Provenance tracking and inspection in lstchain and lstosa

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LST General Meeting – 19/11/2021

What is provenance ?

CTA General Requirement

A-USER-0110 The CTA Observatory must ensure that data processing is traceable and reproducible

Specific Requirements

- Keep the traceability of the data products
- Perform data quality and reliability checks
- Reproduce and reprocess the data
- Debug the pipelines

- Provide provenance information to the final user
- Possibility to filter out results based on provenance analysis

Terminology

Configuration provenance

- software dependencies and execution environment

Data provenance

- usually gives some context and info on last processing step on the dataset
- mostly recorded in FITS HISTORY headers
- also metadata describing the dataset

Execution provenance

- commands and parameters/values with timestamps
- mostly recorded in log files

Full provenance

- provides a graph view of the whole process
- chain of commands datasets parameters/values

Standards in Astronomy

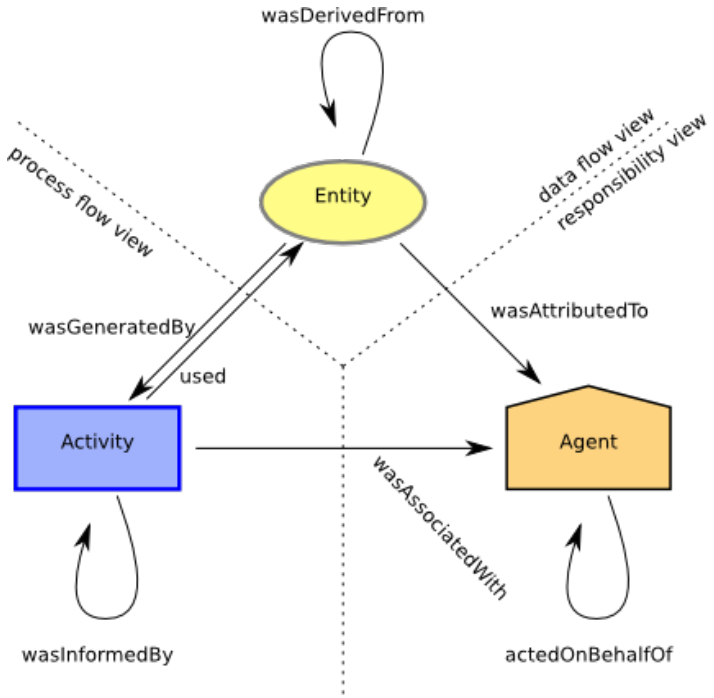
International Virtual Observatory Alliance

IVOA Documents

IVOA Provenance Data Model
Version 1.0

IVOA Recommendation 11 April 2020

https://www.ivoa.net/documents/ProvenanceDM



On-going efforts within IVOA to develop standards for astronomical archives to expose and access provenance information

ProvSAP
Provenance Simple Access Protocol

ProvTAP
Provenance Tabular Access Protocol

voprov
Python package to work with IVOA Provenance Model objects

logprov
Python package to capture provenance following IVOA Provenance Model

work-in-progress

Capturing provenance

On top

- data products collection have been already produced
- extract only information present in data and save it in a structured way elsewhere

Inside

- capture and save provenance at the moment of data processing

Granularity and level of details

- which steps, processes, datasets, ancillary files and parameters
- execution environment and dependencies

Format

- model and syntax that accounts for describing the pipeline components and relationships
- serializing provenance info as attached metadata, structured logs, graphs, relational DB,..

