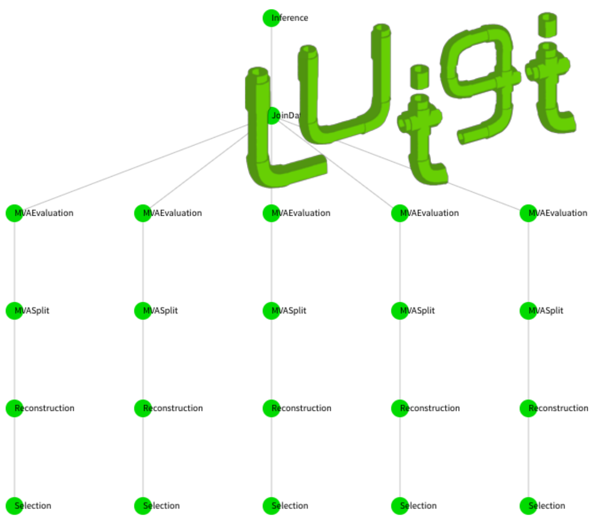
law

luigi analysis workflow



Design Pattern for Analysis Automation on Interchangeable, Distributed Resources using **L**uigi **A**nalysis **W**orkflows

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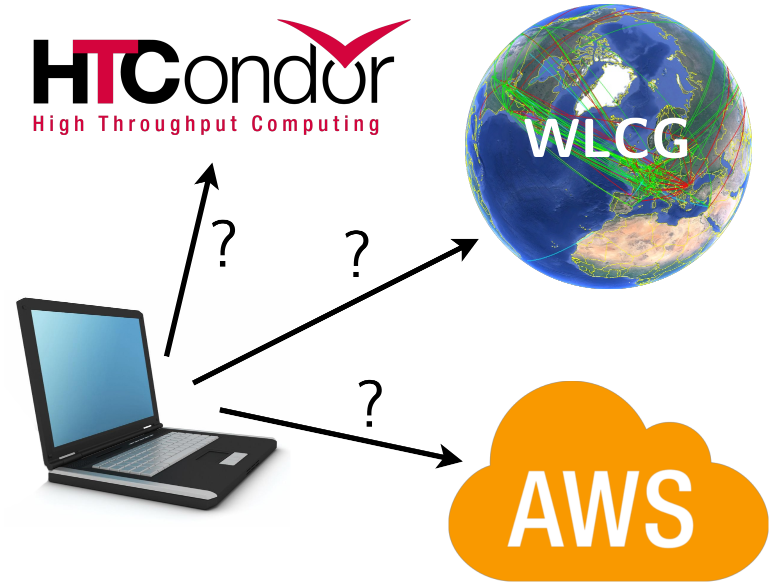
14.03.2019

GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

RWTH AACHEN UNIVERSITY

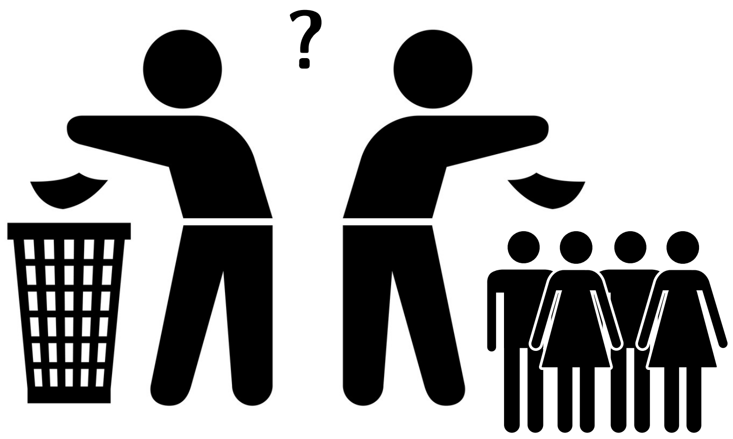
Motivational questions

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



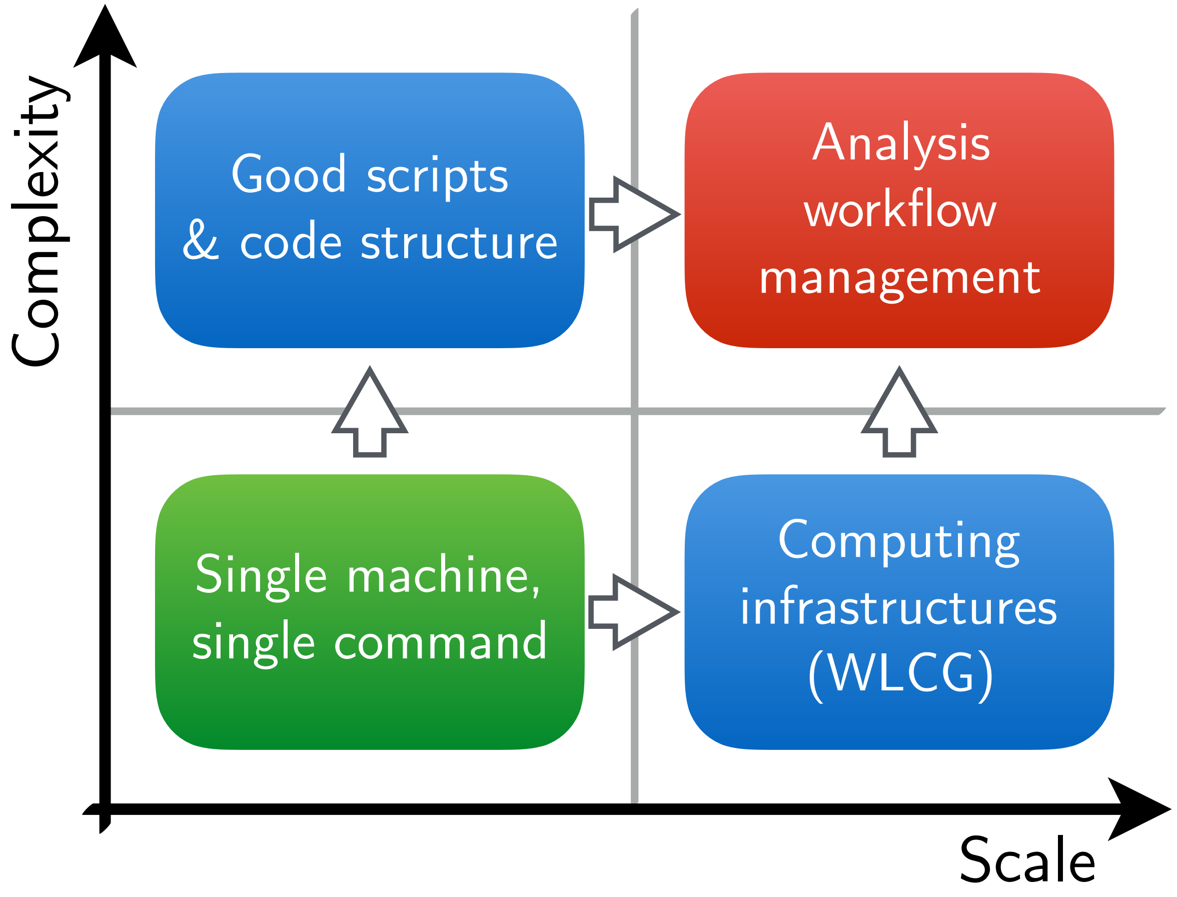
- **Reproducibility**: When a M.Sc. / PhD / Postdoc leaves, ...
  - can someone else run the analysis?
  - is there a loss of information? Is a new *framework* required?
    - ▷ Dependencies often only exist in the physicists head!

- **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!



- Scale: measure of resource consumption and amount of data
- Complexity: measure of granularity and inhomogeneity of workloads

- Future analyses likely to be large and complex, bottlenecks:
  - Undocumented structure & requirements between workloads, only exists in the physicist's head
  - Bookkeeping of data, revisions, ...
  - Manual execution/steering of jobs
  - Error-prone & time-consuming

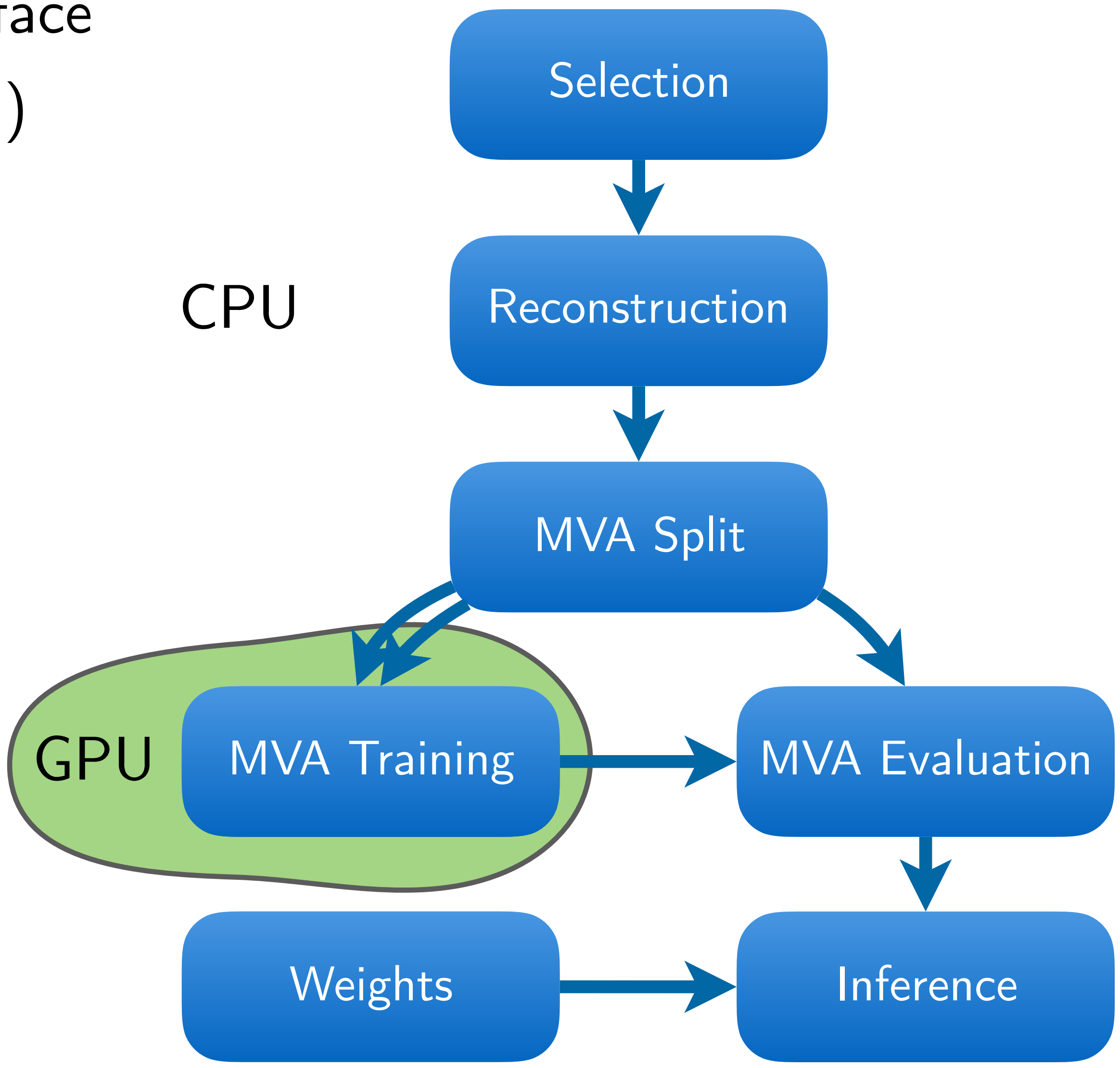

Complexity
Good scripts & code structure
Analysis workflow management
Single machine, single command
Computing infrastructures (WLCG)
Scale

→ Analysis workflow management essential for future measurements!

