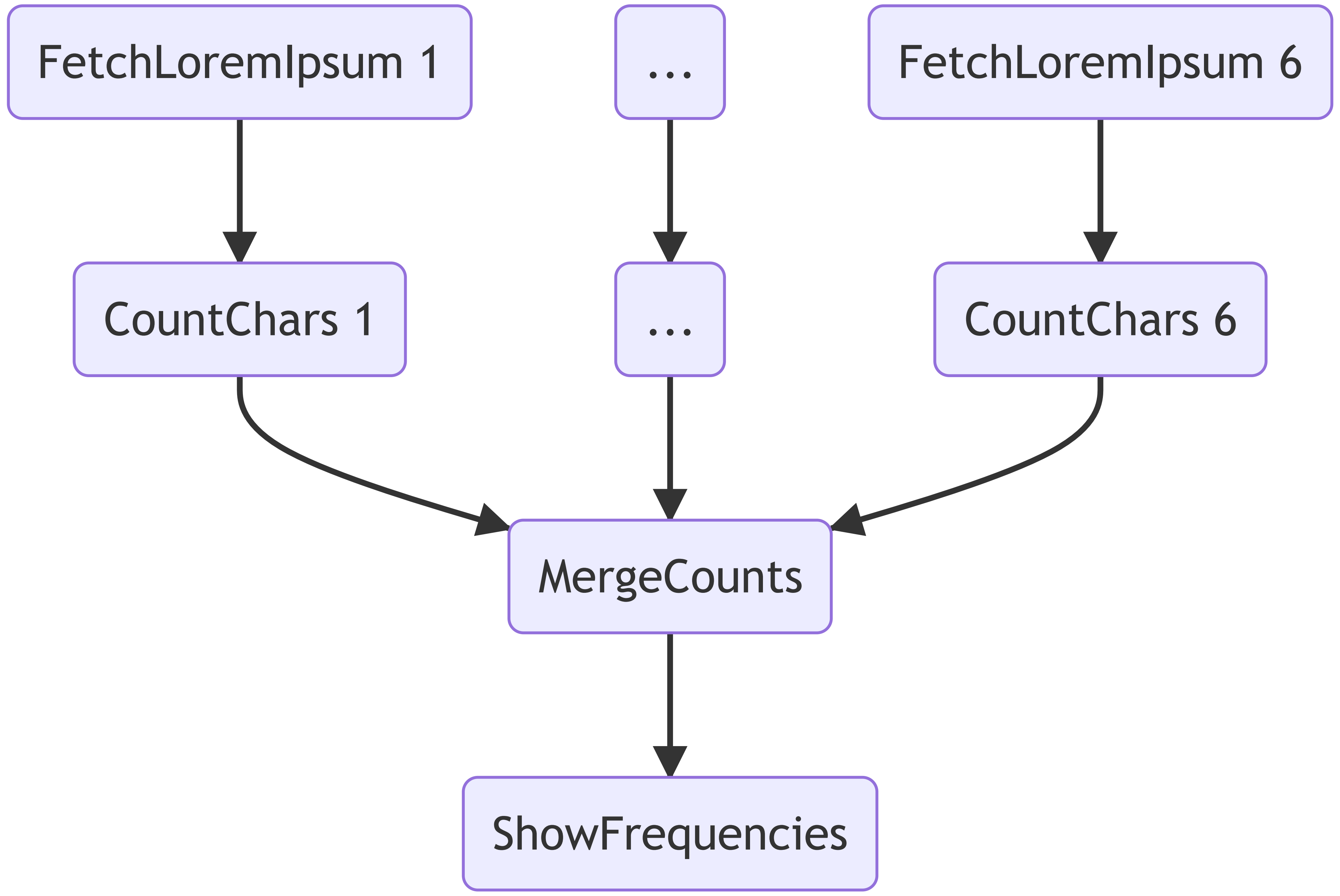
MC with systematic derived from nominal sample

MC, Syst. II


...
Reconstruction
MVA Split
train
test
evaluate
MVA Training
weights
MVA Evaluation
Inference
...
MC with systematic
generated from
new events

- Print character frequencies in the "loremipsum" placeholder text (from examples/loremipsum)

  - ▻ Fetch 6 paragraphs as txt files from some server
  - ▻ Count character frequencies and save them in json
  - ▻ Merge into a single json file
  - ▻ Print frequencies



(graphs via mermaid.live)

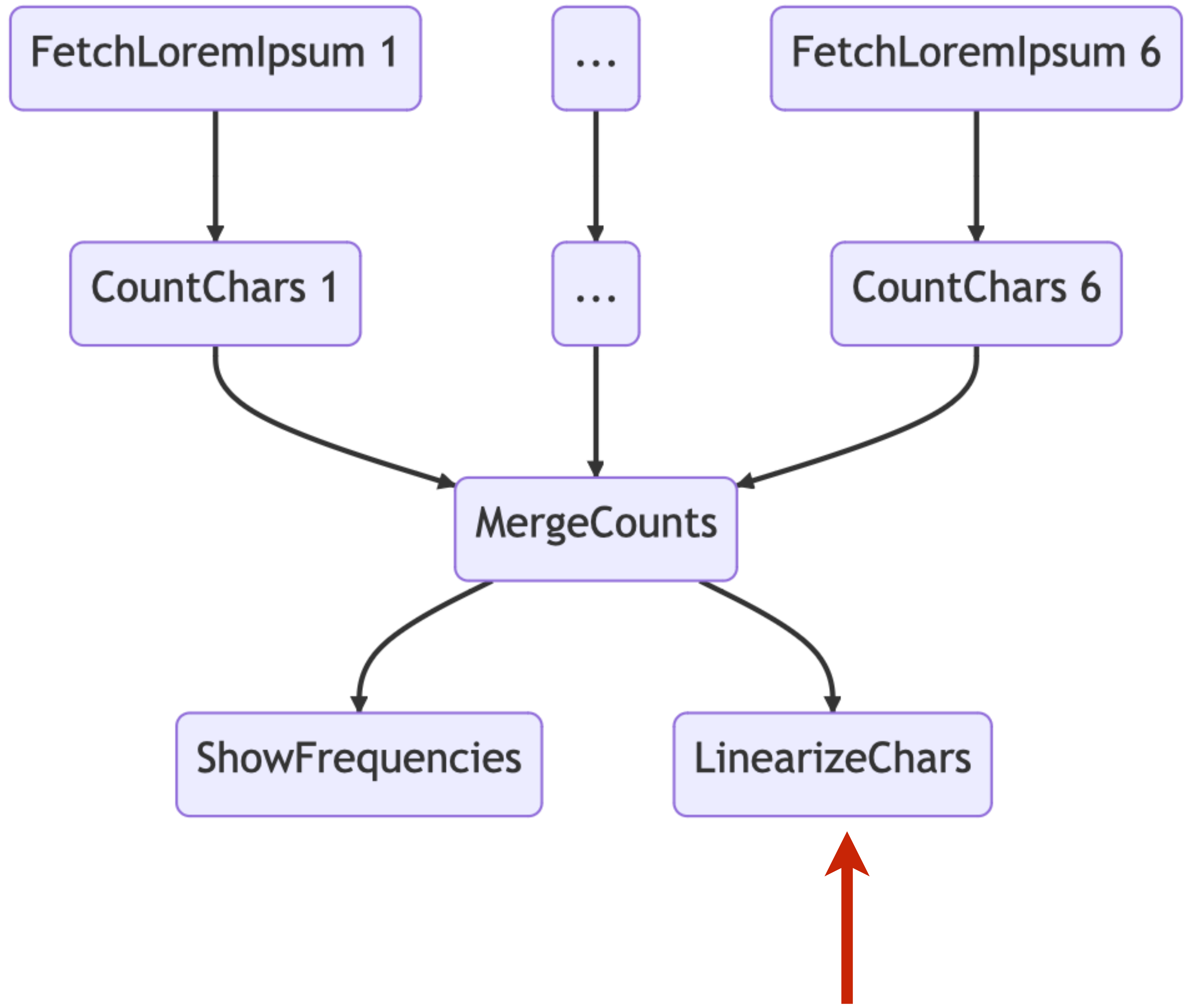
- launch binder for the notebook version

- Additional example: Workflow using CERN HTCondor

- **Interactive parameters**
  - Append `--print-status RECURSION_LEVEL[,TARGET_LEVEL]`
  - Append `--print-deps RECURSION_LEVEL`
  - Append `--remove-output RECURSION_LEVEL[,MODE],[RESTART]`
  - Append `--fetch-output RECURSION_LEVEL[,MODE],[DIRECTORY]`

- **Parallelize**
  - Append `--workers 4`

- **Add a task**
  - LinearizeChars
    - Create an ordered string "aaaaabbbccdddeeeeeeeeee..." from all existing characters and save it in a text file



- **Many tasks exhibit the same overall structure and/or purpose**
  - *"Run over N existing files"* / *"Generate N events/toys"* / *"Merge N into M files"*
  - All these tasks can **profit from the same features**
    - ▻ *"Only process file x and/to y", "Remove outputs of "x, y & z",*
      "Process N files, but consider the task finished once M < N are done", "..."

  → Calls for a generic container object that provides guidance and features for these cases

- **Workflow "containers"**
  - Task that introduces a parameters called `--branch b` (`luigi.IntParameter`)
    - ▻ `b >= 0`: Instantiates particular tasks called "branches"; `run()` will (e.g.) process file `b`
    - ▻ `b = -1`: Instantiates the workflow container itself; `run()` will run* **all branch tasks**
    - * How branch tasks are run is implemented in different workflow types: **local** or several **remote ones**

- **Practical advantages**
  - Convenience: same features available in all workflows (see next slides)
  - **Scalability and versatility for remote workflows**
    - ▻ Jobs: Better control of jobs, submission, task-to-job matching ... (see next slides)
    - ▻ Luigi: Central scheduler breaks when pinged by O(10k) tasks every few seconds
    - ▻ Remote storage: Allows batched file operations instead of file-by-file requests

- Tasks that each write a single character into a text file
- Character assigned to them though the branch map as their "branch data"

```
import luigi
import law

from my_analysis.tasks import AnalysisTask


class WriteAlphabet(AnalysisTask, law.LocalWorkflow):

    def create_branch_map(self):
        chars = "ABCDEFGHIJKLMNOPQRSTUVWXYZ"
        return dict(enumerate(chars))

    def output(self):
        return law.LocalFileTarget(f"char_{self.branch}.txt")

    def run(self):
        # branch_data refers to this branch's value in the branch map
        self.output().dump(f"char: {self.branch_data}", formatter="txt")
```

- **6 remote workflow implementations come with law**
  - htcondor, glite, lsf, arc, slurm, cms-crab (in PR#150)
  - Based on generic "job manager" implementations in contrib packages