Software considered

lstosa

Python **pipeline** for the **On-site Analysis of low-level** data observations from the LST1 curated and developed by GAE-UCM group.
https://github.com/gae-ucm/lstosa

lstchain

Python **library** for the **processing of low-level** data observations from the LST1 curated and developed by the LST Collaboration.
https://github.com/cta-observatory/cta-lstchain

ctapipe

Python **framework** for prototyping the **low-level data processing** algorithms for the Cherenkov Telescope Array.
https://github.com/cta-observatory/ctapipe

ctapipe

Configuration provenance
- software dependencies and execution environment

Execution provenance
- commands and parameters/values with timestamps
- mostly recorded in log files

cta cherenkov telescope array

Provenance in Tools

- provides a very simple API to **code provenance capture features in ctapipe Tools**
- provides serialization in JSON format and as Python dictionaries
- captures execution environment and profiling by default
- allows capture of processes, input and output datasets
- compliant with IVOA Provenance model

Cons

- tracks provenance execution **within a single Tool**
- needs the use of ctapipe Tools

Up to now it **does not allow chaining** provenance products of different Tools but allows concatenation of a provenance records for the same Tool into a single log file

```python
from ctapipe.core import Provenance

prov = Provenance()
 # prov a singleton, so this gives you the same provenance class

prov.start_activitity("some_activity")

... # do things
prov.add_input_file("test.txt")
prov.add_output_file("out.txt")

prov.start_activity("some_sub_activity")

# do more things
prov.add_output_file("out2.txt")

prov.finish_activity() # finish some_activity
prov.finish_activity() # finish some_sub_activity
```

Data provenance

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- also metadata describing the dataset

Store configuration execution metadata in HDF5 files #747

Merged rlopezcoto merged 18 commits into `master` from `metadata` 16 days ago

Conversation 22 | Commits 18 | Checks 8 | Files changed 10

Write | Preview

This PR stores the config execution of scripts as metadata attributes of the HDF5 files and tables produced in the R0->calibration->DL1->DL1AB->DL2 workflow.

The scripts involved in this workflow are:

- `/scripts/lstchain_data_create_time_calibration_file.py`
- `/tools/lstchain_create_calibration_file.py`
- `/scripts/lstchain_data_r0_to_dl1.py`
- `/scripts/lstchain_dl1ab.py`
- `/scripts/lstchain_dl1_to_dl2.py`
- `/scripts/lstchain_add_source_dependent_parameters.py`

The global metadata stored at the root level of the HDF5 files, as well as into each of the tables/containers produced, account for the versions of the software used in the execution of the script that produces de file i.e. `CTAPIPE_VERSION`, `LSTCHAIN_VERSION`, `CTAPIPE_IO_LST`

The configuration parameters used for each script/tool are stored as an attribute `config` of the tables/containers produced.

lstchain

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cherenkov telescope array

These metadata may be easily retrieved with `pytables` library and `vitables` software, as described in the python snippets and screenshots below.

```
with tables.open_file(filename) as file:
   ...:     print(file.root._v_attrs["LSTCHAIN_VERSION"])

0.7.4.post16+git0deb44e
```

```
with tables.open_file(filename) as file:
   ...:     config = yaml.safe_load(file.root.dl1.event.telescope.parameters.LST_LSTCam.attrs["config"])
print(config["tailcut"])

{'picture_thresh': 6,
 'boundary_thresh': 3,
 'keep_isolated_pixels': False,
 'min_number_picture_neighbors': 2,
 'use_only_main_island': False,
 'delta_time': 2}
```

In the case where, during one of the workflow steps, a specific table is directly retrieved from one previous existing file and copied into the new produced HDF5 file, then the software versions and the config execution metadata are kept untouched.