Abstraction: analysis workflows

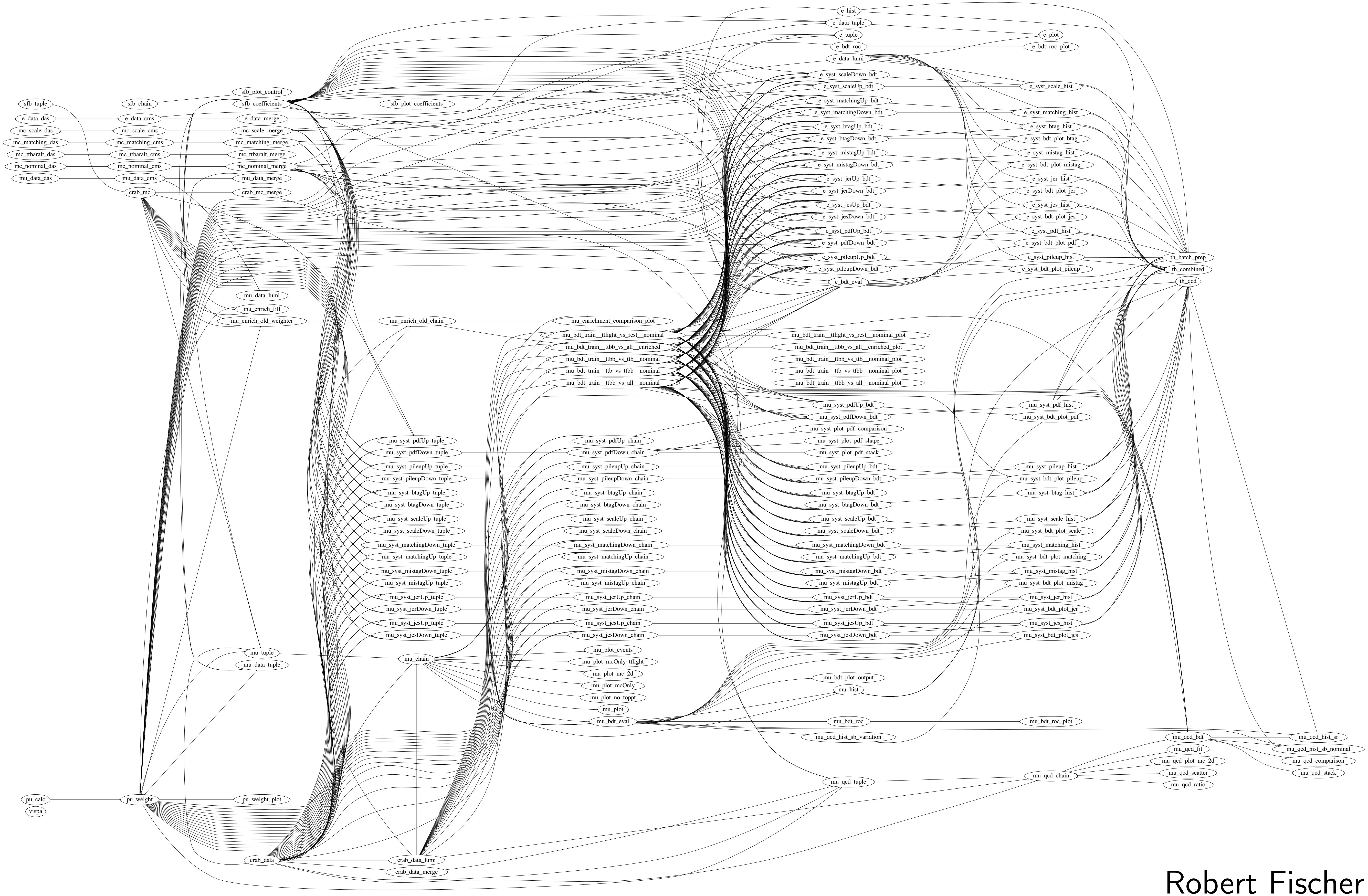
- Workflow, decomposable into particular workloads
- Workloads related to each other by common interface
  - In/outputs define directed acyclic graph (DAG)
- Alter default behavior via parameters
- Computing resources
  - Run location (CPU, GPU, WLCG, ...)
  - Storage location (local, dCache, EOS, ...)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

Example



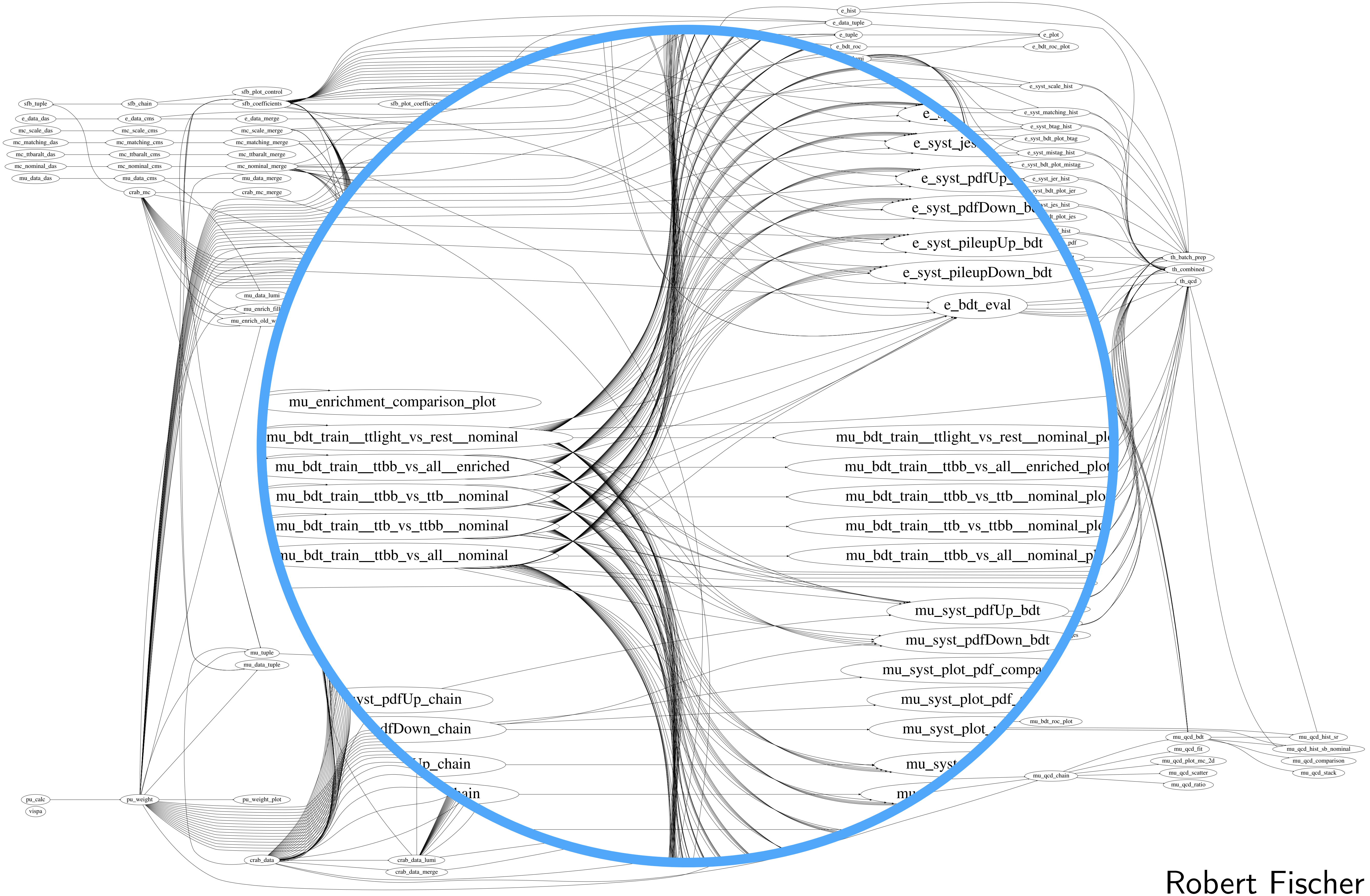
→ Reads like a checklist for analysis workflow management

Example: ttbb cross section measurement



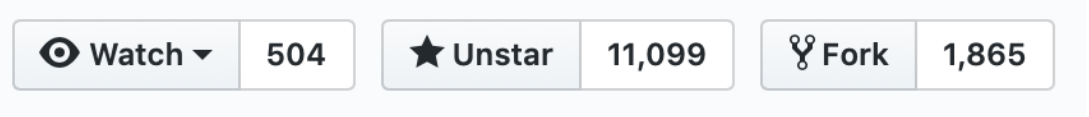
Robert Fischer

Example: ttbb cross section measurement



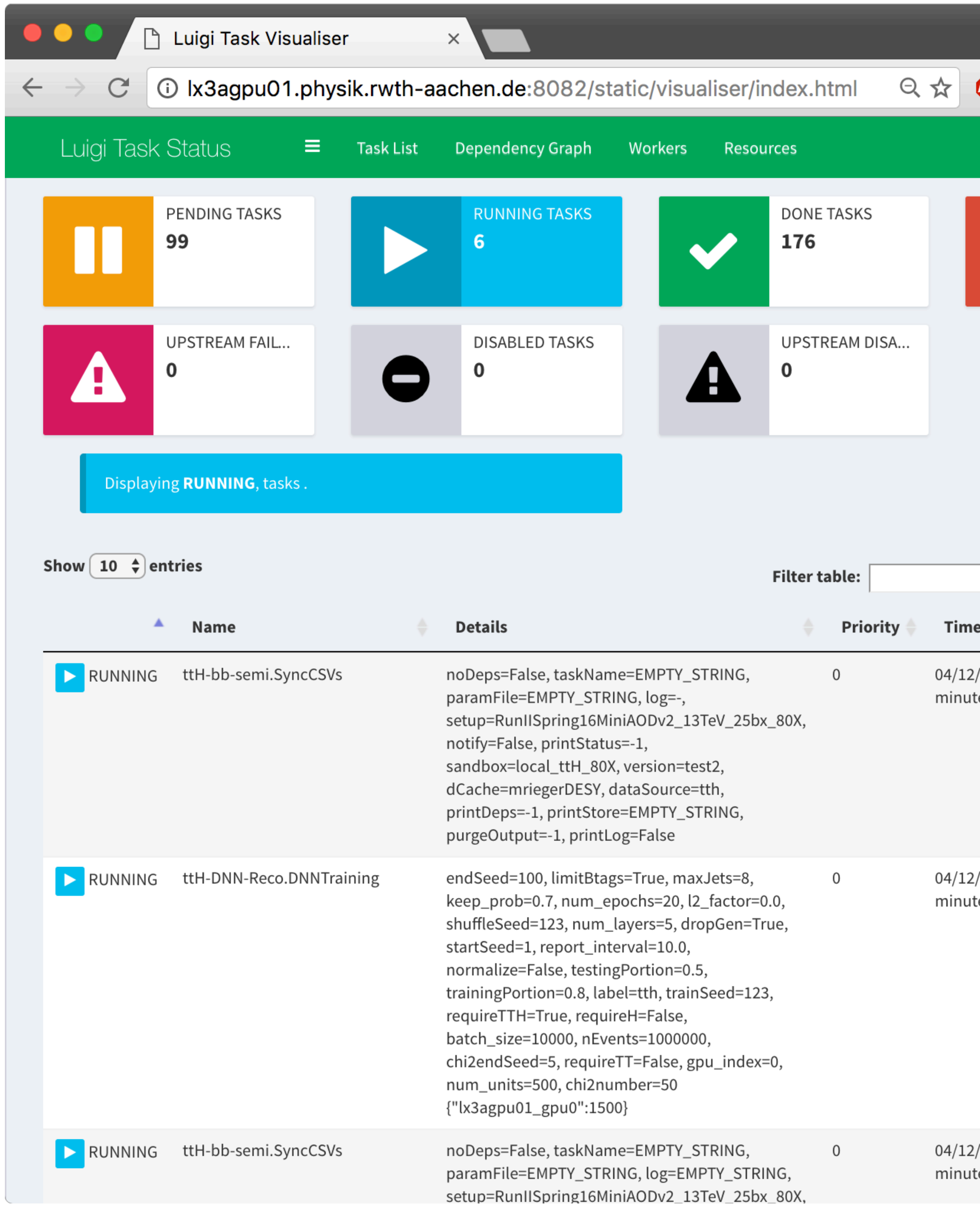
Robert Fischer

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



Building blocks

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



Displaying **RUNNING**, tasks .

	Name	Details	Priority	Time
RUNNING	ttH-bb-semi.SyncCSVs	noDeps=False, taskName=EMPTY_STRING, paramFile=EMPTY_STRING, log=-, setup=RunIISpring16MiniAODv2_13TeV_25bx_80X, notify=False, printStatus=-1, sandbox=local_ttH_80X, version=test2, dCache=mriegerDESY, dataSource=tth, printDeps=-1, printStore=EMPTY_STRING, purgeOutput=-1, printLog=False	0	04/12/ minut

RUNNING	ttH-DNN-Reco.DNNTraining	endSeed=100, limitBtags=True, maxJets=8, keep_prob=0.7, num_epochs=20, l2_factor=0.0, shuffleSeed=123, num_layers=5, dropGen=True, startSeed=1, report_interval=10.0, normalize=False, testingPortion=0.5, trainingPortion=0.8, label=tth, trainSeed=123, requireTTH=True, requireH=False, batch_size=10000, nEvents=1000000, chi2endSeed=5, requireTT=False, gpu_index=0, num_units=500, chi2number=50
		{"lx3agpu01_gpu0":1500}
			0	04/12/
				minut

RUNNING	ttH-bb-semi.SyncCSVs	noDeps=False, taskName=EMPTY_STRING, paramFile=EMPTY_STRING, log=EMPTY_STRING, setup=RunIISpring16MiniAODv2_13TeV_25bx_80X,	0	04/12/ minut

- Web interface, error handling, command line tools, task history, collaborative features, …
- github.com/spotify/luigi