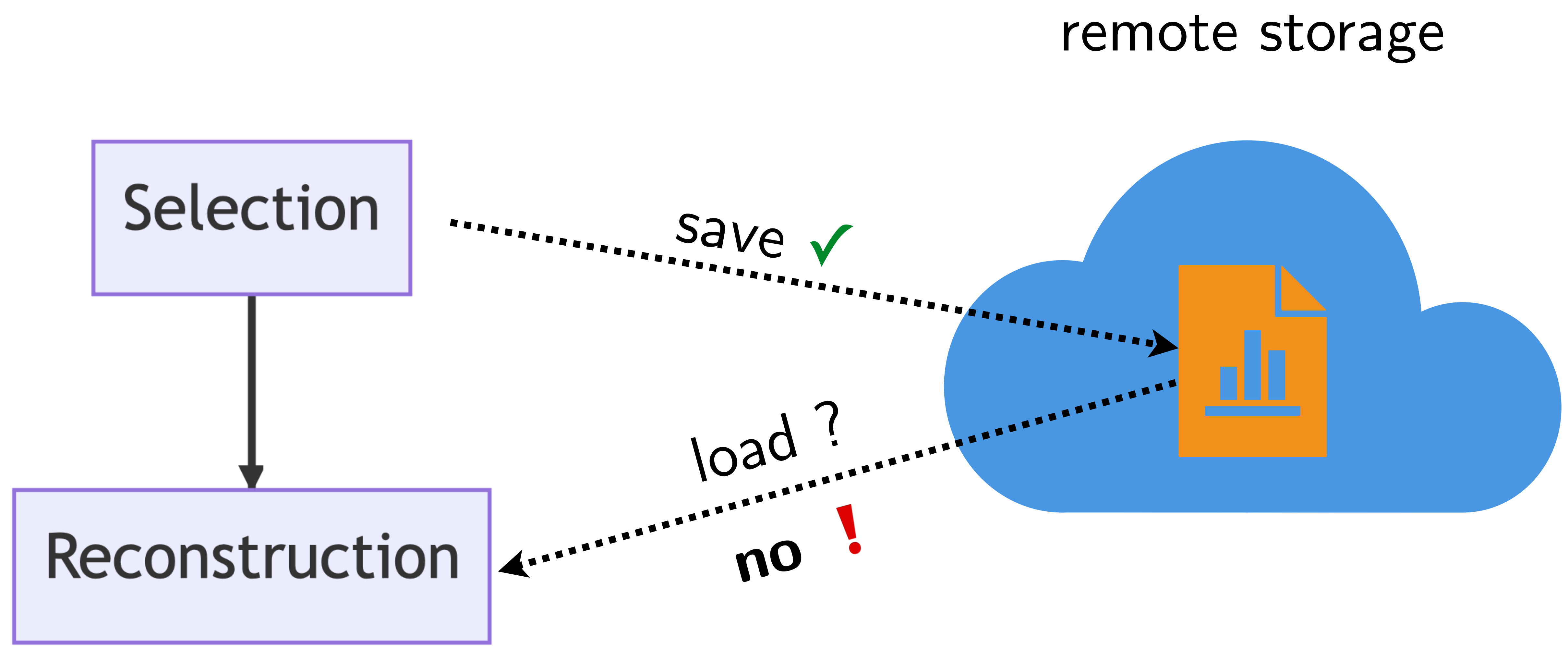
- **Job managers fully decoupled from most law functionality**
  - Simple extensibility
  - No "auto-magic" in submission files, rather minimal and configurable through tasks
  - Usable also without law

- **Most important features**
  - Job submission functionality "declared" via task class inheritance
  - Provision of software and job-specific requirements through `workflow_requires()`
  - Control over remote jobs through parameters:
    - `--branch` `--branches` : granular control of which tasks to process
    - `--acceptance` `--tolerance` : defines when a workflow is complete / failed
    - `--poll-interval` `--walltime` : controls the job status polling interval and runtime
    - `--tasks-per-job` `--parallel-jobs` : control of resource usage at batch systems

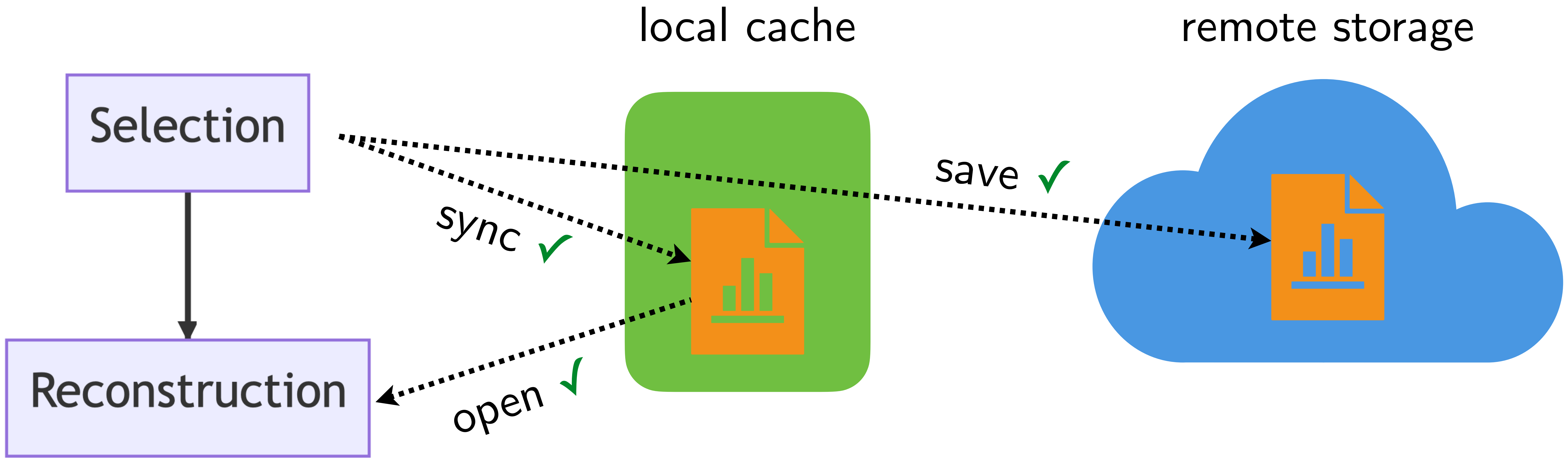
```python
# coding: utf-8
# flake8: noqa

import luigi
import law

from my_analysis.tasks import Selection
from my_analysis.algorithms import awesome_reconstruction


class Reconstruction(law.Task):

    def requires(self):
        return Selection.req(self)

    def output(self):
        return law.wlcg.WLCGFileTarget("/some/remote/path.parquet")

    def run(self):
        # !!!
        # awesome reconstruction is expecting local paths

        with self.input().localize("r") as inp:
            with self.output().localize("w") as outp:
                awesome_reconstruction(inp.path, outp.path)

```

```python
# coding: utf-8
# flake8: noqa

import luigi
import law

from my_analysis.tasks import Selection
from my_analysis.algorithms import awesome_reconstruction


class Reconstruction(law.Task):

    def requires(self):
        return Selection.req(self)

    def output(self):
        return law.wlcg.WLCGFileTarget("/some/remote/path.parquet")

    @law.decorator.localize
    def run(self):
        # !!!
        # awesome reconstruction is expecting local paths

        # but that's ok since the decorator does the localization
        awesome_reconstruction(self.input().path, self.output().path)

```

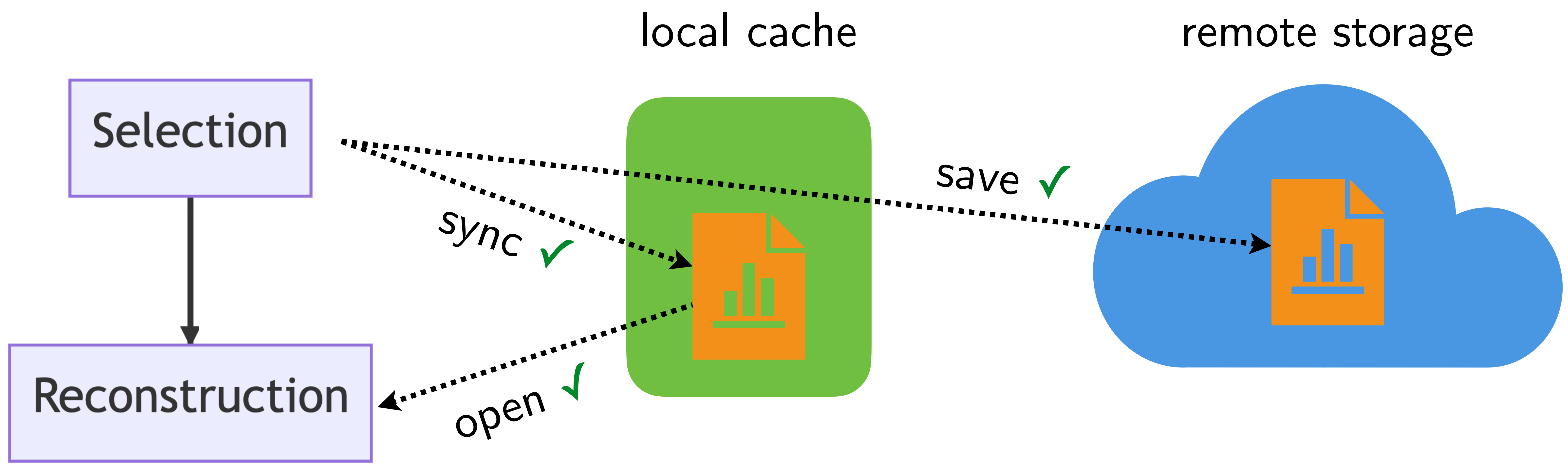
- **Local cache for remote targets**



- **Local cache for remote targets**



- **Local cache for remote targets**



- **Simple configuration**
  - When enabled, all operations on remote targets are cached

law.cfg

```
[wlcg_fs]

base: root://eosuser.cern.ch/eos/user/m/mrieger/myproject
use_cache: True
cache_root: /tmp/mrieger/wlcg_fs_cachhe
cache_max_size: 10GB
```

- **Consider this example again**

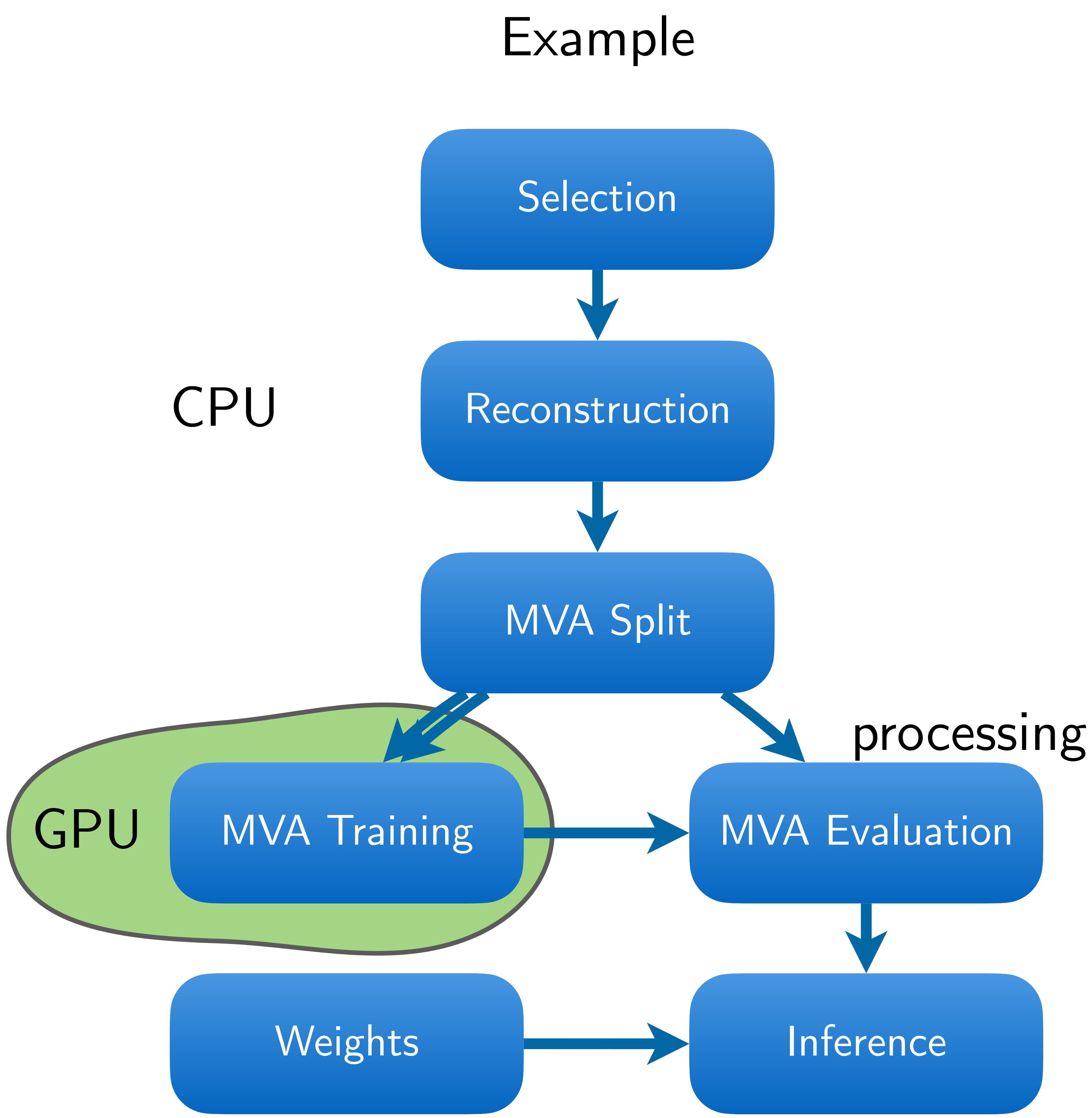
  ```
  > law run Reconstruction --dataset ttbar --workflow htcondor
  ```