lstchain

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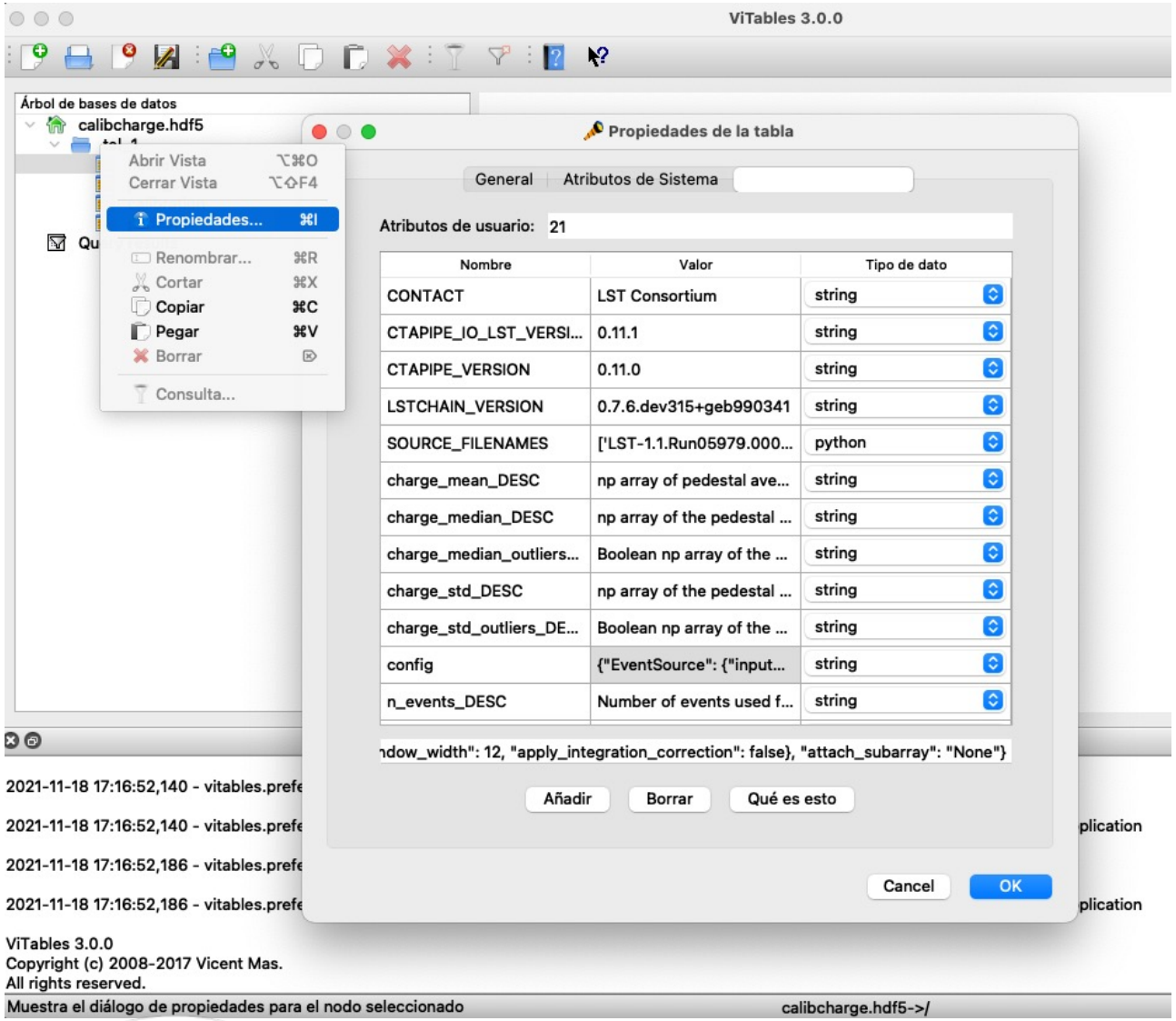
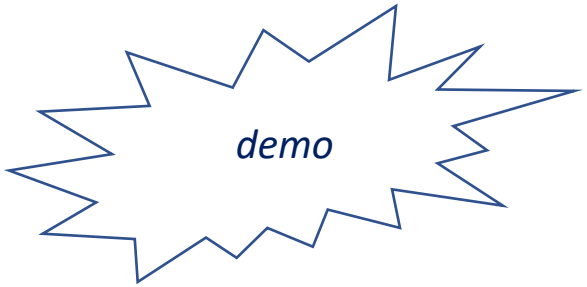



```
CalibrationHDF5Writer:
  output_file: "calibcharge.hdf5"
  config_file: "/Users/jer/git/cta-observatory/cta-lstchain/lstchain/data/onsite_camera_calibration_param.json"
  one_event: true
  events_to_skip: 1000
  calibration_product: "LSTCalibrationCalculator"
  log_level: "DEBUG"
  log_config: {…}
  EventSource:
    input_url: "/Users/jer/DATA/LST/R0/20210902/LST-1.1.Run05979.0000.fits.fz"
LSTEventSource:
  LSTR0Corrections:
    drs4_pedestal_path: "/Users/jer/DATA/LST/calibration/20210902/v0.7.3/drs4_pedestal.Run05978.0000.fits"
    drs4_time_calibration_path: "/Users/jer/DATA/LST/calibration/20210902/v0.7.3/time_calibration.Run05979.0000.hdf5"
    select_gain: false
  EventTimeCalculator:
    run_summary_path: "/Users/jer/DATA/LST/monitoring/RunSummary/RunSummary_20210902.ecsv"
  allowed_tels:
    0: 1
LSTCalibrationCalculator:
  squared_excess_noise_factor: 1.222
  flatfield_product: "FlasherFlatFieldCalculator"
  pedestal_product: "PedestalIntegrator"
PedestalIntegrator:
  sample_duration: 100000
  tel_id: 1
  charge_median_cut_outliers:
    0: -10
    1: 10
  charge_std_cut_outliers:
    0: -10
    1: 10
  charge_product: "FixedWindowSum"
FlasherFlatFieldCalculator:
  sample_duration: 100000
  tel_id: 1
  charge_product: "LocalPeakWindowSum"
  charge_median_cut_outliers:
    0: -0.5
    1: 0.5
  charge_std_cut_outliers:
    0: -10
    1: 10
  time_cut_outliers:
    0: 2
    1: 38
LocalPeakWindowSum:
  window_shift: 5
  window_width: 12
  apply_integration_correction: false
FixedWindowSum:
```