7 Luigi in a nutshell

```
# reco.py

import luigi

from analysis.ttH.tasks import Selection

class Recontruction(luigi.Task):

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


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

    def output(self):
        return luigi.LocalTarget("reco_%s.root" % self.dataset)

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

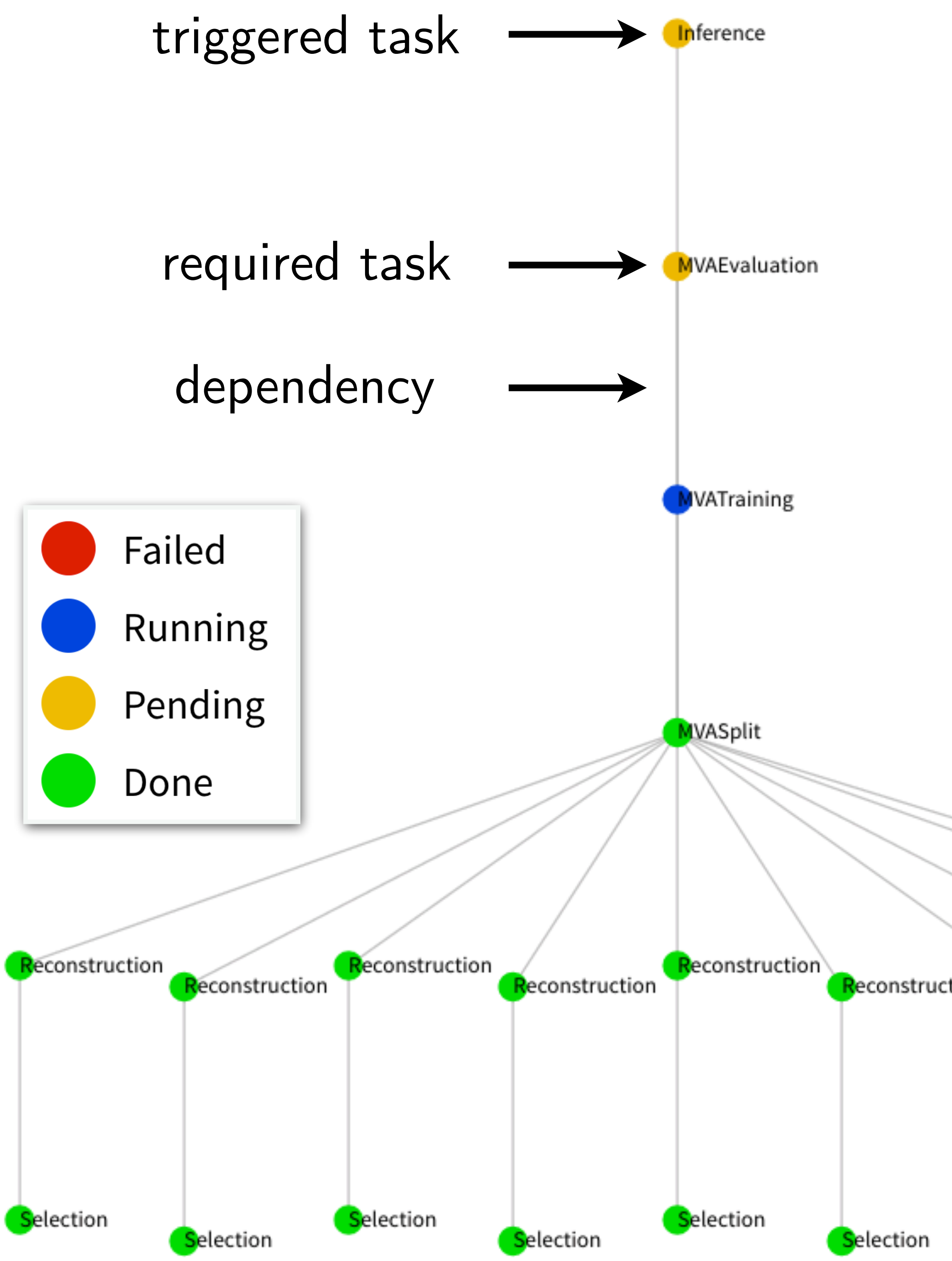
```
> python reco.py Reconstruction --dataset ttJets
```

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 when all output targets of a task exist

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



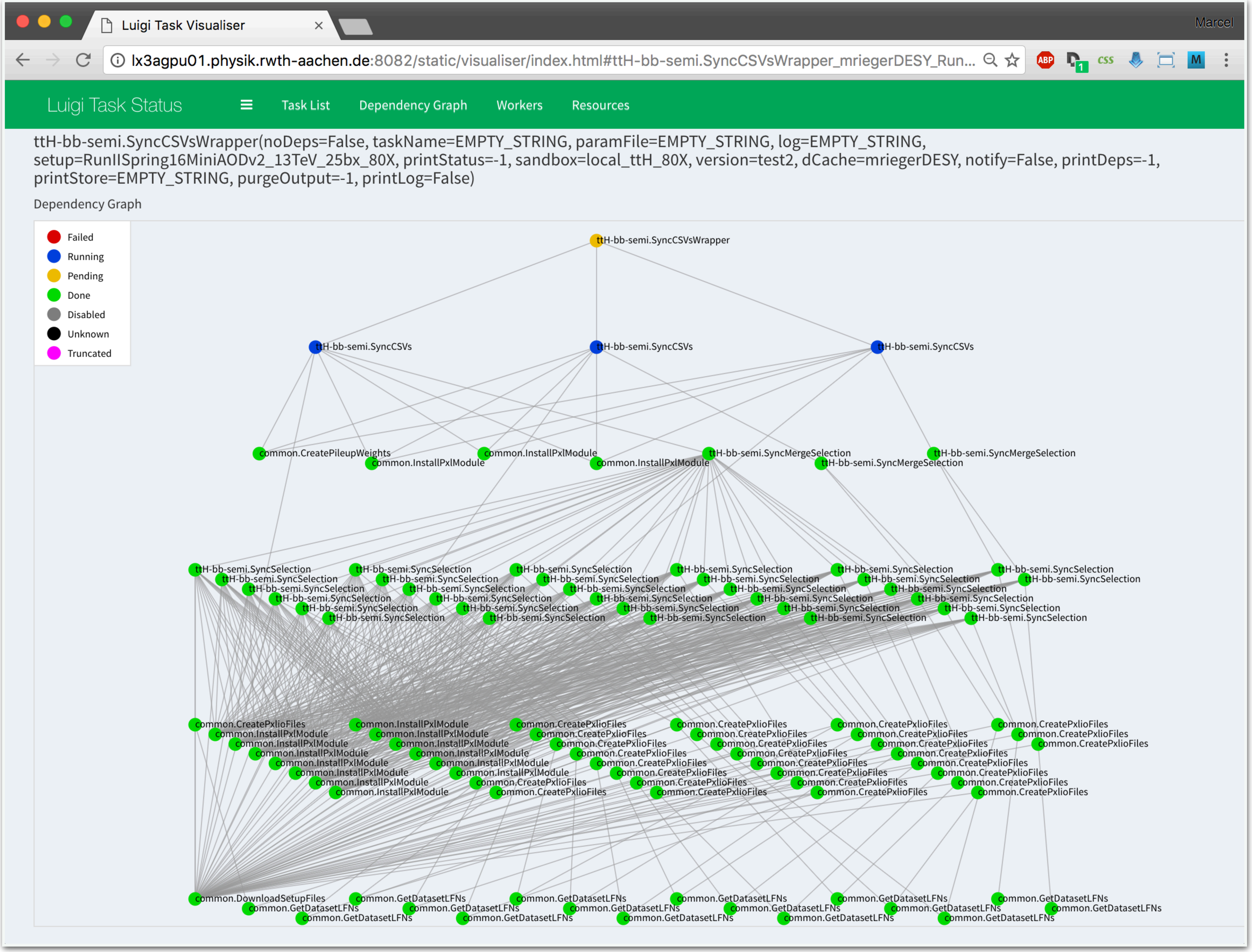
triggered task

required task

dependency

🔴 Failed
🔵 Running
🟡 Pending
🟢 Done

9 Example trees

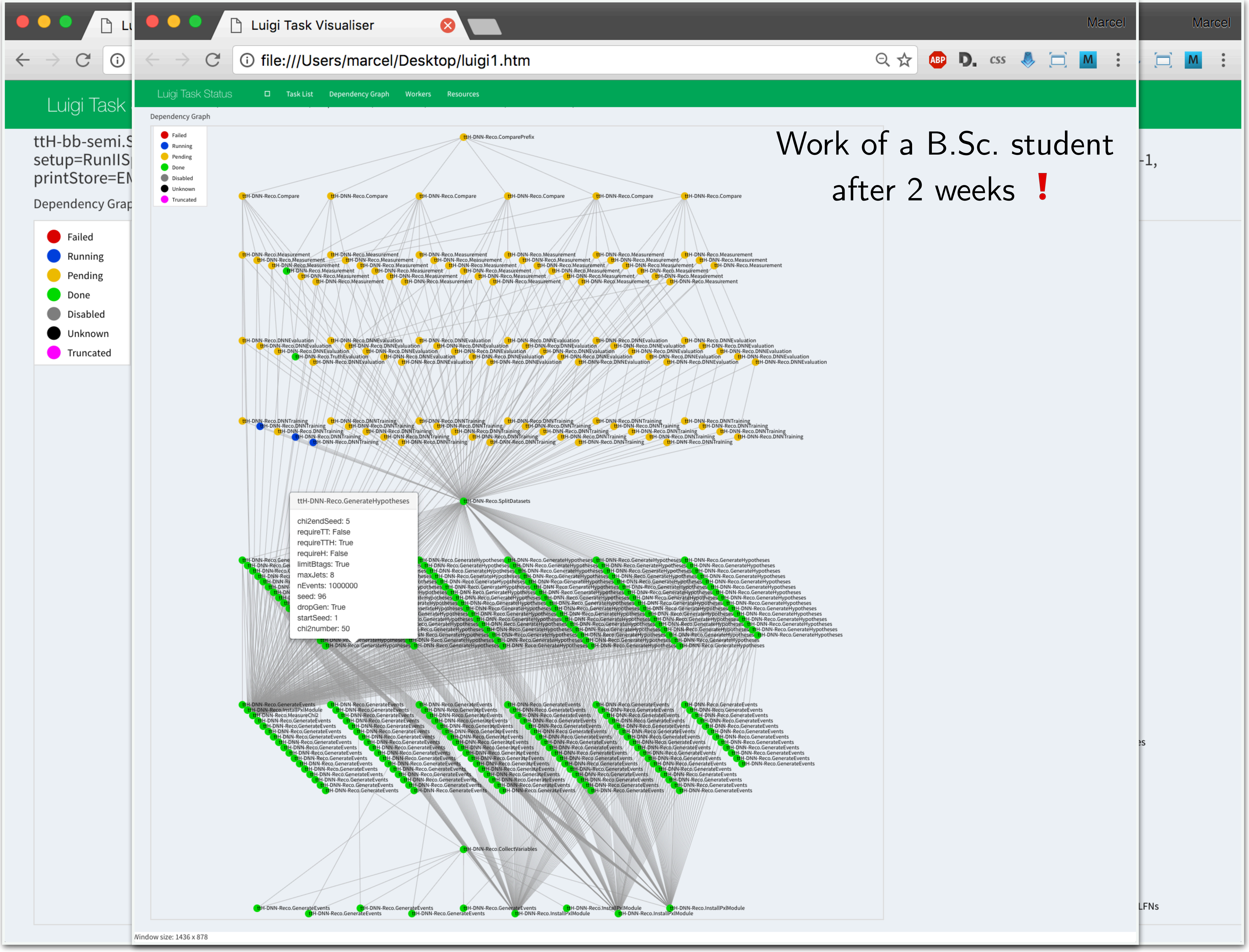


Luigi Task Visualiser
Marcel
lx3agpu01.physik.rwth-aachen.de:8082/static/visualiser/index.html#ttH-bb-semi.SyncCSVsWrapper_mriegerDESY_Run...
Luigi Task Status
Task List
Dependency Graph
Workers
Resources

ttH-bb-semi.SyncCSVsWrapper(noDeps=False, taskName=EMPTY_STRING, paramFile=EMPTY_STRING, log=EMPTY_STRING, setup=RunIISpring16MiniAODv2_13TeV_25bx_80X, printStatus=-1, sandbox=local_ttH_80X, version=test2, dCache=mriegerDESY, notify=False, printDeps=-1, printStore=EMPTY_STRING, purgeOutput=-1, printLog=False)

Dependency Graph

9 Example trees



Luigi Task Visualiser

file:///Users/marcel/Desktop/luigi1.htm

Luigi Task Status □ Task List Dependency Graph Workers Resources

Dependency Graph

● Failed
● Running
● Pending
● Done
● Disabled
● Unknown
● Truncated

ttH-DNN-Reco.GenerateHypotheses

chi2endSeed: 5
requireTT: False
requireTTH: True
requireH: False
limitBtags: True
maxJets: 8
nEvents: 1000000
seed: 96
dropGen: True
startSeed: 1
chi2number: 50

Window size: 1436 x 878

Marcel
ttH-DNN-Reco.ComparePrefix
ttH-DNN-Reco.Compare
ttH-DNN-Reco.Measurement
ttH-DNN-Reco.DNNEvaluation
ttH-DNN-Reco.TruthEvaluation
ttH-DNN-Reco.DNNTraining
ttH-DNN-Reco.SplitDatasets
ttH-DNN-Reco.GenerateHypotheses
ttH-DNN-Reco.GenerateEvents
ttH-DNN-Reco.InstallPxlModule
ttH-DNN-Reco.MeasureChi2
ttH-DNN-Reco.CollectVariables
Luigi Task
ttH-bb-semi.S
setup=RunIIS
printStore=EM
Dependency Grap
-1,
es
LFNs

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

law

luigi analysis workflow

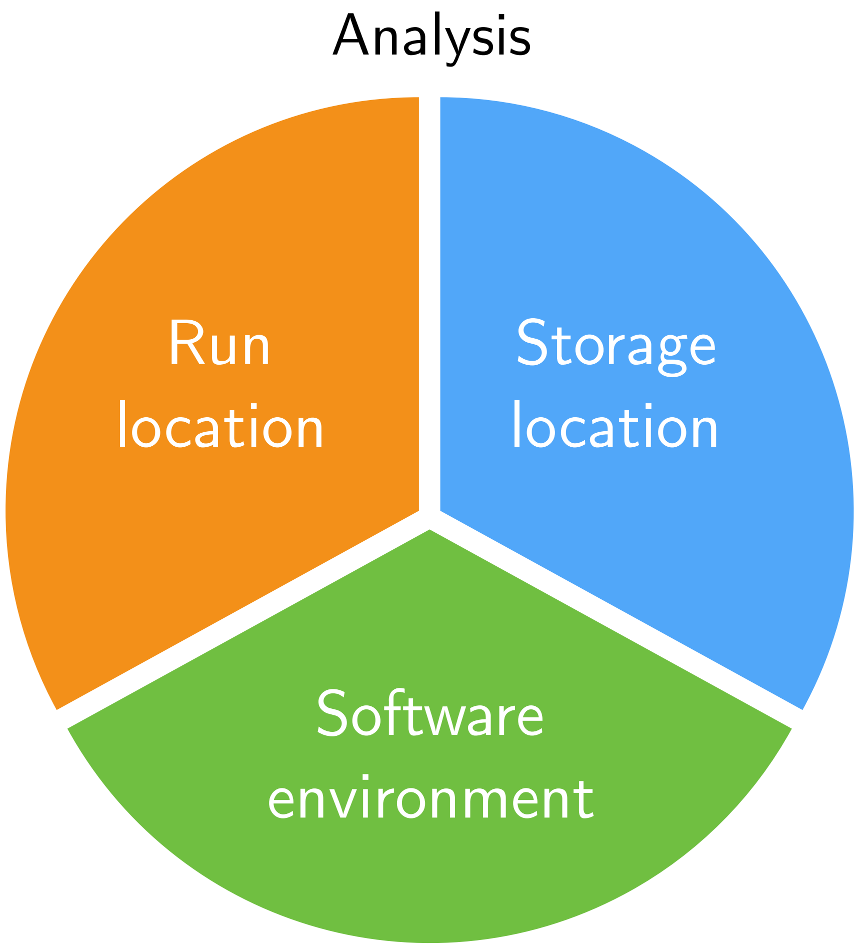
law - *luigi* analysis workflow

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