  - $\mathcal{O}$(500 - 4k) files, stored either locally or remotely
  - Any workflow engine will first check if things need to be rerun
    - $\mathcal{O}$(500 - 4k) file requests (**via network**)!
    - Prepare for admins to find you 👀
  - *What* law *does*
    - Reconstruction is a workflow
    - Workflows output a so-called **TargetCollection**'s, containing all outputs of its branch tasks
    - **TargetCollection**'s can check if their files are located in the same directory
    - If they do, perform a single (remote) **listdir** and compare basenames → **single request**

- **There is no free lunch**
  - Our HEP resources (clusters, grid, storage elements, software environments) are very **inhomogeneous**
  - A **realistic** workflow engine
    - can make some good, simple assumptions based on known best-practices

      BUT
    - it should **always** allow users to transparently **change decisions** & **configure every single aspect!**

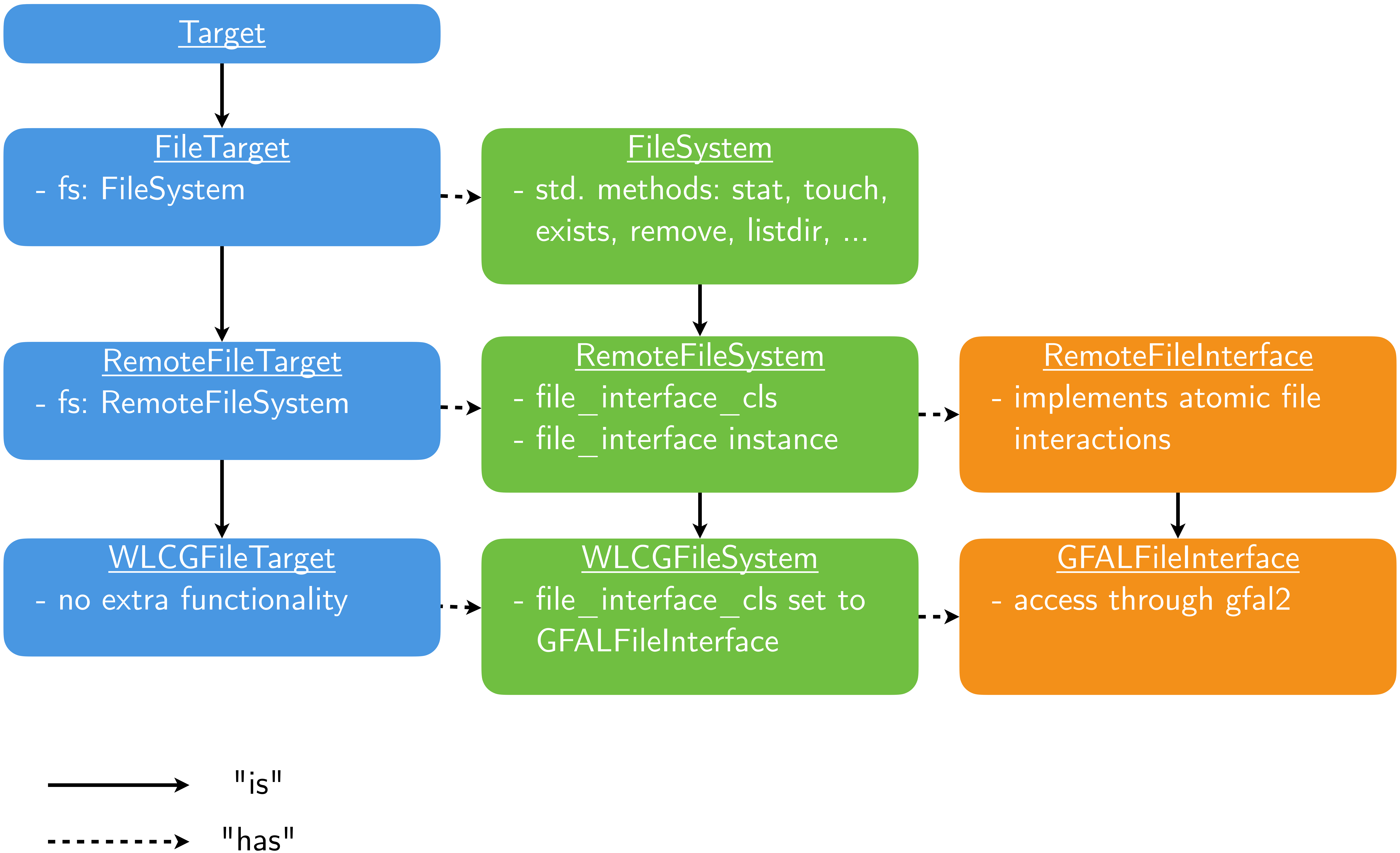
- Workflow, decomposable into particular workloads
- Workloads related to each other by common interface
  - In/outputs define directed acyclic graph (DAG)
- Alter default behavior via parameters
- Computing resources
  - Run location (CPU, GPU, WLCG, ...)
  - Storage location (local, dCache, EOS, ...)
- Software environment
- Collaborative development and
- Reproducible intermediate and



→ Reads like a checklist for analysis workflow management

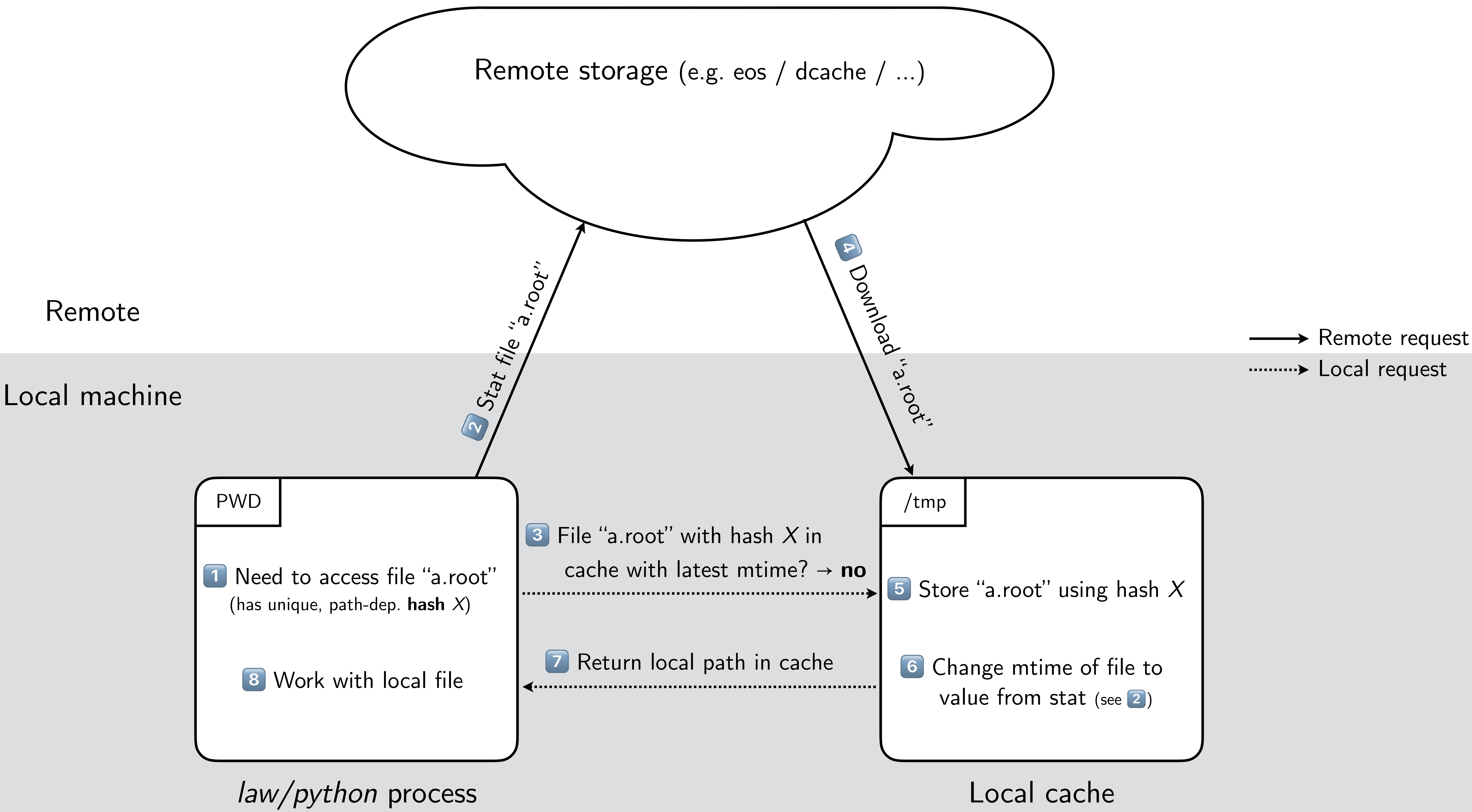
(Remote) targets

```python
import law

from my_analysis import SomeTaskWithROOTOutput, some_executable

law.contrib.load("wlcg")


class MyTask(law.Task):

    def requires(self):
        return SomeTaskWithROOTOutput.req(self)

    def output(self):
        return law.wlcg.WLCGFileTarget("large_root_file.root")

    def run(self):
        # using target formatters for loading and dumping
        with self.input().load(formatter="uproot") as in_file:
            with self.output().dump(formatter="root") as out_file:
                ...

        # using localized representation of (e.g.) output
        # to use its local path for some executable
        # (the referenced file is automatically moved to the
        # remote location once the context exits)
        with self.output().localize("w") as tmp_output:
            some_executable(tmp_output.path)

    @law.decorator.localize
    def run(self):
        # when wrapped by law.decorator.localize
        # self.input() and self.output() returns localized
        # representations already and deals with subsequent copies
        some_executable(self.output().path)
```