demo

Full provenance
- provides a graph view of the whole process
- chain of commands datasets parameters/values

Provenance capture

structured logging

How?
- Using standard Python logging mechanism and a **provenance model defined in a YAML file**
- Non-intrusive implementation with **function/class decoration** in existing code
- Info within decorated functions can be extracted and mapped into W3C/IVOA Prov syntax
- Python **logging configuration** is set in an independent configuration file

Which info?
- Used and produced datasets, input parameters, config files and processes

What do we get?
- **Post-processed** log files as merged/filtered logs with info in W3C/IVOA Prov syntax
- W3C provenance **JSON** files and **PDF** graphs as final provenance products

lstosa

Full provenance
- provides a graph view of the whole process
- chain of commands datasets parameters/values

cta cherenkov telescope array

Detailed considerations

- Captured **subrun-wise** and post-processed to **run-wise**
- Post-processing/merging yields provenance products at **different levels of granularity**
  - calibration
  - r0_to_dl1
  - dl1_to_dl2
  - all processes
- Execution **environment** is captured and stored as a session property
- Info *hidden* in **configuration files**
  - compared with hash-content algorithm and **copied** for reproducibility purposes
- Montecarlo simulated training datasets are not copied but **referenced**
- **Dry execution** mechanism allows provenance capture and merging avoiding data processing
- **Session properties**: observation date, run number, lstosa config file, lstchain version