- Software design follows 2 primary goals:

  1. Scalability on HEP infrastructure (but not limited to)
  2. Decoupling of **run locations**, **storage locations** & **software environments**
     - ▹ No fixation on dedicated resources
     - ▹ All components interchangeable

- Provides a toolbox to follow an **analysis design pattern**
  - ▪ No constraint on language or data structures
  - → Not a *framework*!



law features (1)

1. Job submission

- Idea: submission built into tasks, **no need to write extra code**
- Currently supported job systems: HTCondor, LSF, gLite, ARC, (CRAB)
  - Backend not hard-coded, selectable at runtime
- Mandatory features
  - Automatic resubmission, dashboard interface
- From the htcondor_at_cern example:

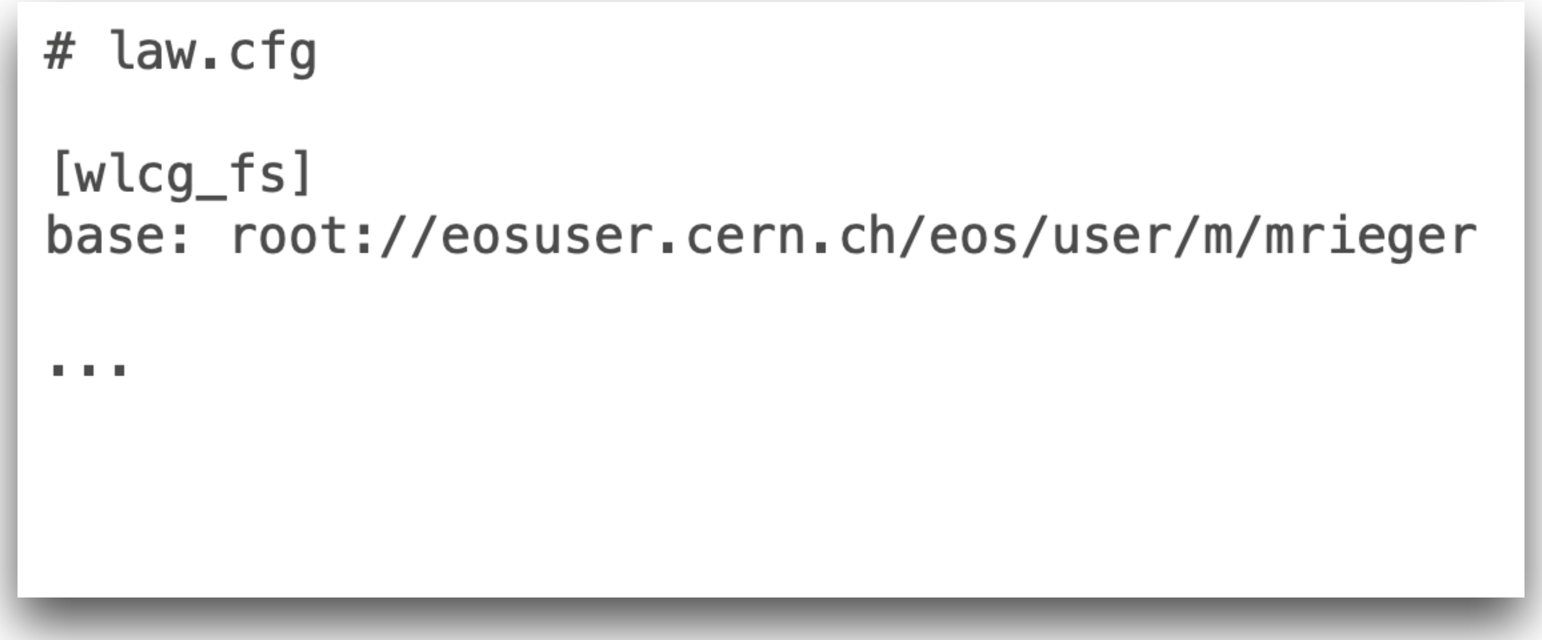
```
lxplus129:law_test > law run CreateChars --version v1 --poll-interval 0.5 --workflow htcondor
INFO: [pid 30564] Worker Worker(host=lxplus129.cern.ch, username=mrieger) running
                  CreateChars(branch=-1, start_branch=0, end_branch=26, version=v1)
going to submit 26 htcondor job(s)
submitted 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 >
```

13 *law* features (2)

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 (dCache, XRootD, GridFTP, SRM, ...) + DropBox
  - API **identical** to local targets
- Mandatory features
  - Automatic retries, local caching
- Example: working with files on EOS

"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 directories above

13 *law* features (2)

2. Remote targets

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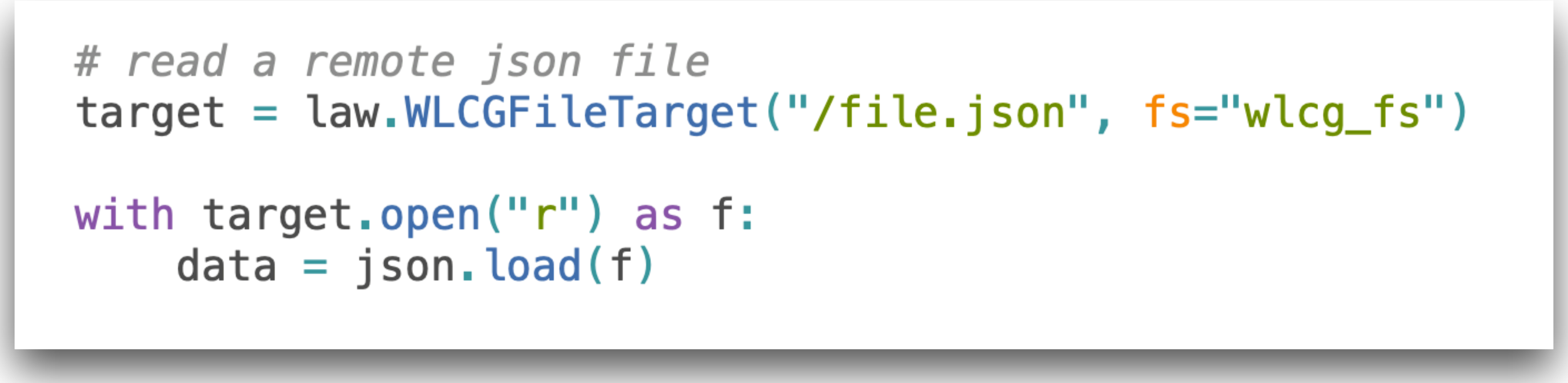
Reading remote files (json)



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

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

13 *law* features (2)

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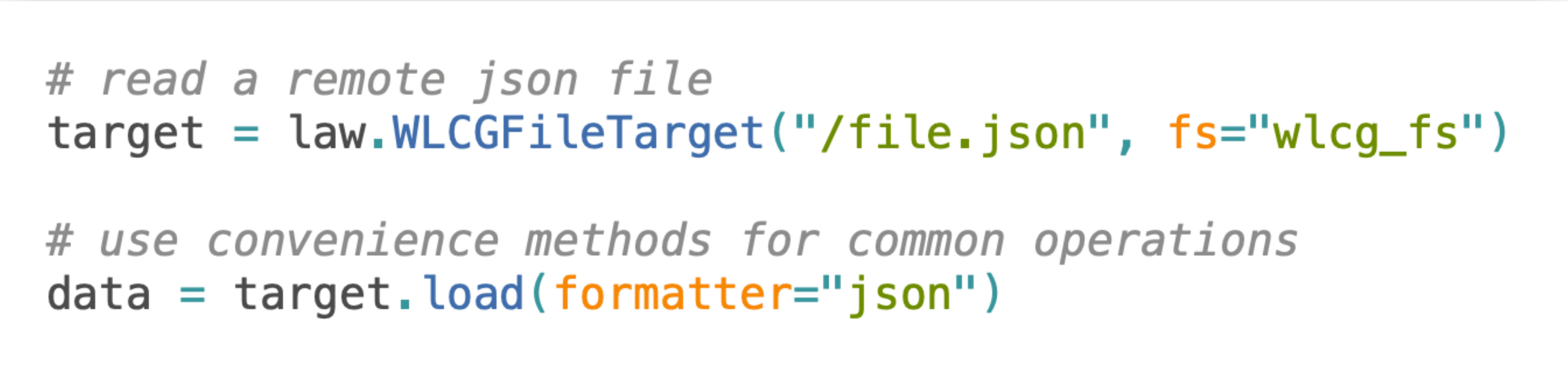
- Example: working with files on EOS

Conveniently reading remote files (json)



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

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

13 *law* features (2)

2. Remote targets

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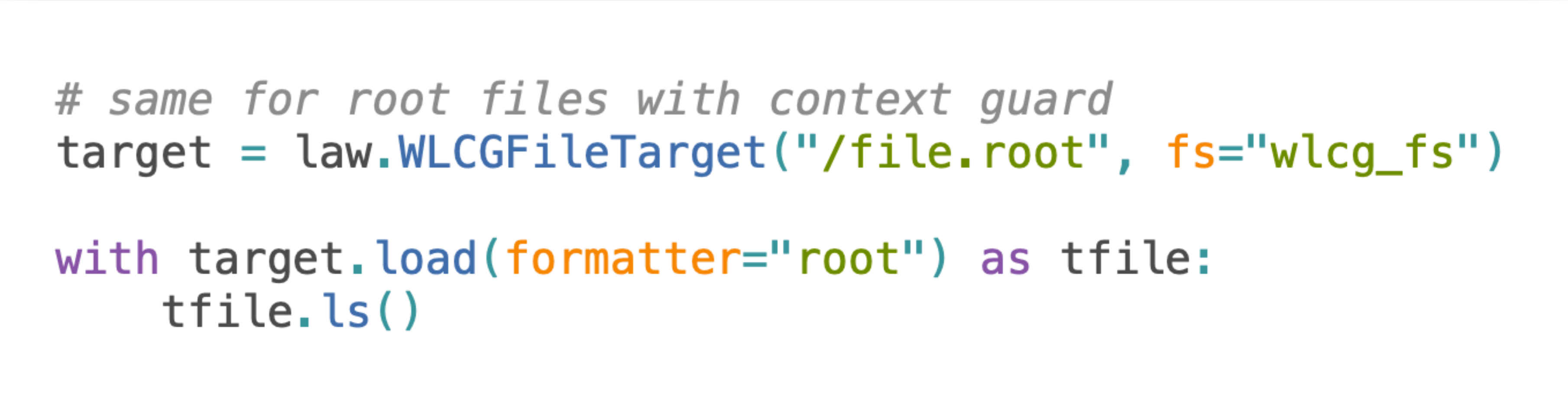
Conveniently reading remote files



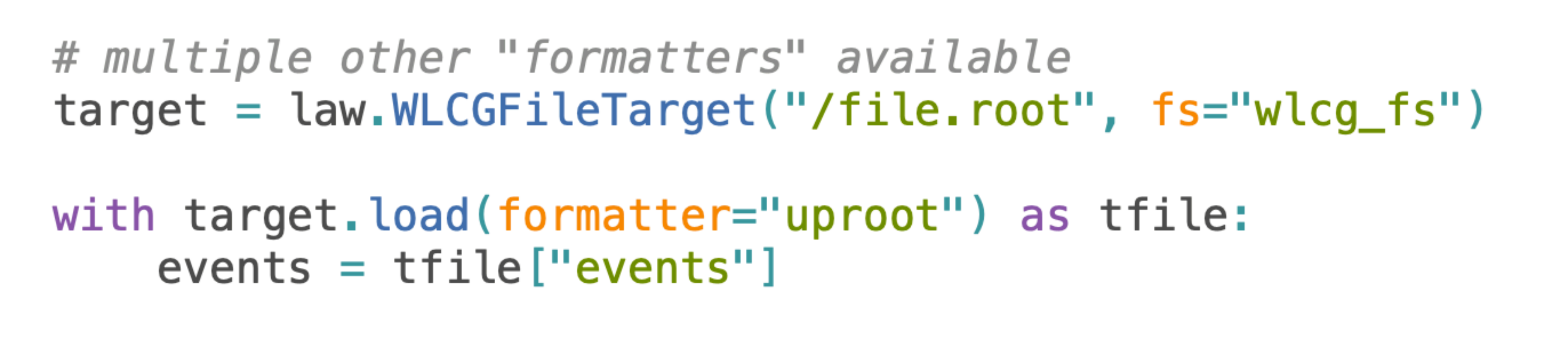
```python
# same for root files with context guard
target = law.WLCGFileTarget("/file.root", fs="wlcg_fs")