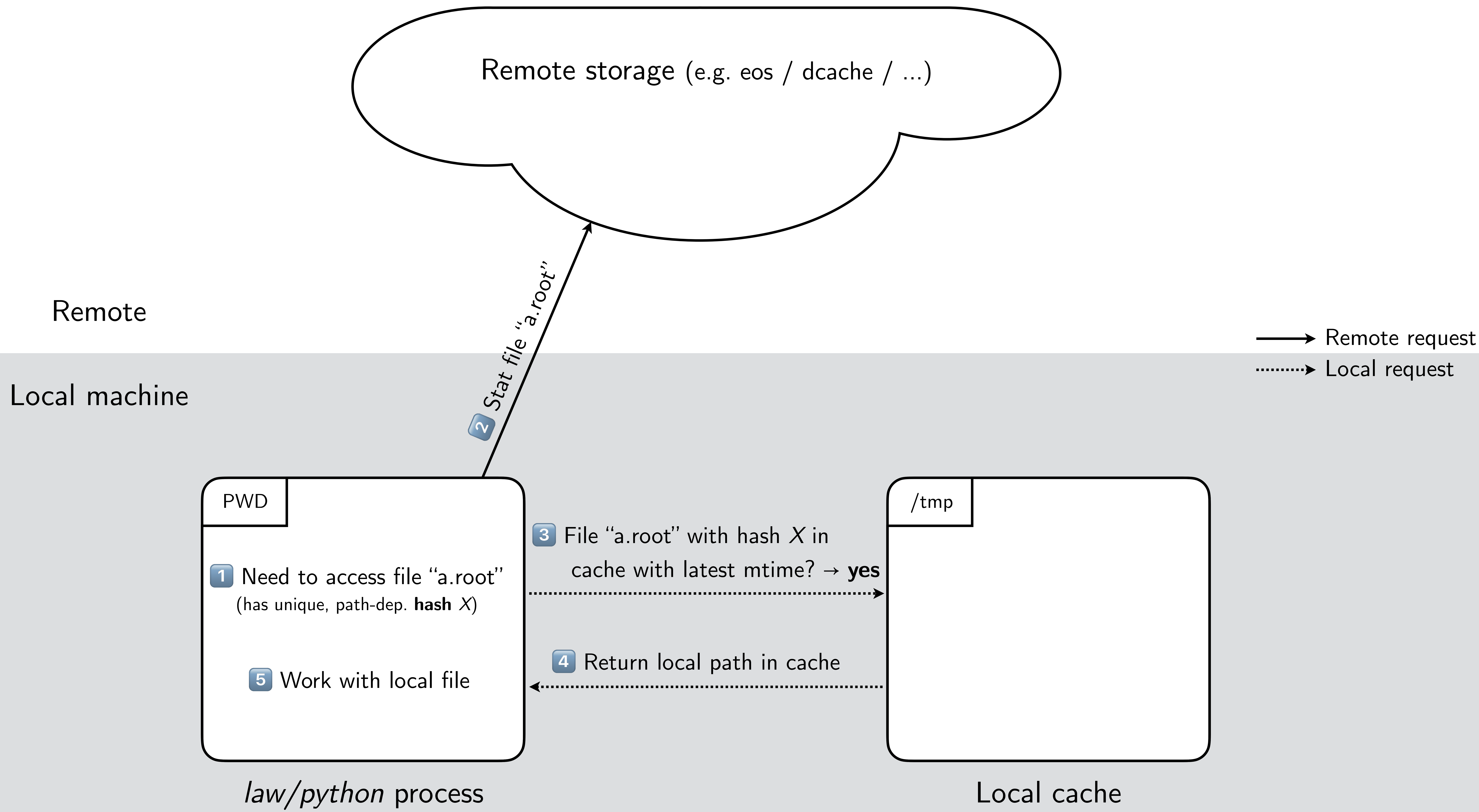

Target
FileTarget
- fs: FileSystem
FileSystem
- std. methods: stat, touch, exists, remove, listdir, ...
RemoteFileTarget
- fs: RemoteFileSystem
RemoteFileSystem
- file_interface_cls
- file_interface instance
RemoteFileInterface
- implements atomic file interactions
WLCGFileTarget
- no extra functionality
WLCGFileSystem
- file_interface_cls set to GFALFileInterface
GFALFileInterface
- access through gfal2
"is"
"has"

Local caching (1)

Configuration ☞



Configuration ☞



Workflows

- **Many tasks exhibit the same overall structure and/or purpose**
  - *"Run over N existing files"* / *"Generate N events/toys"* / *"Merge N into M files"*
  - All these tasks can **profit from the same features**
    - ▻ *"Only process file x and/to y", "Remove outputs of "x, y & z",*
      "Process N files, but consider the task finished once M < N are done", "..."

  → Calls for a generic container object that provides guidance and features for these cases

- **Workflow "containers"**
  - Task that introduces a parameters called `--branch b` (`luigi.IntParameter`)
    - ▻ `b >= 0`: Instantiates particular tasks called "branches"; `run()` will (e.g.) process file `b`
    - ▻ `b = -1`: Instantiates the workflow container itself; `run()` will run* all branch tasks
    - * How branch tasks are run is implemented in different workflow types: local or several remote ones

- **Practical advantages**
  - Convenience: same features available in all workflows (see next slides)
  - **Scalability and versatility for remote workflows**
    - ▻ Jobs: Better control of jobs, submission, task-to-job matching ... (see next slides)
    - ▻ Luigi: Central scheduler breaks when pinged by O(10k) tasks every few seconds
    - ▻ Remote storage: allows batched file operations instead of file-by-file requests

Common

```python
class Workflow(law.BaseTask):

    branch = luigi.IntParameter(default=-1)

    @property
    def is_workflow(self):
        return self.branch == -1

    def branch_tasks(self):
        return [self.req(self, branch=b) for b in self.create_branch_map()]
```

Workflow specific

```python
    def workflow_requires(self):
        """ requirements to be resolved before the workflow starts """

    def workflow_output(self):
        """ output of the workflow (usually a collection of branch outputs) """

    def workflow_run(self):
        """ run implementation """
```

When "`is_workflow`", seen by luigi as `requires()`, `output()` and `run()`

Implemented by task

```python
    def create_branch_map(self):
        """ Maps branch numbers to arbitrary payloads, e.g.
            ``return {0: "file_A.txt", 1: "file_C.txt", 2: ...}``
            To be implemented by inheriting tasks.
        """
        raise NotImplementedError

    def requires(self):
        """ usual requirement definition """

    def output(self):
        """ usual output definition """

    def run(self):
        """ usual run implementation """
```

- Tasks that each write a single character into a text file
- Character assigned to them though the branch map as their "branch data"

```python
import luigi
import law

from my_analysis.tasks import AnalysisTask


class WriteAlphabet(AnalysisTask, law.LocalWorkflow):

    def create_branch_map(self):
        chars = "ABCDEFGHIJKLMNOPQRSTUVWXYZ"
        return dict(enumerate(chars))

    def output(self):
        return law.LocalFileTarget(f"char_{self.branch}.txt")

    def run(self):
        # branch_data refers to this branch's value in the branch map
        self.output().dump(f"char: {self.branch_data}", formatter="txt")
```

- 6 **remote workflow implementations come with law**
  - htcondor, glite, lsf, arc, slurm, cms-crab (in PR#150)
  - Based on generic "job manager" implementations in contrib packages

- **Job managers fully decoupled from most law functionality**
  - Simple extensibility
  - No "auto-magic" in submission files, rather minimal and configurable through tasks
  - Usable also without law

- **Most important features**
  - Job submission functionality "declared" via task class inheritance
  - Provision of software and job-specific requirements through `workflow_requires()`
  - Control over remote jobs through parameters:
    - `--branch` `--branches` : granular control of which tasks to process
    - `--acceptance` `--tolerance` : defines when a workflow is complete / failed
    - `--poll-interval` `--walltime` : controls the job status polling interval and runtime
    - `--tasks-per-job` `--parallel-jobs` : control of resource usage at batch systems

Miscellaneous

Package structure

Command-line interface

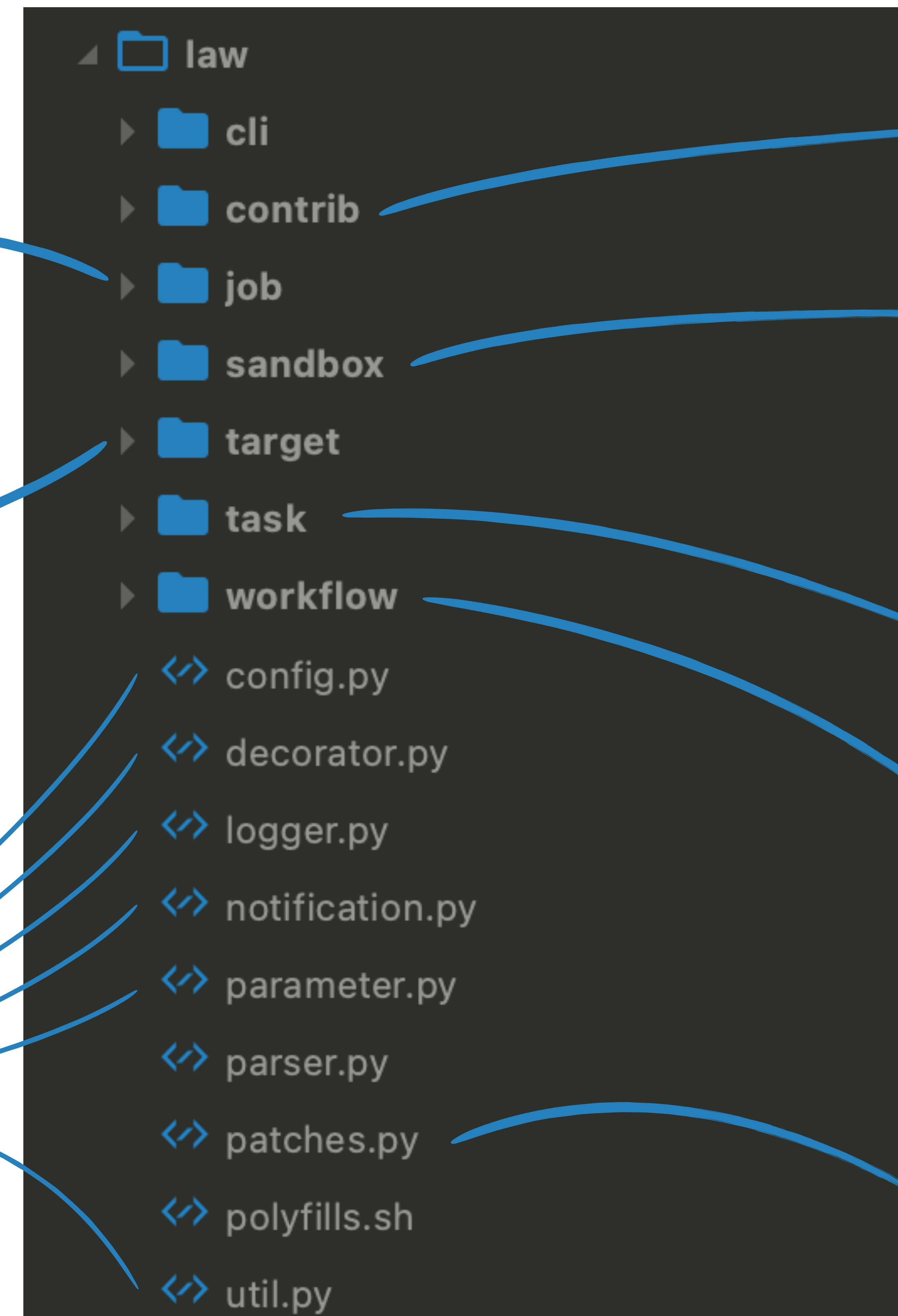
Job interface

- Job file factory interface
- Job manager interface
- Generic remote job script

Target definitions

- Generic + file interace
- Local target impl.
- Remote target interfaces

Config parsing & tools
Task decorators
Custom loggers
Notification tools (for e.g. slack/telegram)
Custom parameters
Utilities & helpers



3rd party tools

Sandboxing mechanism

- Sandbox task
- Sandbox interface
- Bash sandbox impl.