run wise at different processing levels

config/definition.yaml

```yaml
activities:
    r0_to_dl1:
        description:
            "Create DL1 files for an observation run and subrun"
        parameters:
            - name: ObservationRun
              description: "Observation run number"
              value: ObservationRun
            - name: ObservationSubRun
              description: "Observation subrun number"
              value: ObservationSubRun
            - name: CalibrationRun
              description: "Calibration run number"
              value: CalibrationRun
            - name: PedestalRun
              description: "Pedestal run number"
              value: PedestalRun
            - name: ProdID
              description: "Production ID"
              value: ProdID
        usage:
            - role: "Observation subrun"
              description: "Observation subrun used"
              entityName: R0SubrunDataset
              value: R0SubrunDataset
              # filepath: /fefs/aswg/data/real/R0/20200218/LST1.1Run02006.0001.fits.fz
            - role: "Pedestal file"
              description: "Pedestal file used"
              entityName: PedestalFile
              value: PedestalFile
              # filepath: /fefs/aswg/data/real/calibration/20200218/v00/drs4_pedestal.Run02005.0000.fits
            - role: "Coefficients calibration file"
              description: "Coefficients calibration file"
              entityName: CoefficientsCalibrationFile
              value: CoefficientsCalibrationFile
              # filepath: /fefs/aswg/data/real/calibration/20200218/v00/calibration.Run02006.0000.hdf5
            - role: "Time calibration file"
              description: "Time calibration file"
              entityName: TimeCalibrationFile
              value: TimeCalibrationFile
              # filepath: /fefs/aswg/data/real/calibration/20191124/v00/time_calibration.Run1625.0000.hdf5
            - role: "Pointing file"
              description: "Pointing filename for DL1"
              entityName: PointingFile
              value: PointingFile
              ath: /fefs/home/lapp/DrivePositioning/drive_log_20_02_18.txt
              iguration file"
```

config/logger.yaml

```yaml
version: 1
formatters:
    simple:
        format: '%(levelname)s %(name)s %(message)s'
        #format: '%(asctime)s.%(msecs)03d%(message)s'
        datefmt: '%Y-%m-%dT%H:%M:%S'
handlers:
    provHandler:
        class: logging.handlers.WatchedFileHandler
        level: INFO
        formatter: simple
        filename: prov.log
loggers:
    provLogger:
        level: INFO
        handlers: [provHandler]
        propagate: False
disable_existing_loggers: False
PREFIX: __PROV__
HASH_METHOD: md5
HASH_BUFFER: path
capture: True
```

config/environment.yaml

```yaml
# Conda environment for provenance package
# conda env update -f environment.yaml

channels:
  - conda-forge

dependencies:
  - python
  - pyyaml
  - prov
  - pydot
  - pydotplus
  # dev dependencies
  - pytest
  - pytest-cov
  - black
  - isort
```