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

law features (2)

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 (dCache, XRootD, GridFTP, SRM, ...) + DropBox
  - API **identical** to local targets
- Mandatory features
  - Automatic retries, local caching
- Example: working with files on EOS

Conveniently reading remote files



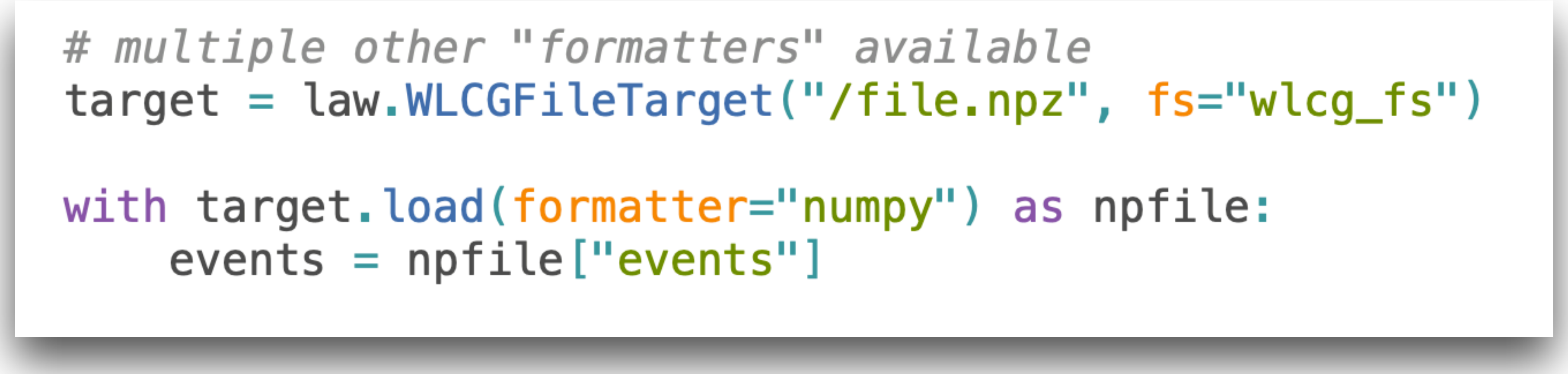
```python
# multiple other "formatters" available
target = law.WLCGFileTarget("/file.root", fs="wlcg_fs")

with target.load(formatter="uproot") as tfile:
    events = tfile["events"]
```

13 *law* features (2)

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 (dCache, XRootD, GridFTP, SRM, ...) + DropBox
  - ▹ API **identical** to local targets
- Mandatory features
  - ▹ Automatic retries, local caching
- Example: working with files on EOS

Conveniently reading remote files



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

with target.load(formatter="numpy") as npfile:
    events = npfile["events"]
```

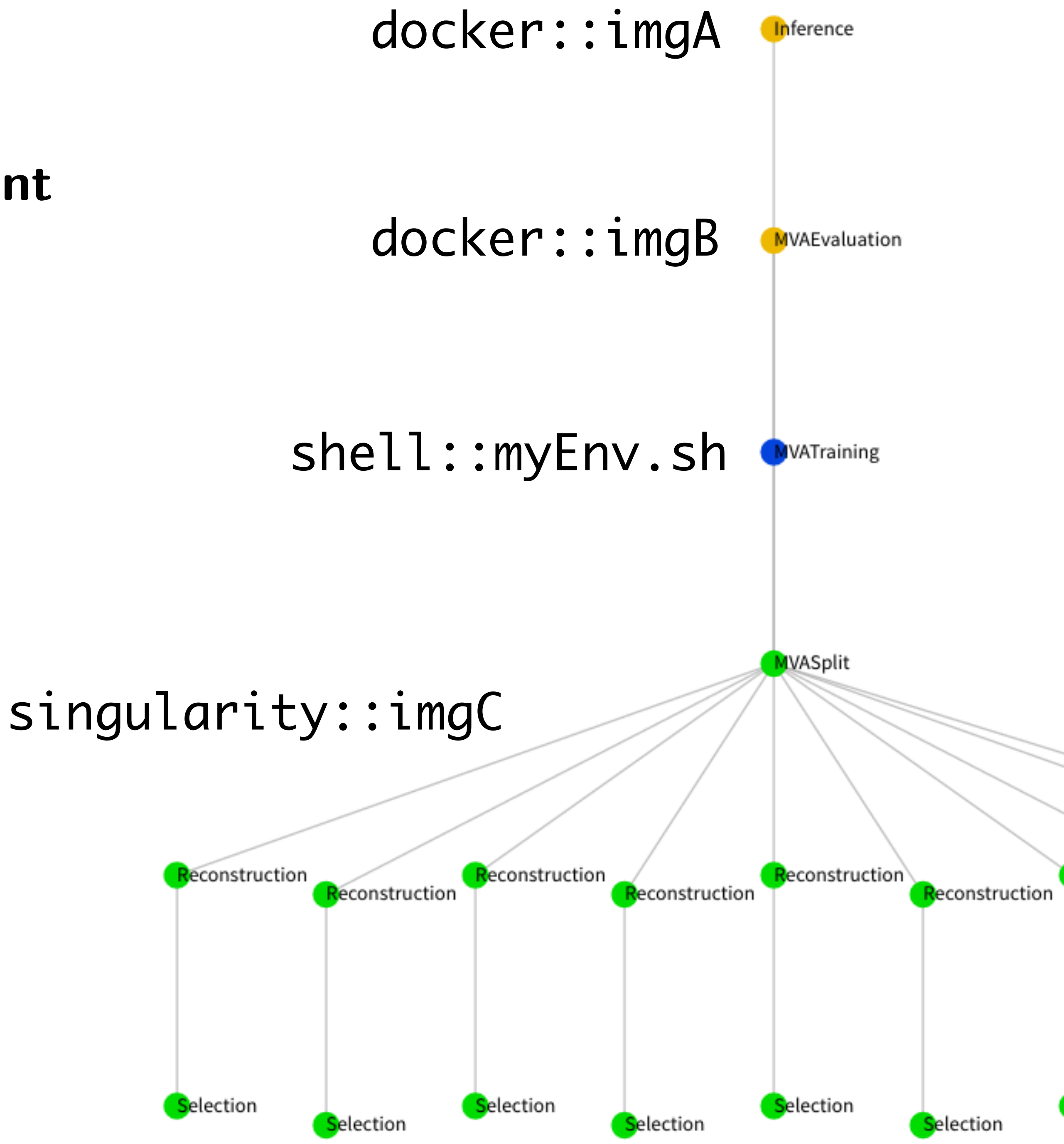
law features (3)

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
  - ▹ Docker images
  - ▹ Singularity images



docker::imgA

docker::imgB

shell::myEnv.sh

singularity::imgC

Singularity

15 *law* in action

```python
# reco.py

import luigi

from analysis.ttH.tasks import Selection

class Recontruction(luigi.Task):

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


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

    def output(self):
        return luigi.LocalTarget("reco_%s.root" % self.dataset)

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

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

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

15 *law* in action

```python
# reco.py

import luigi
import law
from analysis.ttH.tasks import Selection

class Recontruction(law.Task):

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


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

    def output(self):
        return law.LocalFileTarget("reco_%s.root" % self.dataset)

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

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

```
> law run Reconstruction --dataset ttJets
```

15 *law* in action

```python
# reco.py

import luigi
import law
from analysis.ttH.tasks import Selection

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

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


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

    def output(self):
        return law.LocalFileTarget("reco_%s.root" % self.dataset)

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

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

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

15 *law* in action

```python
# reco.py

import luigi
import law
from analysis.ttH.tasks import Selection

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

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


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

    def output(self):
        return law.WLCGFileTarget("reco_%s.root" % self.dataset, fs="eos")

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

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

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

law in action

```
# reco.py

import luigi
import law
from analysis.ttH.tasks import Selection

class Recontruction(law.SandboxTask, law.HTCondorWorkflow):

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

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

    def output(self):
        return law.WLCGFileTarget("reco_%s.root" % self.dataset, fs="eos")

    def run(self):
        inp = self.input()  # this is "output()" of Selection
        outp = self.output()

        # run the reconstruction based on "inp" to create "outp"
```

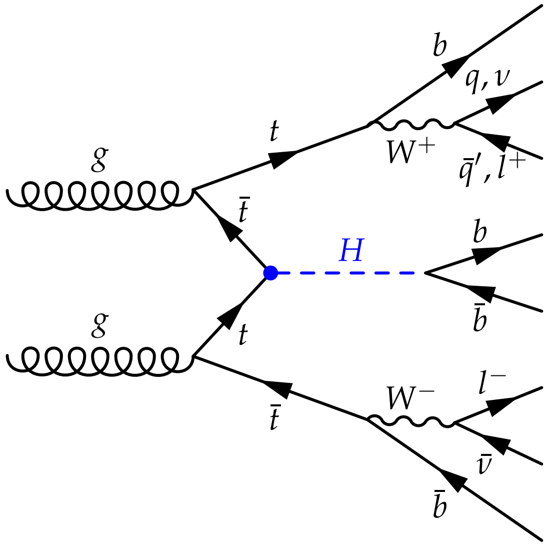
- ☑ luigi task
- ☑ law task
- ☑ Run on HTCondor
- ☑ Store on EOS
- ☑ Run in docker

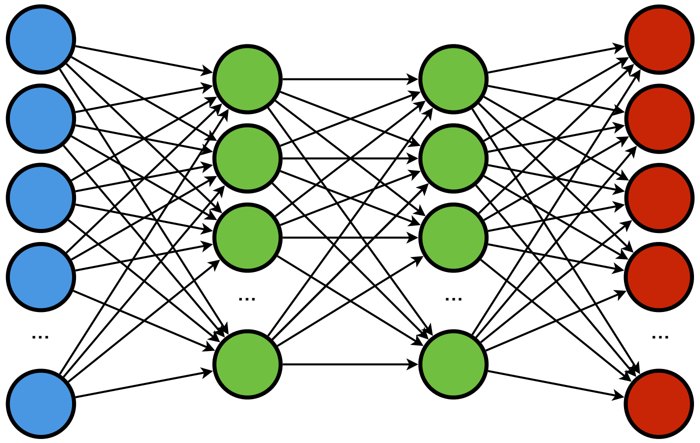
```
> law run Reconstruction --dataset ttJets --workflow htcondor
```

Successful applications

- ttH analysis at CMS (JHEP 03 (2019) 026)
  - Large-scale:
    - ~100 TB of storage, ~500k tasks
  - Complex:
    - DNNs/BDTs/MEM
    - ~80 systematic variations
  - Distributed:
    - 7 CEs, (GPU) clusters, local machines
    - 2 SEs (dCache), local disk, Dropbox, CERNBox
  - Clear separation of duties within group
  - Entire analysis operable by everyone at any time

- DeepCSV + DeepJet b-tagging scale factors at CMS
- Multiple theses





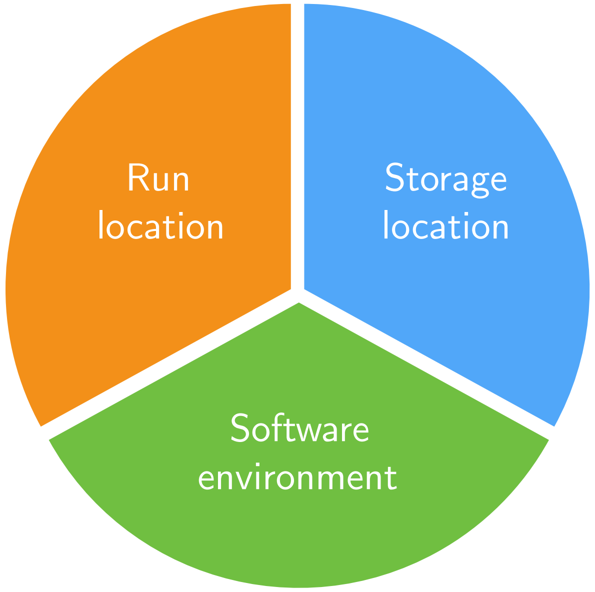
Summary

- HEP analyses likely to increase in scale and complexity
  - Analysis workflow management **essential**
  - Need for toolbox providing a design pattern, **not a framework**

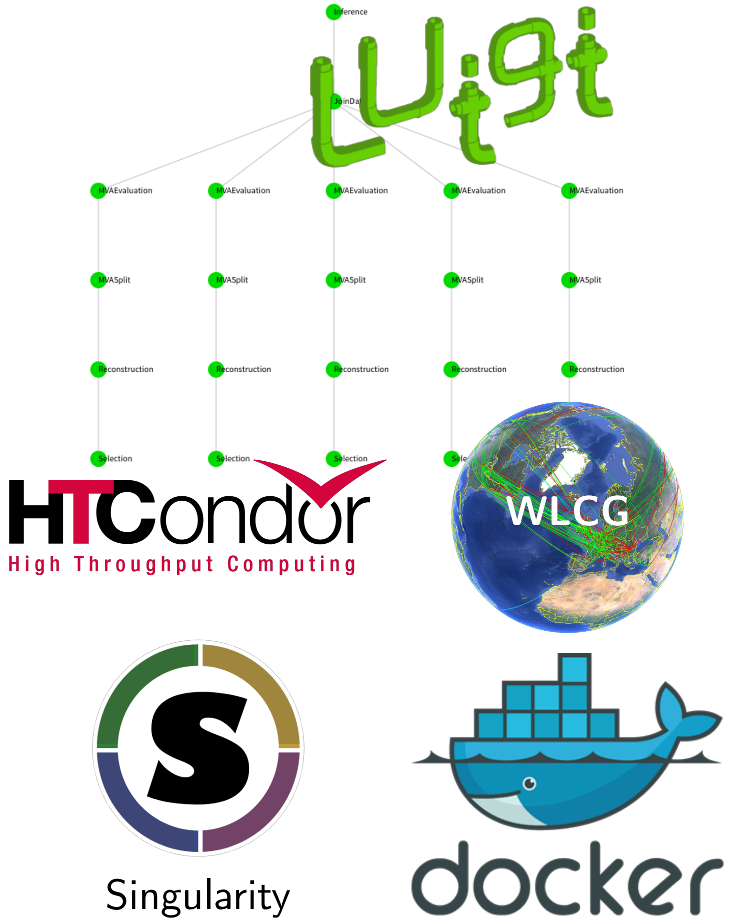
- Luigi is able to model even complex workflows
- Law adds convenience & scalability in the HEP context

- **All** information transparently encoded in tasks, targets & dependencies
- Aim for out-of-the-box preservation

- github.com/riga/law, law.readthedocs.io



law
luigi analysis workflow



Backup

Links

- *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

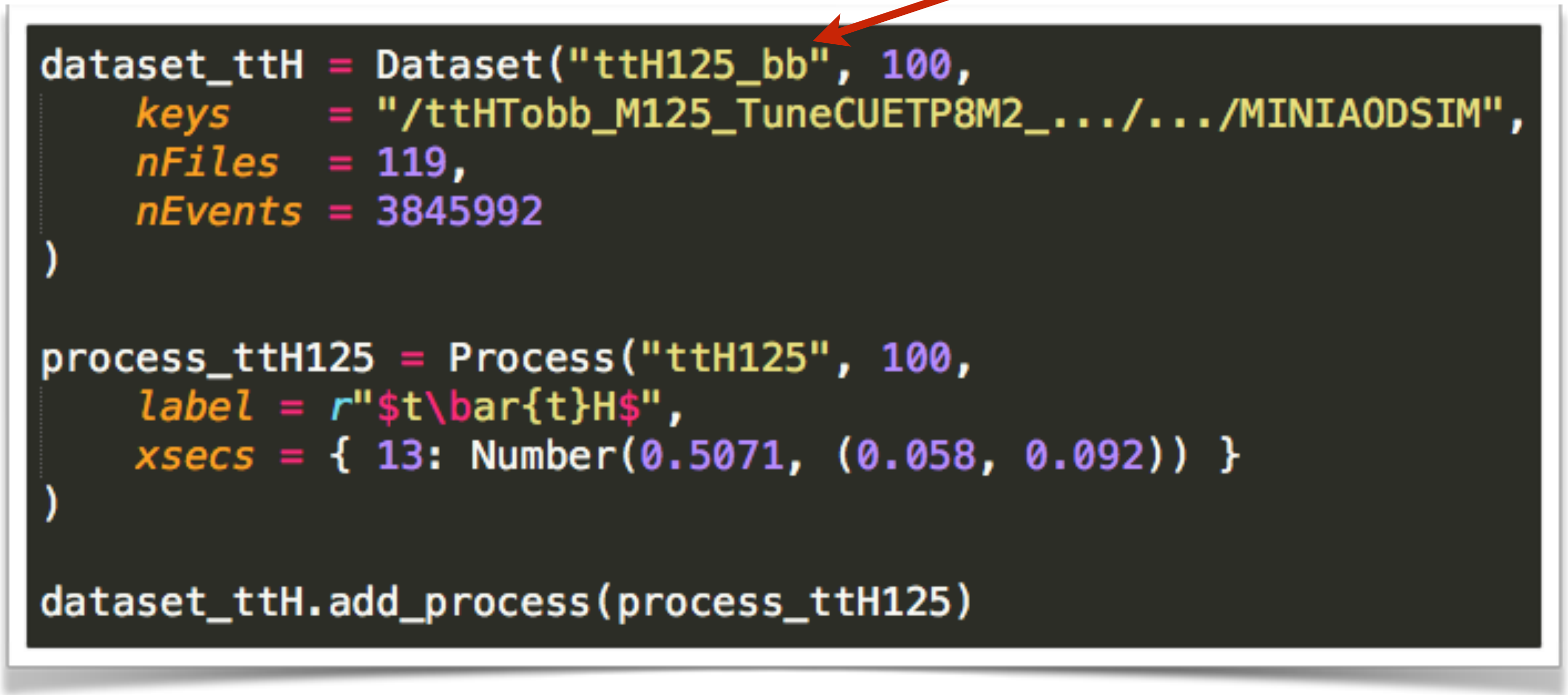
order: structure external HEP data

order

github.com/riga/order

- Pythonic class collection to order “soft”, external HEP data
  - physics processes & cross sections
  - campaigns & datasets
  - channels & categories
  - variables & systematics
- Some data could be centrally managed, some is analysis specific
- Run the example: launch binder
- Use as data backend:

```
> law run Reconstruction --dataset ttH125_bb --...
```



```
dataset_ttH = Dataset("ttH125_bb", 100,
    keys    = "/ttHTobb_M125_TuneCUETP8M2_.../.../MINIAODSIM",
    nFiles  = 119,
    nEvents = 3845992
)

process_ttH125 = Process("ttH125", 100,
    label = r"$t\bar{t}H$",
    xsecs = { 13: Number(0.5071, (0.058, 0.092)) }
)

dataset_ttH.add_process(process_ttH125)
```

Thoughts on HEP analyses

- What is a *framework*?
  - → Bash scripts, python tools, crab configs, CMSSW modules, magic
  - → Connections mostly exist in the physicists head

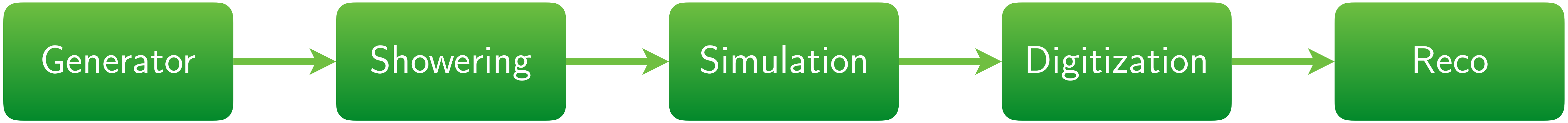
- Documentation?
  - → Not the most beloved hobby in the physics community

- When a M.Sc. / PhD / Postdoc leaves ...
  - → Can someone else run the analysis?
  - → Is this information lost? Is a new framework required?

- Does execution dictate code design?
  - → Does the analysis depend on where it runs?

- From *my* experience: ⅔ of time required for technicalities, ⅓ for physics
  - → Physics output doubled if it was the other way round?

Existing WMS: MC production

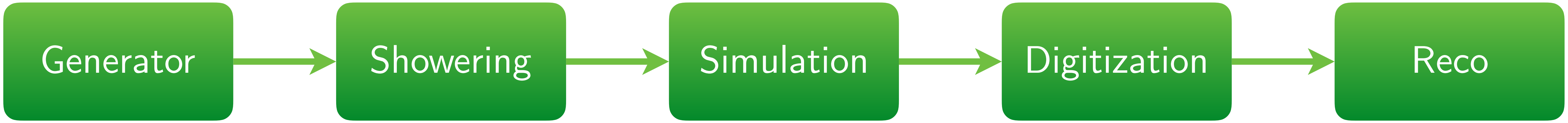


Tailored systems

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

→ Requirements for HEP analyses mostly orthogonal

Existing WMS: MC production



Generator → Showering → Simulation → Digitization → Reco

Tailored systems

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

Wishlist for end-user analyses

- Structure “iterative”, a-priori unknown
- Dynamic workflows, fast R&D cycles
- Tree design, arbitrary dependencies
- Incorporate existing infrastructure
- Use custom software, everywhere

→ Requirements for HEP analyses mostly orthogonal

WMS comparison

	Existing WMS e.g. MC Management	Generic Analysis WMS
Development Process	final objective known in advance	iterative, final composition a priori unknown
Workflow Structure	chain structure, mostly one-dimensional	tree structure, arbitrarily branched
Evolution	static over time, recurrent execution	dynamic, fast R&D cycles
Infrastructure	specially tailored, e.g. storage systems, DBs	incorporate existing, quickly adapt to changes
Applicability	tuned to particular use case	flexible, able to model every possible workflow

→ Existing WMS highly specialized for designated use case