Base task definitions

Base workflow definition

- Local workflow impl.
- Remote workflow interface

Lightweight patches of luigi, e.g.:

- Disable dep. checks in sandboxes
- Colorize logs

→ Could be added directly to luigi

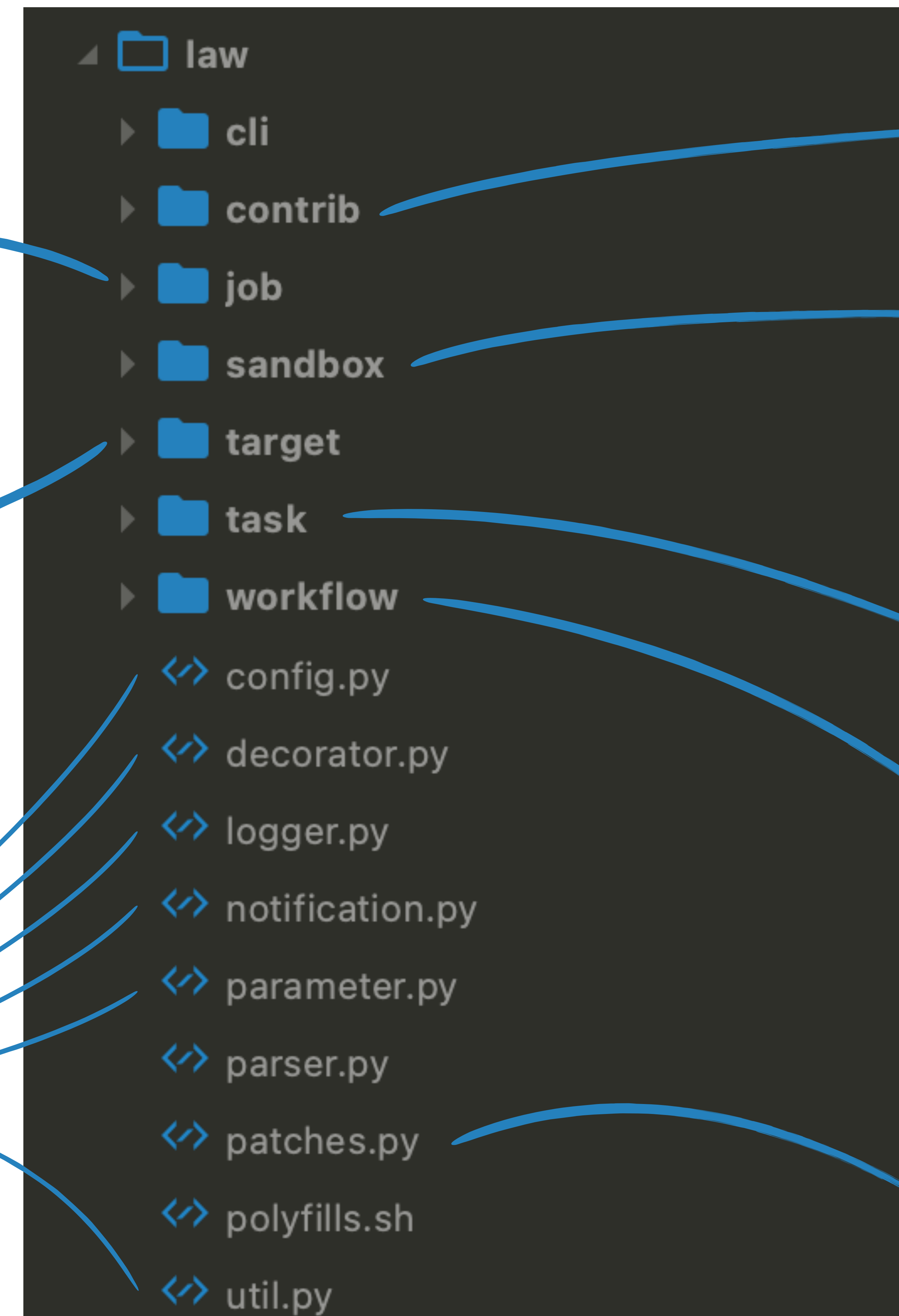
Package structure

Command-line interface

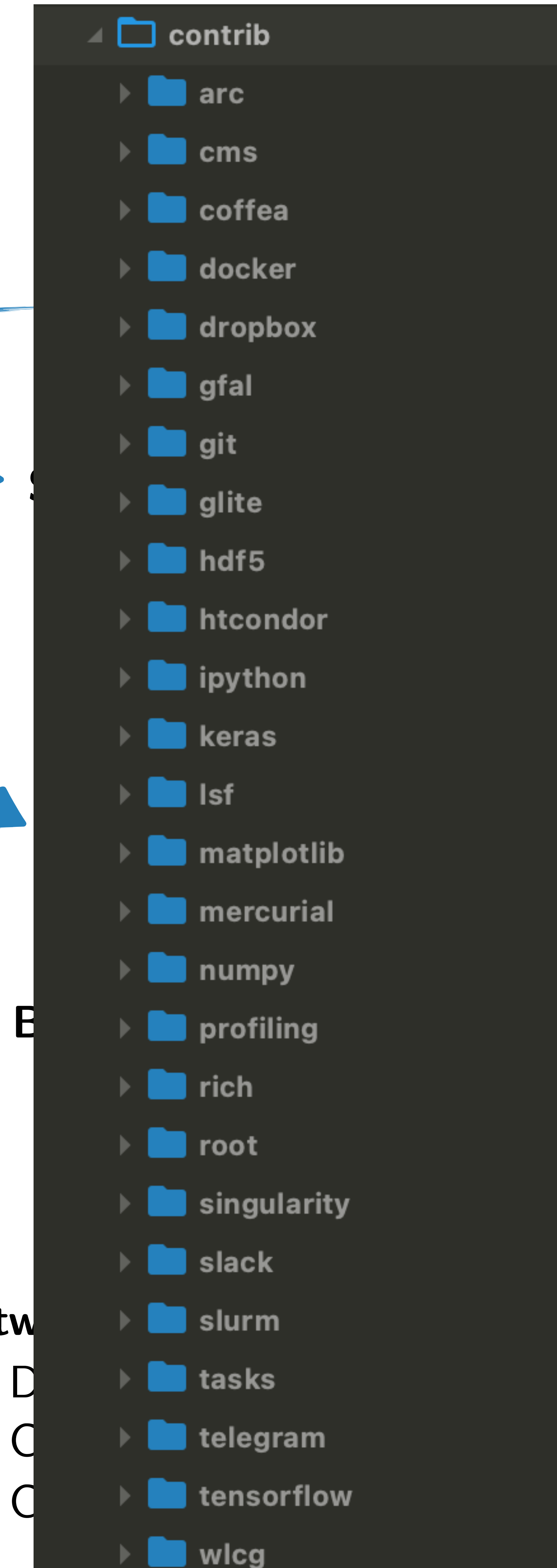
Job interface
- Job file factory interface
- Job manager interface
- Generic remote job script

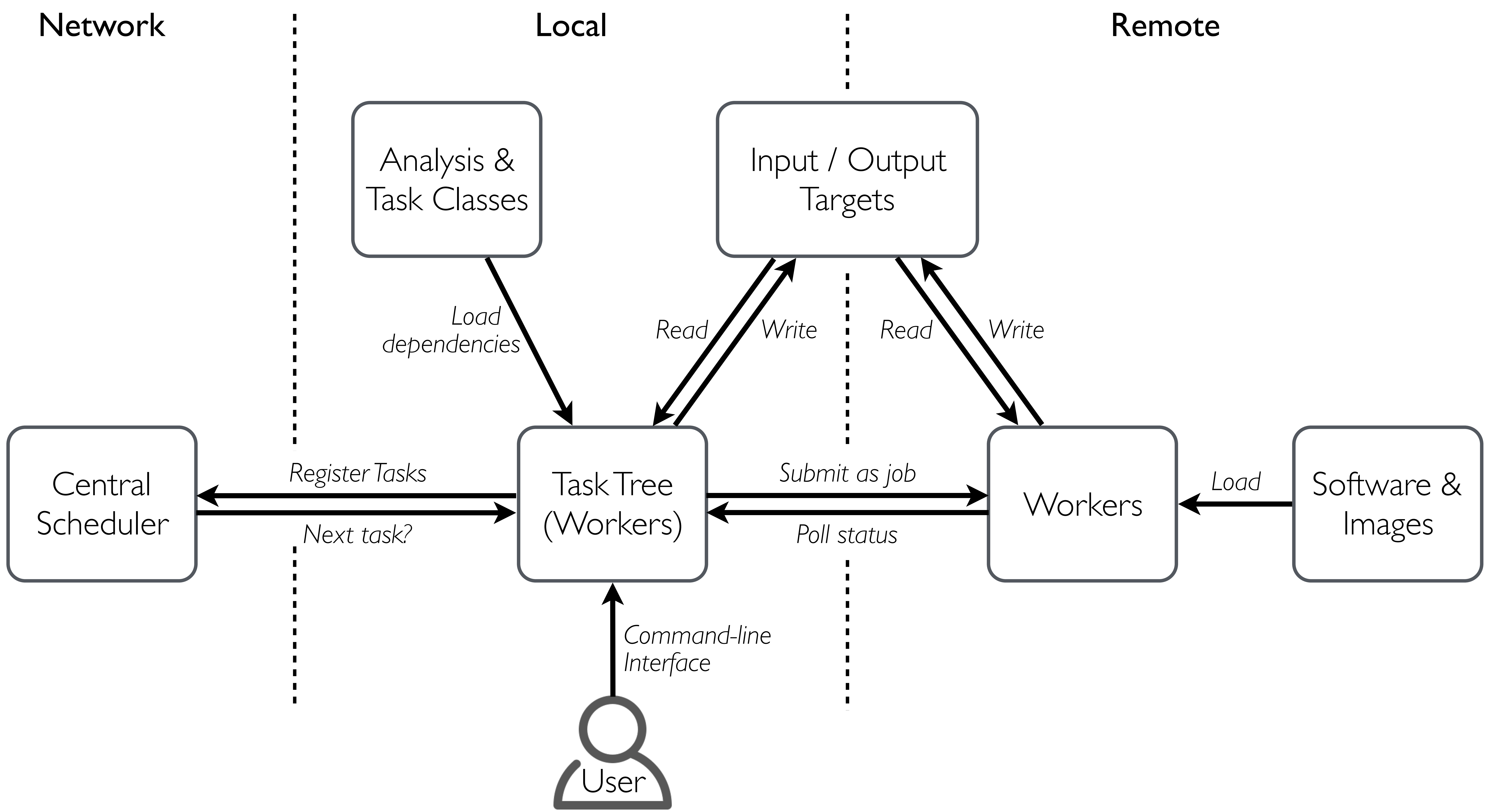
Target definitions
- Generic + file interace
- Local target impl.
- Remote target interfaces