prov.log


```
INFO provLogger __PROV__2020-05-18T14:18:30.445713__PROV__{'session_id': 8739478486569, 'name': '01618', 'startTime': '2020-05-18T14:18:06.362321', 'system': {'executable':
'/fefs/aswg/software/virtual_env/anaconda3/envs/osa/bin/python', 'platform': {'architecture_bits': '64bit', 'architecture_linkage': '', 'machine': 'x86_64', 'processor':
'x86_64', 'node': 'cp15', 'version': '#1 SMP Thu Nov 8 23:39:32 UTC 2018', 'system': 'Linux', 'release': '3.10.0-957.el7.x86_64', 'libcver': "('glibc', '2.10')", 'num_cpus':
32, 'boot_time': '2020-03-24T03:48:43'}, 'python': {'version_string': '3.7.6 | packaged by conda-forge | (default, Mar 23 2020, 23:03:20) \n[GCC 7.3.0]', 'version': '3.7.6',
'compiler': 'GCC 7.3.0', 'implementation': 'CPython'}, 'environment': {'CONDA_DEFAULT_ENV': 'osa', 'CONDA_PREFIX': '/fefs/aswg/software/virtual_env/anaconda3/envs/osa',
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'(osa) ', 'CONDA_SHLVL': '2', 'PATH': '/local/home/lstanalyzer/usr/bin:/local/home/lstanalyzer/.local/bin:/fefs/aswg/software/virtual_env/anaconda3/envs/osa/bin:/fefs/aswg/
software/virtual_env/anaconda3/condabin:/usr/lib64/qt-3.3/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/ibutils/bin:/local/home/lstanalyzer/.local/bin:/local/
home/lstanalyzer/bin', 'LD_LIBRARY_PATH': '/local/home/lstanalyzer/usr/lib:', 'DYLD_LIBRARY_PATH': None, 'USER': 'lstanalyzer', 'HOME': '/local/home/lstanalyzer', 'SHELL':
'/bin/bash'}, 'arguments': ['/fefs/aswg/lstosa/datasequence.py', '-c', 'cfg/sequencer_Nov2019_dragontime_v03.cfg', '-d', '2019_11_23', '--prod_id', 'v0.5.1_v03', '/fefs/
aswg/data/real/calibration/20191123/v03/calibration.Run1614.0000.hdf5', '/fefs/aswg/data/real/calibration/20191123/v03/drs4_pedestal.Run1611.0000.fits', '/fefs/aswg/data/
real/calibration/20191123/v03/time_calibration.Run1614.0000.hdf5', '/fefs/aswg/scripts-osa/corrected_drive_logs_Nov19/drive_log_19_11_23.txt', '0', '0', '0', '0', '--
stderr=sequence_LST1_01618_2432982.err', '--stdout=sequence_LST1_01618_2432982.out', '01618.0008', 'LST1'], 'start_time_utc': '2020-05-18T14:18:30.445684'},
'software_version': 'v0.5.1', 'observation_date': '20191123', 'observation_run': '01618', 'session_tag': 'r0_to_dl1:01618'}
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8739478486569, 'agent_name': 'lstanalyzer', 'script': '/fefs/aswg/lstosa/datasequence.py', 'session_tag': 'r0_to_dl1:01618'}
INFO provLogger __PROV__2020-05-18T14:18:30.447499__PROV__{'activity_id': '621ca2', 'parameters': {'ObservationRun': '01618', 'ObservationSubRun': '0008', 'CalibrationRun':
'01614', 'PedestalRun': '01611', 'ProdID': '03'}, 'session_tag': 'r0_to_dl1:01618'}
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R0/20191123/LST-1.1.Run01618.0008.fits.fz', 'hash': '446f45dd1c878559585395eedce5bc7a', 'hash_type': 'md5', 'type': 'File', 'contentType': 'application/fits', 'session_tag':
'r0_to_dl1:01618'}
INFO provLogger __PROV__2020-05-18T14:18:30.447752__PROV__{'activity_id': '621ca2', 'used_id': '446f45dd1c878559585395eedce5bc7a', 'used_role': 'Observation subrun',
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'session_tag': 'r0_to_dl1:01618'}