→ Requirements for HEP analyses mostly orthogonal

Achievements

1. Toolbox providing building blocks for analyses
   - → Design pattern, **not a framework** (no constraint on language or data structure)
   - → Full decoupling of run locations, storage locations and software environments

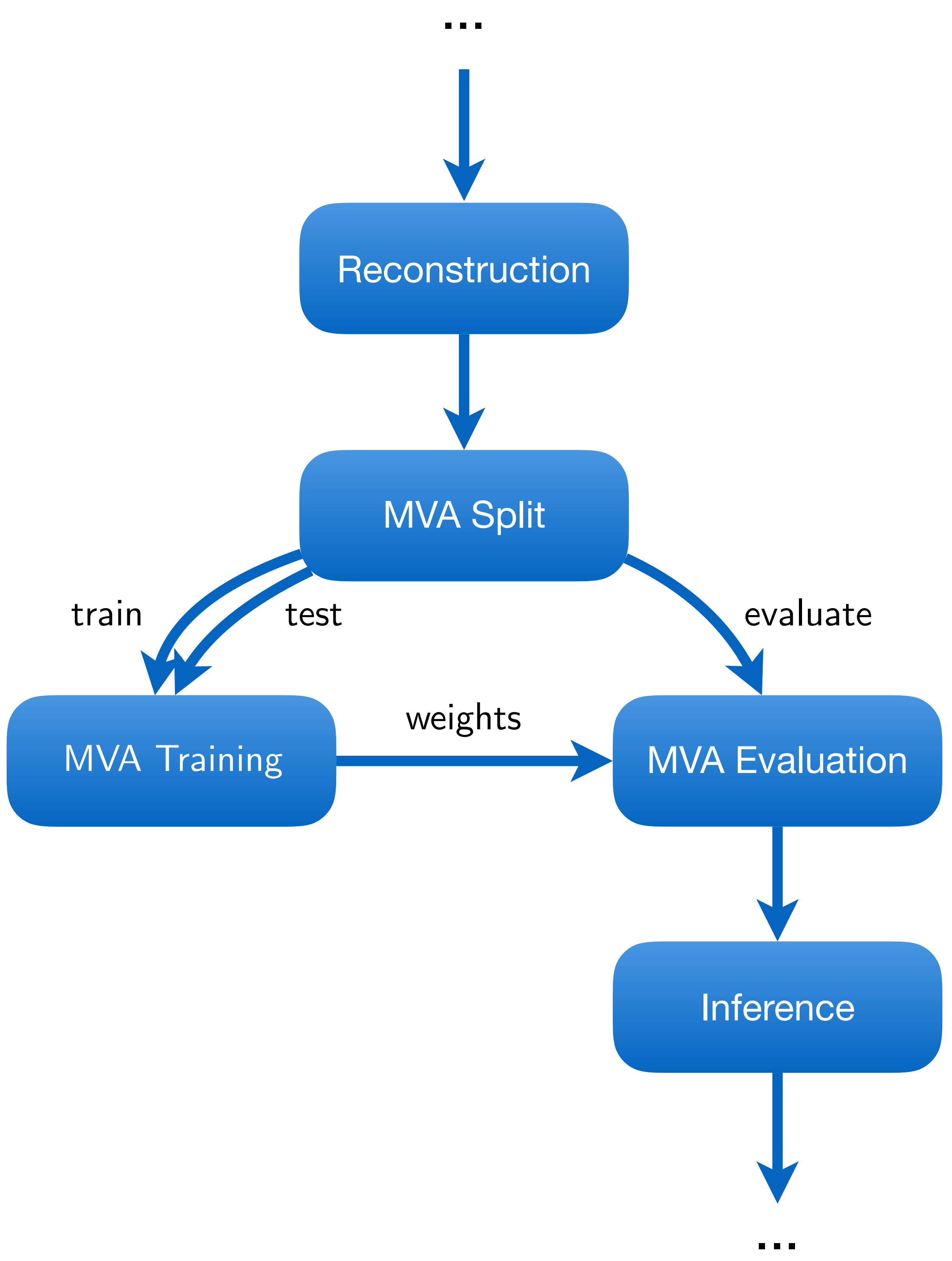
2. **All** information transparently encoded in tasks, targets & dependencies
   - → Results **reproducible** by developer, groups, collaboration, ...
   - → Analysis preservation out-of-the-box

3. make-like execution across distributed resources
   - → Reduces overhead of manual management
   - → Improves cycle times & error-proneness

→ Changed paradigm from executing to defining an analysis
→ Move focus back to physics

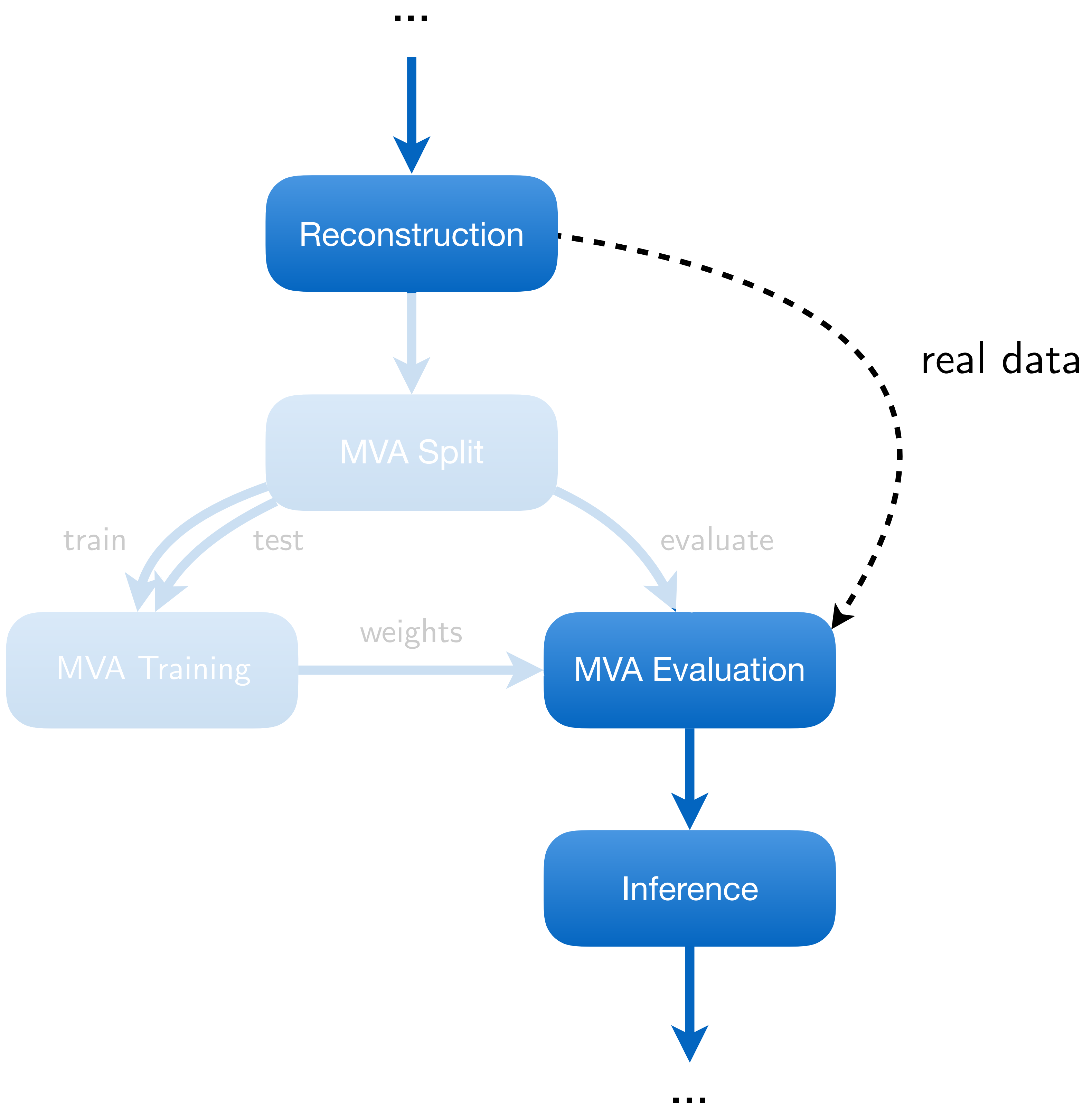
A typical example: ML workflow with uncertainties

Nominal MC



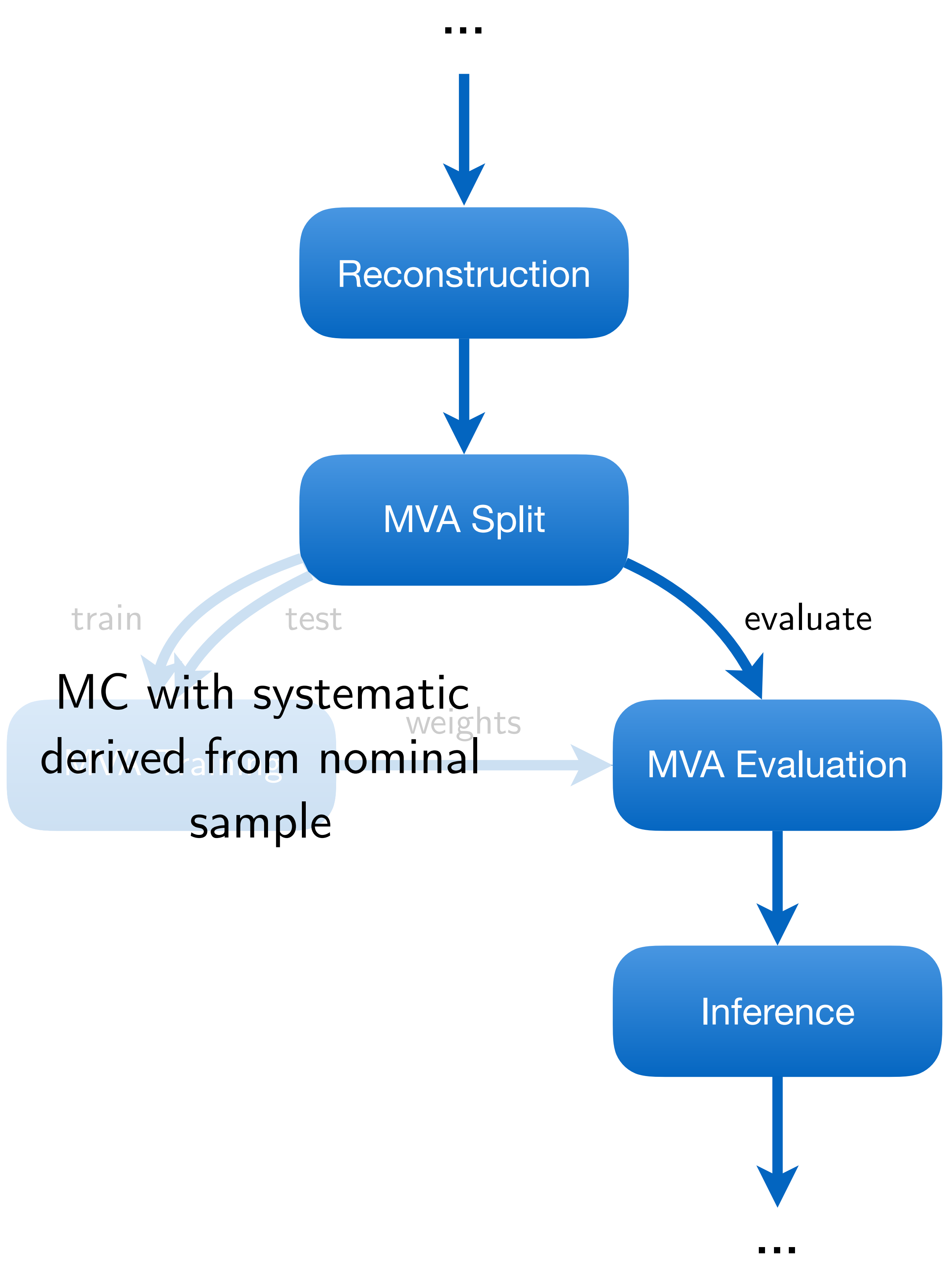
A typical example: ML workflow with uncertainties

Data



A typical example: ML workflow with uncertainties

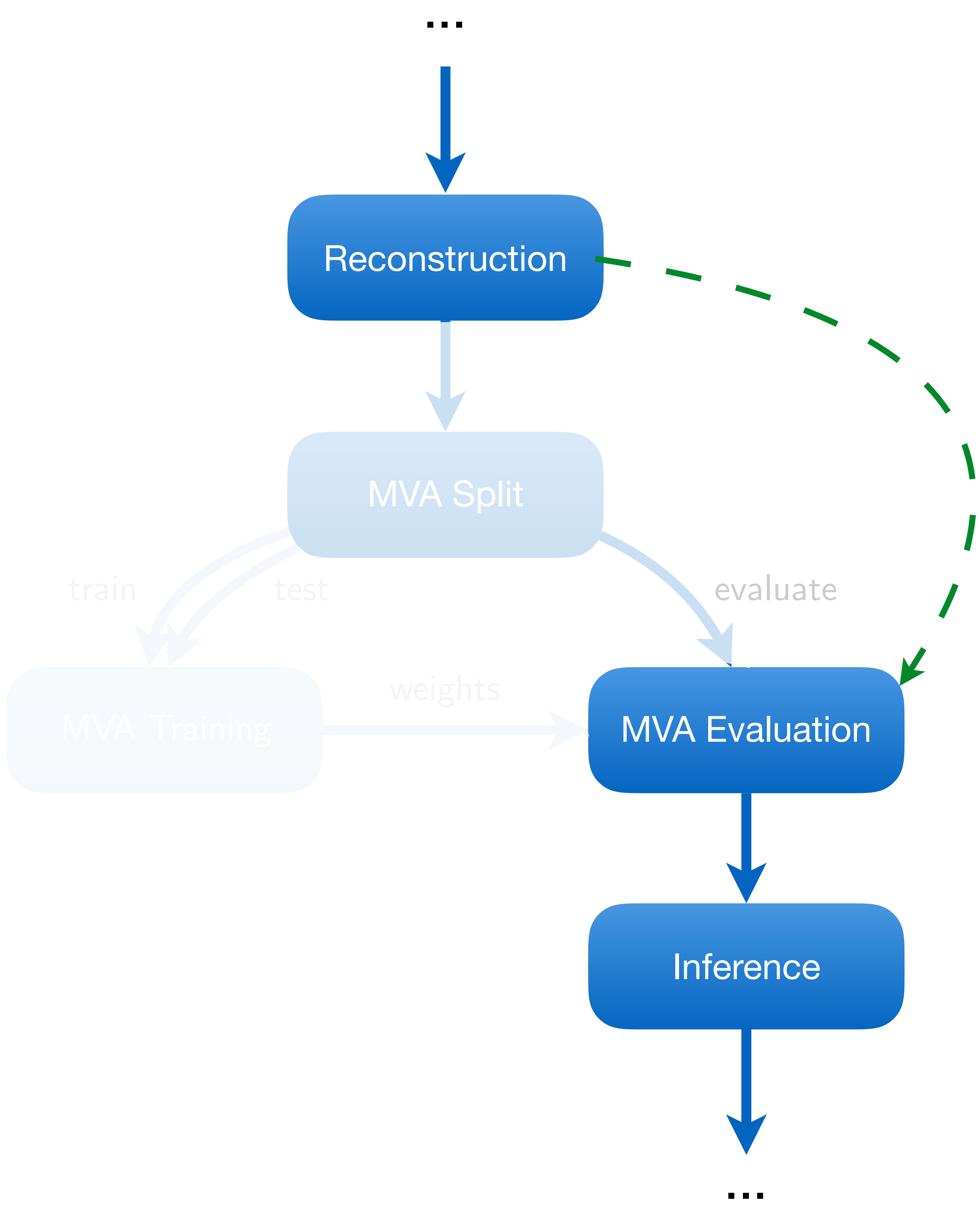
MC, Syst. I



MC with systematic derived from nominal sample

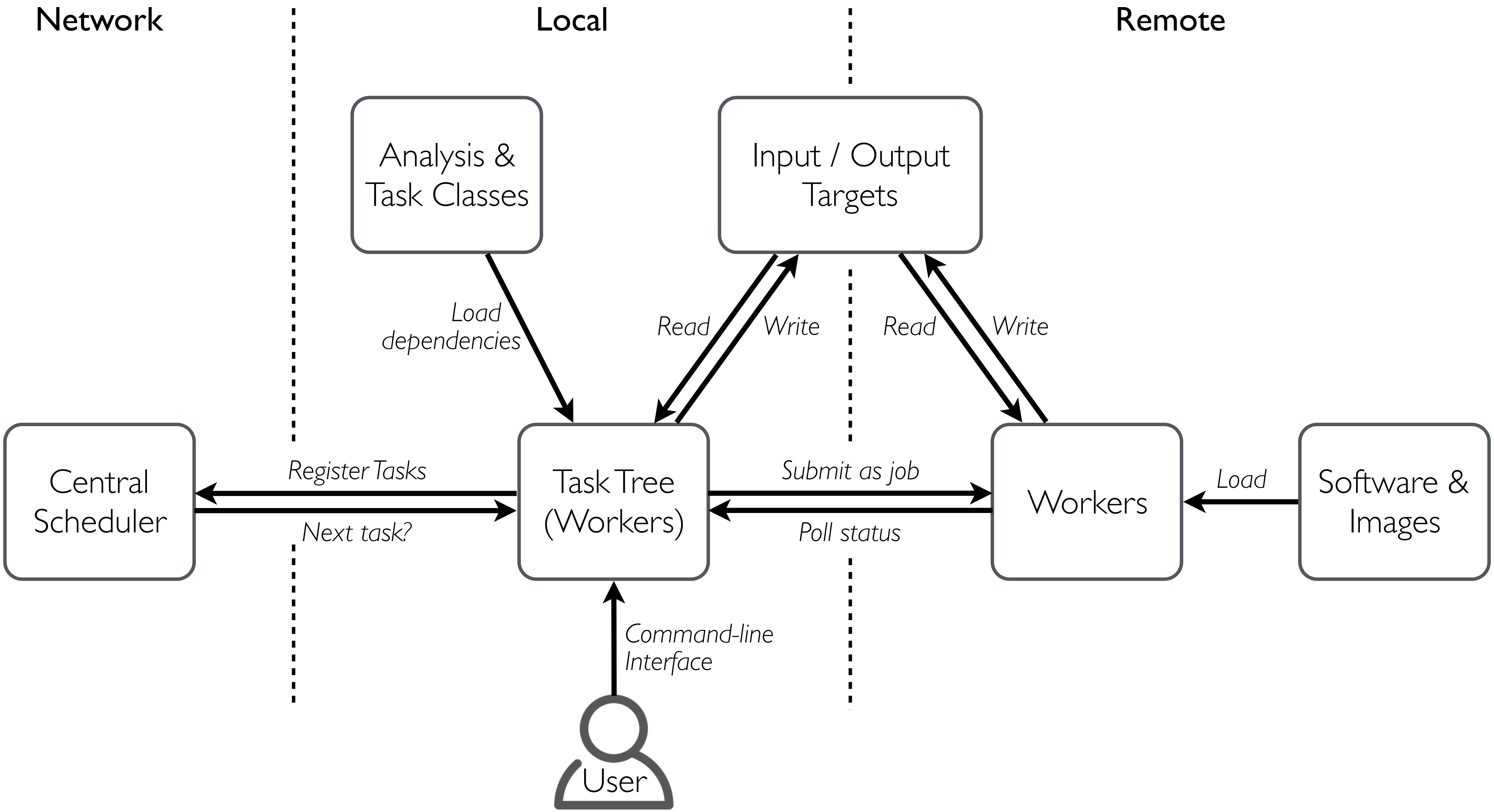
A typical example: ML workflow with uncertainties

MC, Syst. II



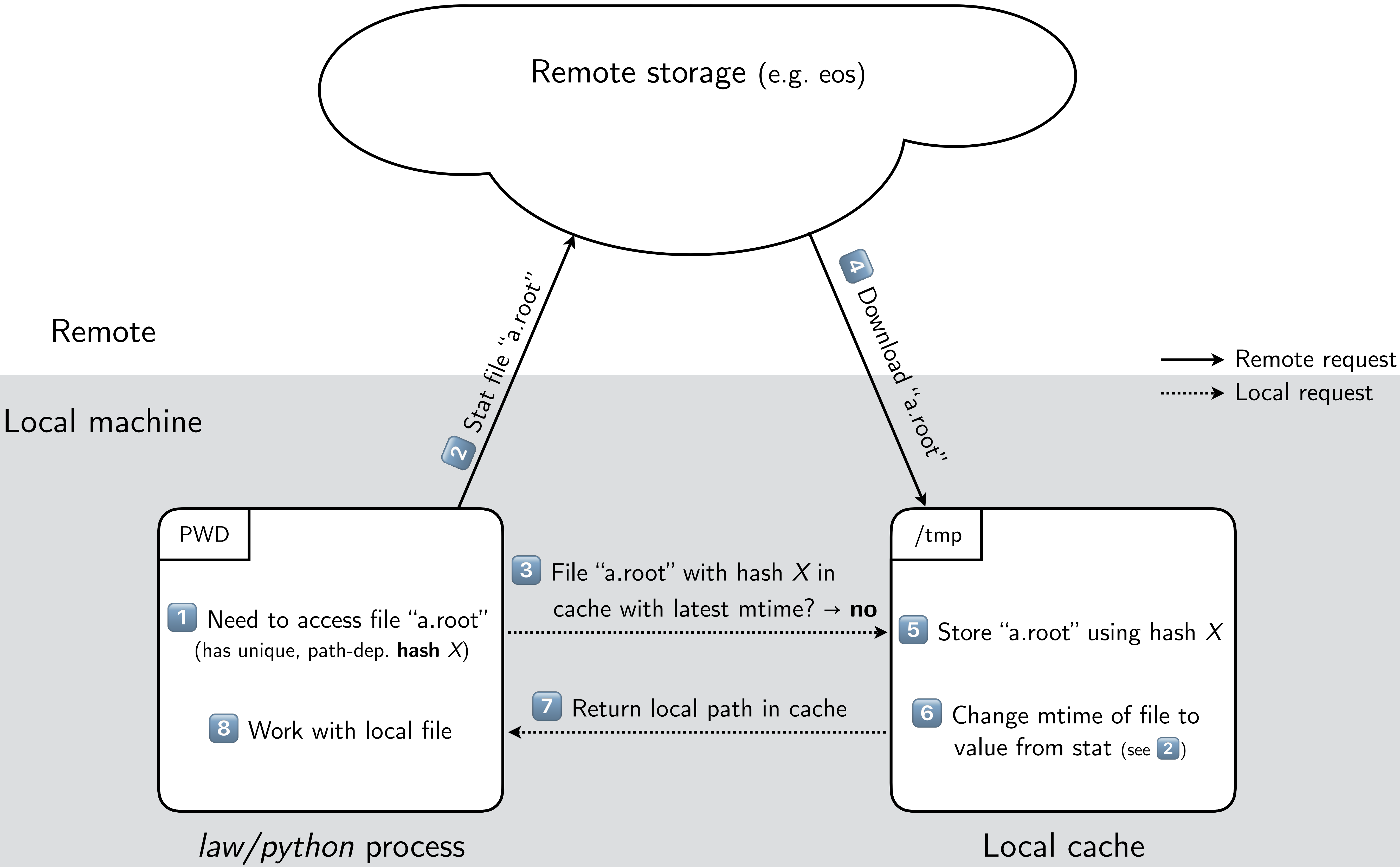
MC with systematic generated from new events

luigi/law architecture

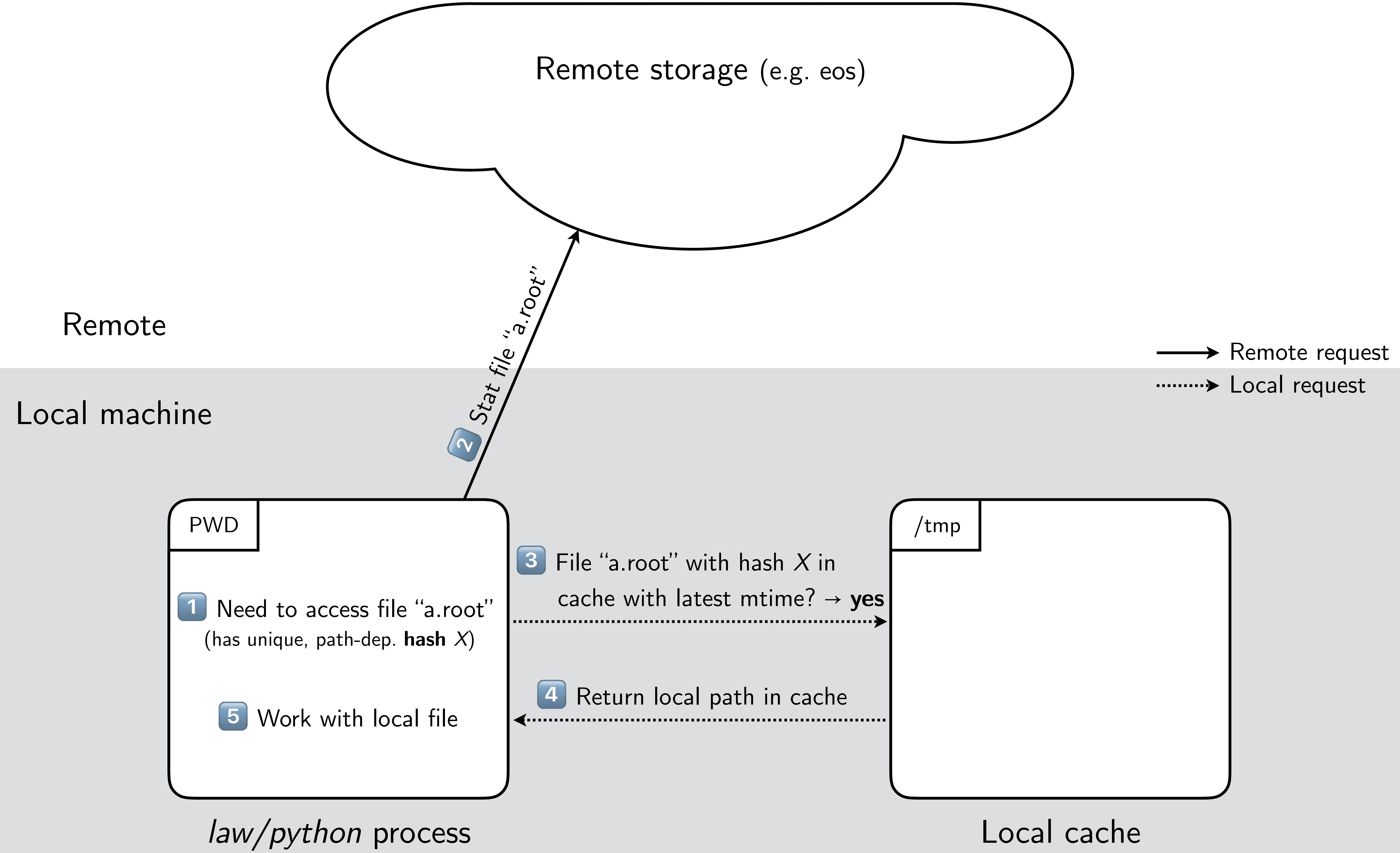


Local caching

Scenario A: file not cached *yet*

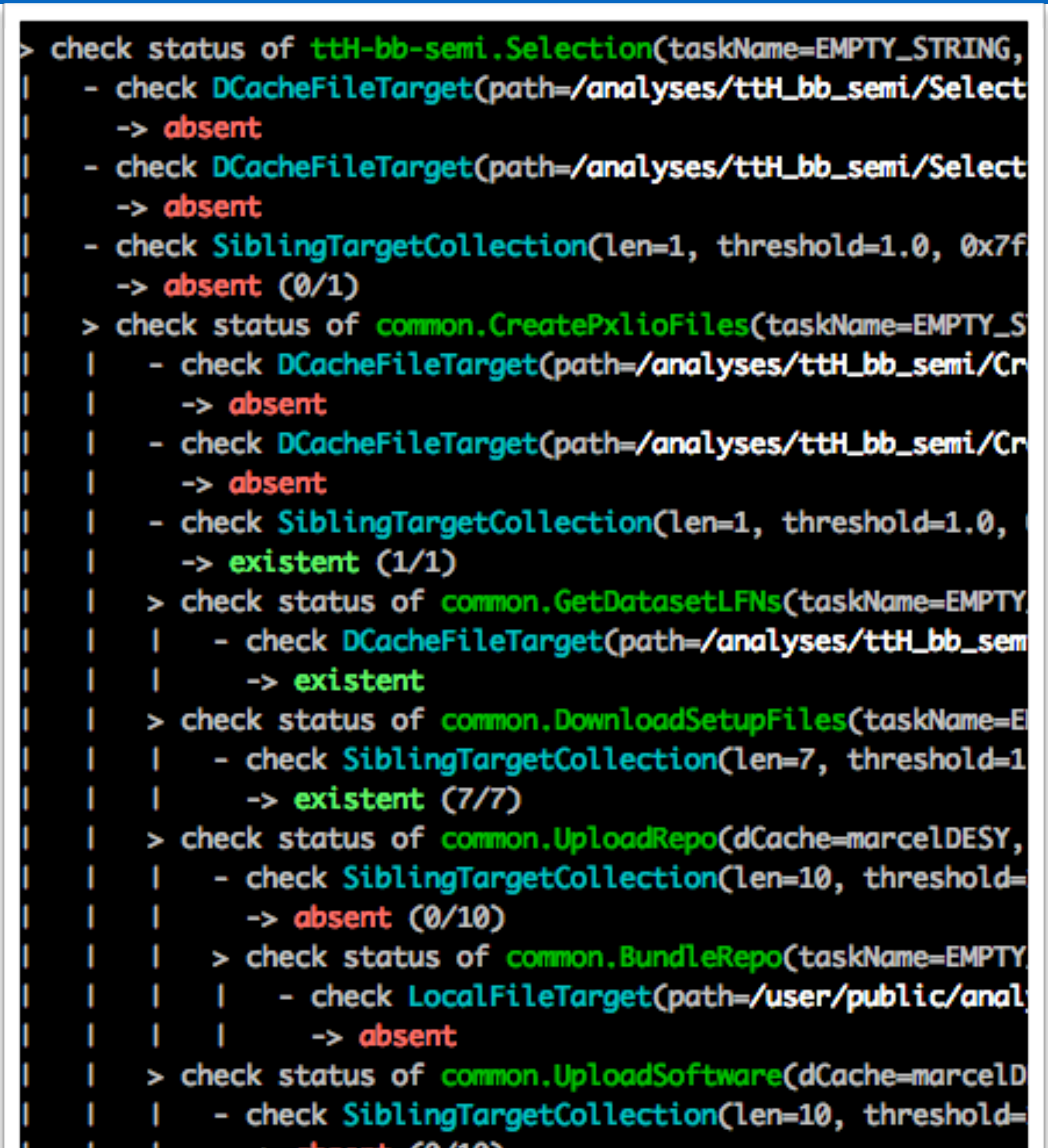

Remote storage (e.g. eos)
Remote
Local machine
2 Stat file "a.root"
4 Download "a.root"
Remote request
Local request
PWD
1 Need to access file "a.root"
(has unique, path-dep. **hash** *X*)
8 Work with local file
3 File "a.root" with hash *X* in
cache with latest mtime? → **no**
7 Return local path in cache
/tmp
5 Store "a.root" using hash *X*
6 Change mtime of file to
value from stat (see 2)
law/python process
Local cache

Scenario B: file *already* cached



Remote storage (e.g. eos)
Remote
Local machine
2 Stat file "a.root"
→ Remote request
⋯→ Local request
PWD
1 Need to access file "a.root"
(has unique, path-dep. **hash** X)
5 Work with local file
3 File "a.root" with hash X in cache with latest mtime? → **yes**
4 Return local path in cache
/tmp
law/python process
Local cache

CLI