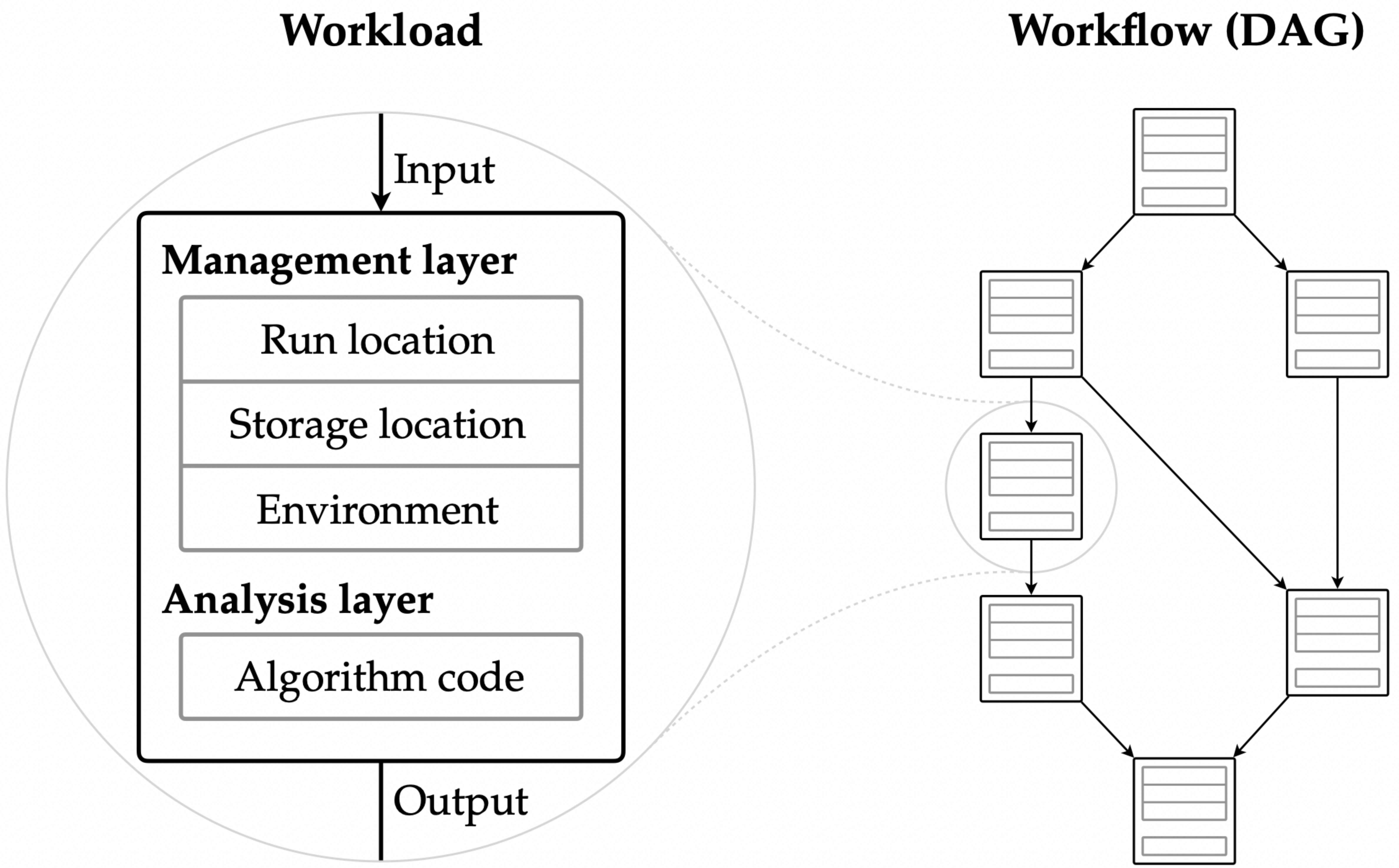
Config parsing & tools
Task decorators
Custom loggers
Notification tools (for e.g. slack/telegram)
Custom parameters
Utilities & helpers



S
E
e
Lightw :
- D xes
- C
→ C gi




Network
Local
Remote
Analysis & Task Classes
Input / Output Targets
Load dependencies
Read
Write
Read
Write
Central Scheduler
Task Tree (Workers)
Workers
Software & Images
Register Tasks
Next task?
Submit as job
Poll status
Load
Command-line Interface
User


Workload
Input
Management layer
Run location
Storage location
Environment
Analysis layer
Algorithm code
Output
Workflow (DAG)

- *law* - *luigi* analysis workflow
  - Repository ☞ github.com/riga/law
  - Paper ☞ arXiv:1706.00955 (CHEP16 proceedings)
  - Documentation ☞ law.readthedocs.io (in preparation)
  - Minimal example ☞ github.com/riga/law/tree/master/examples/loremipsum
  - HTCondor example ☞ github.com/riga/law/tree/master/examples/htcondor_at_cern
  - Contact ☞ Marcel Rieger

- *luigi* - Powerful Python pipelining package (by Spotify)
  - Repository ☞ github.com/spotify/luigi
  - Documentation ☞ luigi.readthedocs.io
  - "Hello world!" ☞ github.com/spotify/luigi/blob/master/examples/hello_world.py

- Technologies
  - GFAL2 ☞ dmc.web.cern.ch/projects/gfal-2/home
  - Docker ☞ docker.com
  - Singularity ☞ singularity.lbl.gov

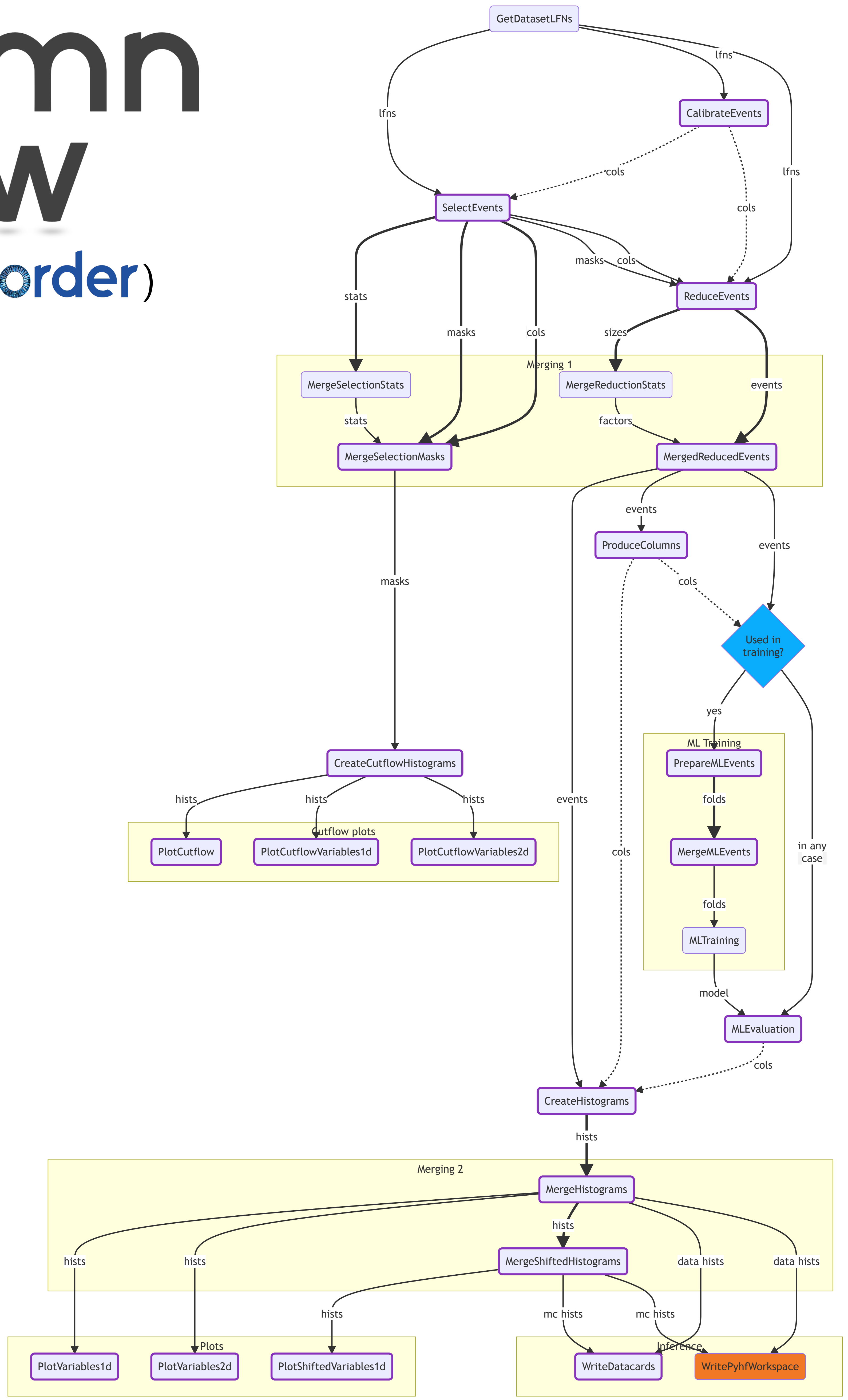
columnflow

- **columnflow**: Backend for large-scale columnar analyses
  - Reads and writes columns only if necessary
  - Creates new columns and merges with existing ones at the **latest possible instance**

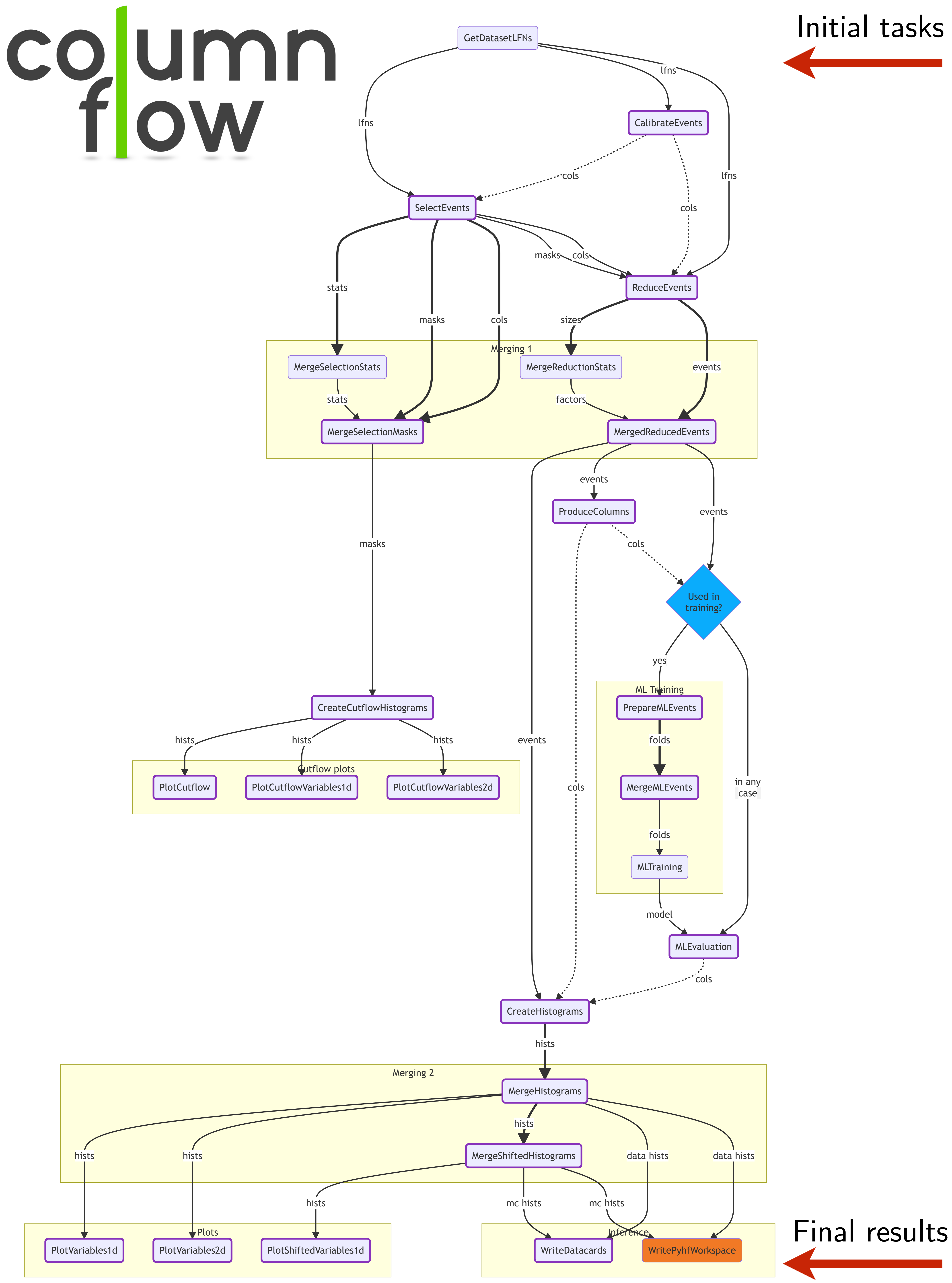
  - Stores intermediate outputs for
    - ▻ computations downstream
    - ▻ sharing results of same computations across groups
    - ▻ applications requiring per-event info (ML)
    - ▻ studies done by students
    - ▻ debugging purposes
    - → difference to map-reduce pattern in coffea processors
  - Heavy use of bare NumPy & TensorFlow & awkward, plus coffea NanoScheme behavior