```
> check status of ttH-bb-semi.Selection(taskName=EMPTY_STRING,
|   - check DCacheFileTarget(path=/analyses/ttH_bb_semi/Select
|     -> absent
|   - check DCacheFileTarget(path=/analyses/ttH_bb_semi/Select
|     -> absent
|   - check SiblingTargetCollection(len=1, threshold=1.0, 0x7f
|     -> absent (0/1)
|   > check status of common.CreatePxlioFiles(taskName=EMPTY_S
|   |   - check DCacheFileTarget(path=/analyses/ttH_bb_semi/Cr
|   |     -> absent
|   |   - check DCacheFileTarget(path=/analyses/ttH_bb_semi/Cr
|   |     -> absent
|   |   - check SiblingTargetCollection(len=1, threshold=1.0,
|   |     -> existent (1/1)
|   |   > check status of common.GetDatasetLFNs(taskName=EMPTY
|   |   |   - check DCacheFileTarget(path=/analyses/ttH_bb_sem
|   |   |     -> existent
|   |   > check status of common.DownloadSetupFiles(taskName=E
|   |   |   - check SiblingTargetCollection(len=7, threshold=1
|   |   |     -> existent (7/7)
|   |   > check status of common.UploadRepo(dCache=marcelDESY,
|   |   |   - check SiblingTargetCollection(len=10, threshold=
|   |   |     -> absent (0/10)
|   |   |   > check status of common.BundleRepo(taskName=EMPTY
|   |   |   |   - check LocalFileTarget(path=/user/public/anal
|   |   |   |     -> absent
|   |   > check status of common.UploadSoftware(dCache=marcelD
|   |   |   - check SiblingTargetCollection(len=10, threshold=
|   |   |     -> absent (0/10)
```