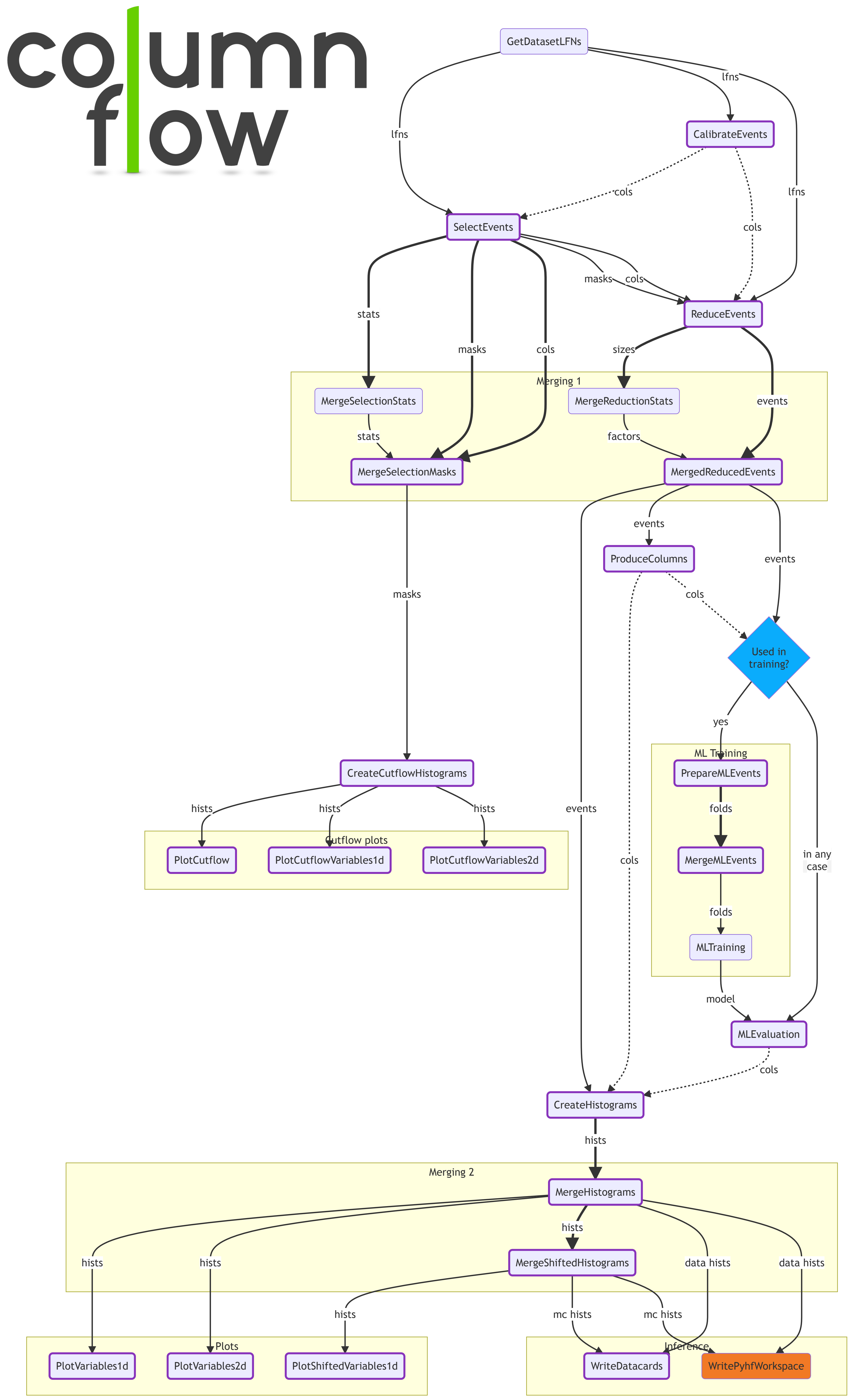
  - Full resolution of systematic uncertainties (next slide)
  - Checks 15/17 points of the CMS analysis wishlist in the ATTF report

columnflow
(using law & order)



workflow *suggested* by columnflow, but can be fully customized


GetDatasetLFNs
lfns
CalibrateEvents
lfns
cols
SelectEvents
cols
lfns
masks
cols
ReduceEvents
stats
masks
cols
sizes
Merging 1
MergeSelectionStats
MergeReductionStats
events
stats
factors
MergeSelectionMasks
MergedReducedEvents
events
ProduceColumns
events
masks
cols
Used in training?
yes
ML Training
CreateCutflowHistograms
PrepareMLEvents
hists
hists
hists
events
folds
Cutflow plots
PlotCutflow
PlotCutflowVariables1d
PlotCutflowVariables2d
cols
MergeMLEvents
in any case
folds
MLTraining
model
MLEvaluation
cols
CreateHistograms
hists
Merging 2
MergeHistograms
hists
hists
hists
MergeShiftedHistograms
data hists
data hists
hists
mc hists
mc hists
Plots
inference
PlotVariables1d
PlotVariables2d
PlotShiftedVariables1d
WriteDatacards
WritePyhfWorkspace
Initial tasks
Final results

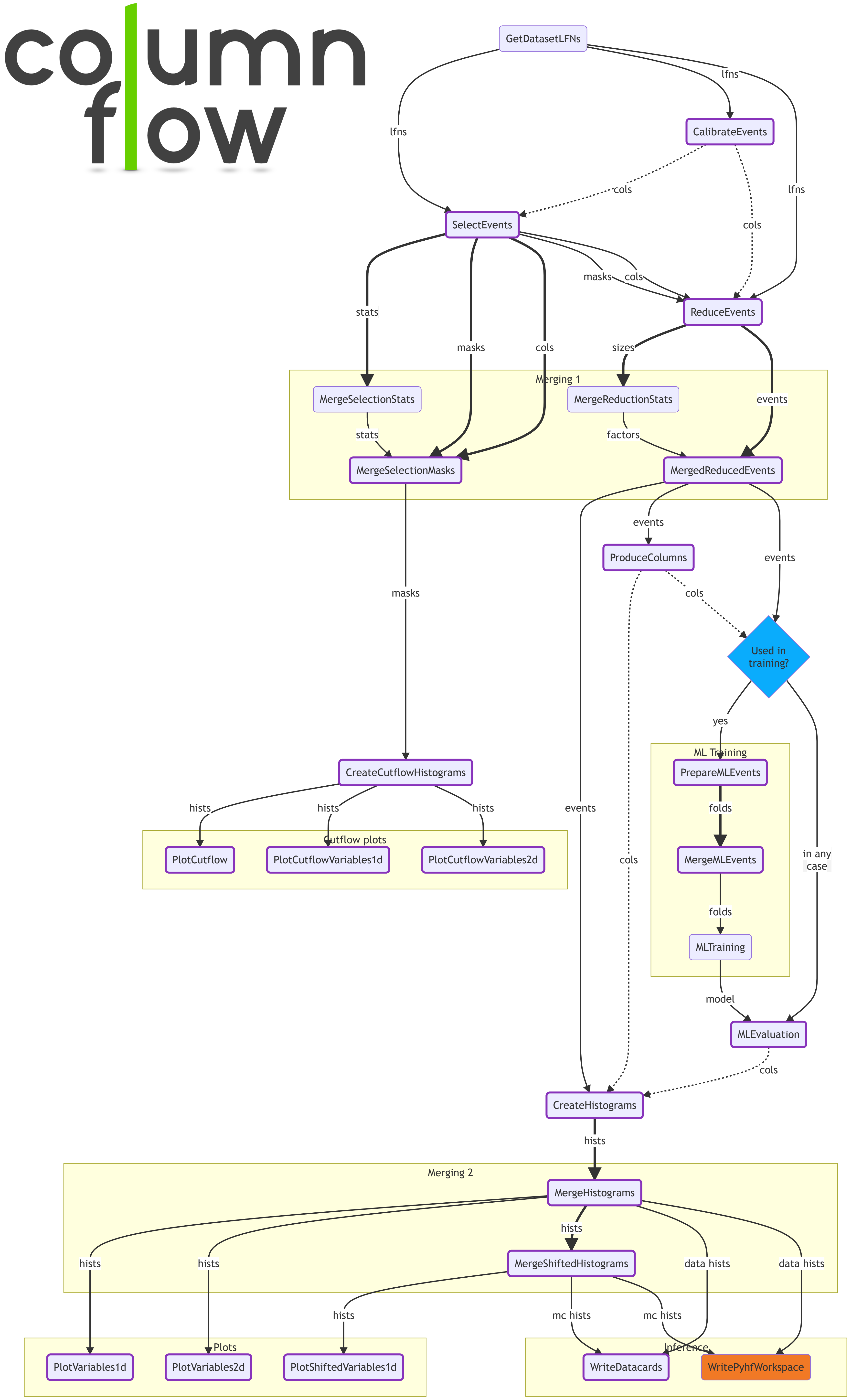


Initial tasks

Final results

"nominal"

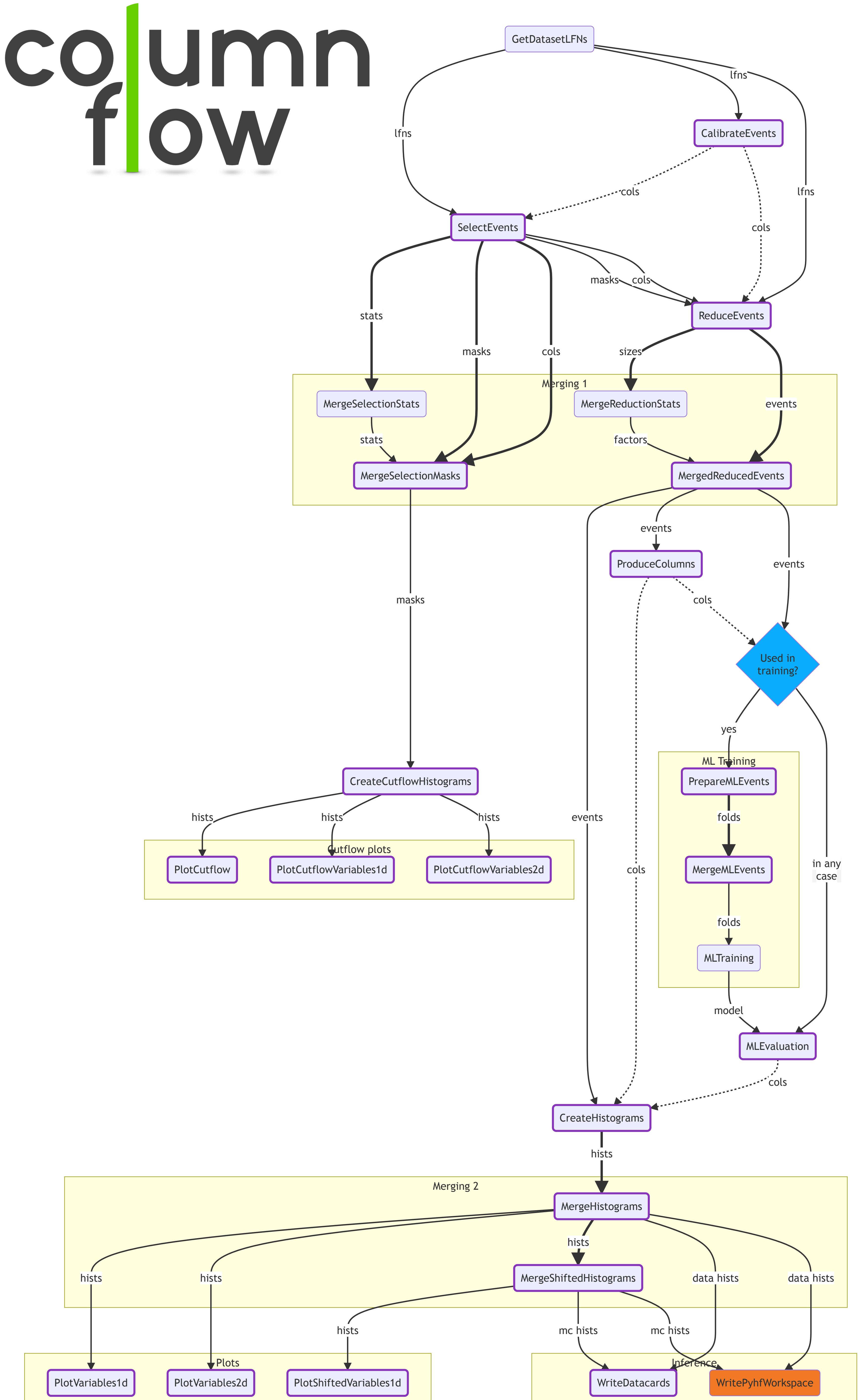
Example: Resolution of systematic uncertainties



Initial tasks

Final results

"nominal" "tune(up|down)" "jec(up|down)" "pileup(up|down)" ...



Initial tasks

Final results

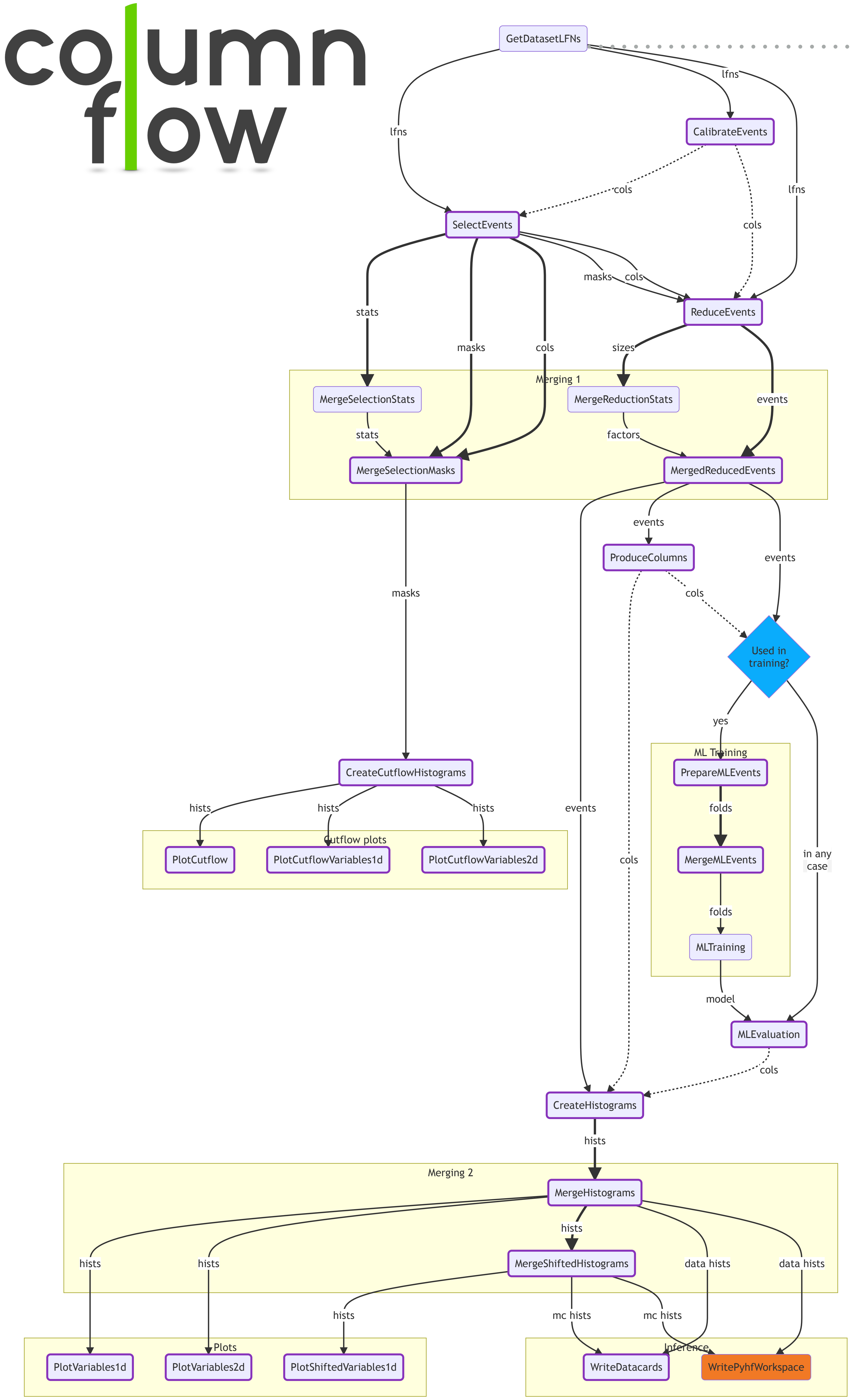
"nominal" "tune(up|down)" "jec(up|down)" "pileup(up|down)" ...

Key idea

Tasks *know* which uncertainties

- *they implement*
- they *depend on* (through upstream tasks)

columnflow



Initial tasks

Final results

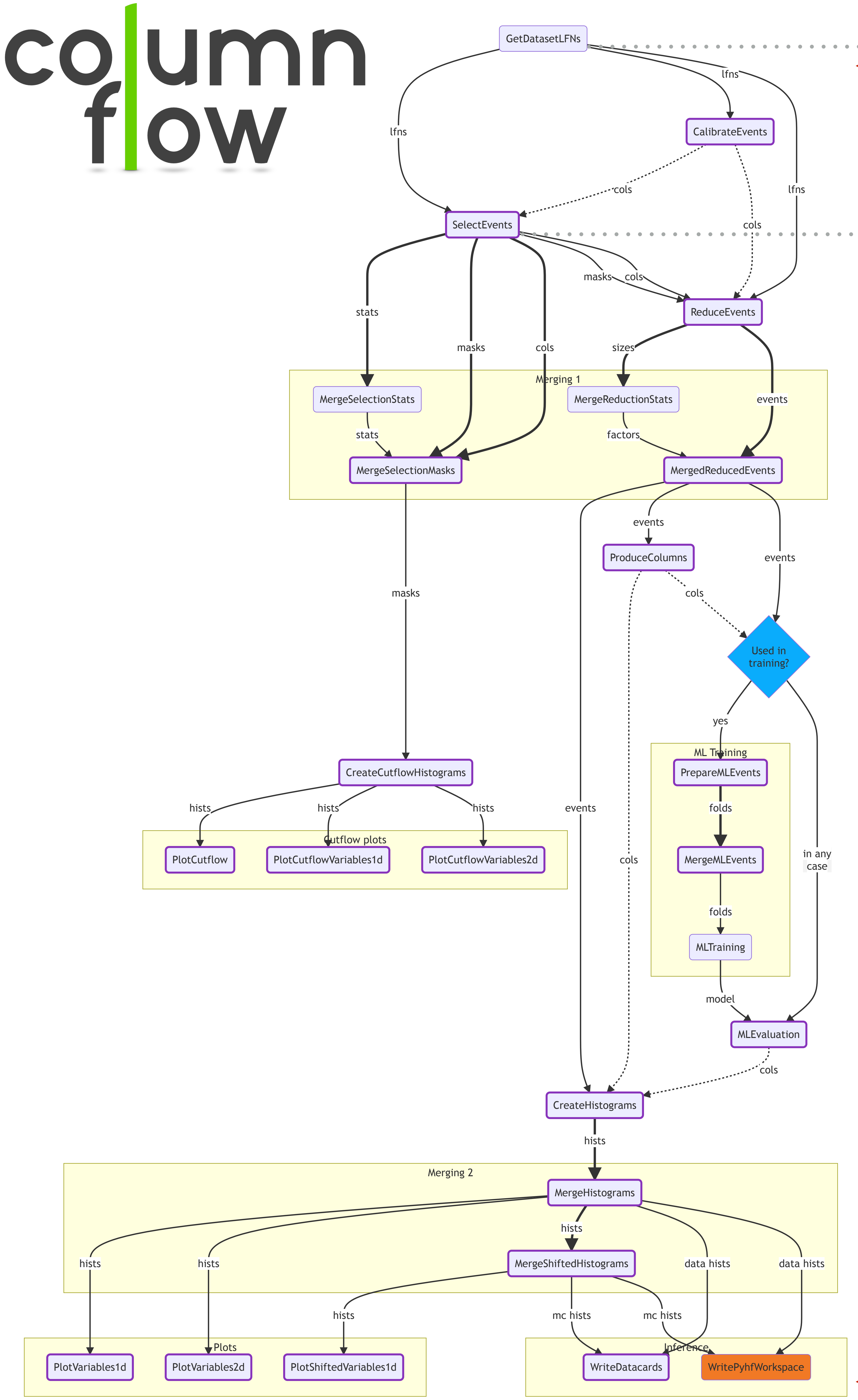
"nominal" "tune(up|down)" "jec(up|down)" "pileup(up|down)" ...

Key idea

Tasks *know* which uncertainties

- *they implement*
- they *depend on* (through upstream tasks)

columnflow



Initial tasks

reuses all "nominal" outputs above

SelectEvents

Final results

"nominal" "tune(up|down)" "jec(up|down)" "pileup(up|down)" ...

Key idea

Tasks *know* which uncertainties

- *they implement*
- they *depend on* (through upstream tasks)

Key idea

Tasks *know* which uncertainties

- *they implement*
- they *depend on* (through upstream tasks)