INFO provLogger __PROV__2020-05-18T14:18:30.447966__PROV__{'activity_id': '621ca2', 'used_id': '7404bb00748454d63badfe247c774a13', 'used_role': 'Pedestal file',
'session_tag': 'r0_to_dl1:01618'}
INFO provLogger __PROV__2020-05-18T14:18:30.448065__PROV__{'entity_id': 'd8077e3bbdcb371f688ae65b0972e212', 'name': 'CoefficientsCalibrationFile', 'filepath': '/fefs/aswg/
data/real/calibration/20191123/v03/calibration.Run1614.0000.hdf5', 'hash': 'd8077e3bbdcb371f688ae65b0972e212', 'hash_type': 'md5', 'type': 'File', 'contentType':
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'x86_64', 'node': 'cp15', 'version': '#1 SMP Thu Nov 8 23:39:32 UTC 2018', 'system': 'Linux', 'release': '3.10.0-957.el7.x86_64', 'libcver': "('glibc', '2.10')", 'num_cpus':
32, 'boot_time': '2020-03-24T03:48:43'}, 'python': {'version_string': '3.7.6 | packaged by conda-forge | (default, Mar 23 2020, 23:03:20) \n[GCC 7.3.0]', 'version': '3.7.6',
'compiler': 'GCC 7.3.0', 'implementation': 'CPython'}, 'environment': {'CONDA_DEFAULT_ENV': 'osa', 'CONDA_PREFIX': '/fefs/aswg/software/virtual_env/anaconda3/envs/osa',
'CONDA_PYTHON_EXE': '/fefs/aswg/software/virtual_env/anaconda3/bin/python', 'CONDA_EXE': '/fefs/aswg/software/virtual_env/anaconda3/bin/conda', 'CONDA_PROMPT_MODIFIER':
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software/virtual_env/anaconda3/condabin:/usr/lib64/qt-3.3/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/ibutils/bin:/local/home/lstanalyzer/.local/bin:/local/
home/lstanalyzer/bin', 'LD_LIBRARY_PATH': '/local/home/lstanalyzer/usr/lib:', 'DYLD_LIBRARY_PATH': None, 'USER': 'lstanalyzer', 'HOME': '/local/home/lstanalyzer', 'SHELL':
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aswg/data/real/calibration/20191123/v03/calibration.Run1614.0000.hdf5', '/fefs/aswg/data/real/calibration/20191123/v03/drs4_pedestal.Run1611.0000.fits', '/fefs/aswg/data/
real/calibration/20191123/v03/time_calibration.Run1614.0000.hdf5', '/fefs/aswg/scripts-osa/corrected_drive_logs_Nov19/drive_log_19_11_23.txt', '0', '0', '0', '0', '--
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hdf', 'session_tag': 'r0_to_dl1:01618'}
```
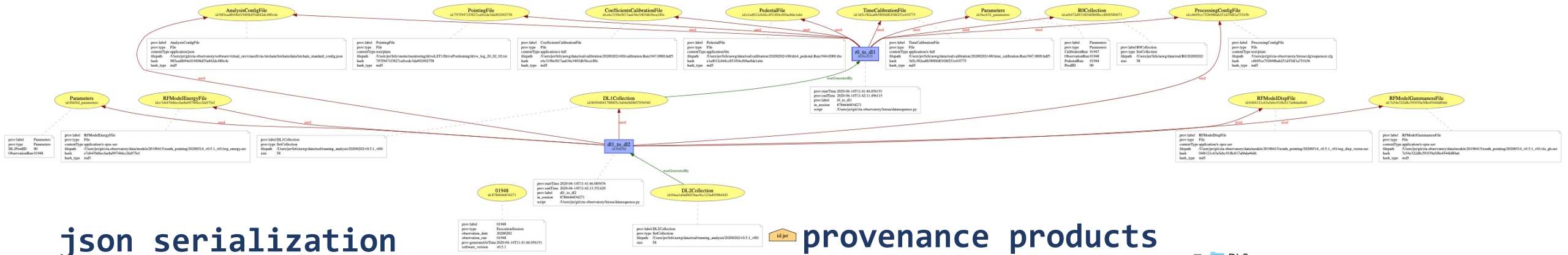

data processing provenance graph



json serialization


```
{
    "prefix": {
        "id": "id:",
        "default": "param:"
    },
    "entity": {
        "id:8756102484710": {
            "prov:label": "r0_to_dl1",
            "prov:type": "ExecutionSession",
            "prov:generatedAtTime": "2020-05-08T11:51:47.051025",
            "script": "/home/daniel.morcuende/lstosa/datasequence.py",
            "software_version": "v0.4.5.post566+gite395ef2",
            "observation_date": "20200118",
            "observation_run": "01832"
        },
        "id:4b1e22_parameters": {
            "ObservationRun": "01832",
            "CalibrationRun": "01831",
            "PedestalRun": "01830",
            "ProdID": "02",
            "prov:type": "Parameters",
            "prov:label": "Parameters"
        },
        "id:6d23620c4d92ef92b642a0116908fad1": {
            "prov:label": "PedestalFile",
            "prov:type": "File",
            "filepath": "/fefs/aswg/workspace/daniel.morcuende/data/real/calibration/20200118/v02/drs4_pedestal.Run1830.0000.f
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```
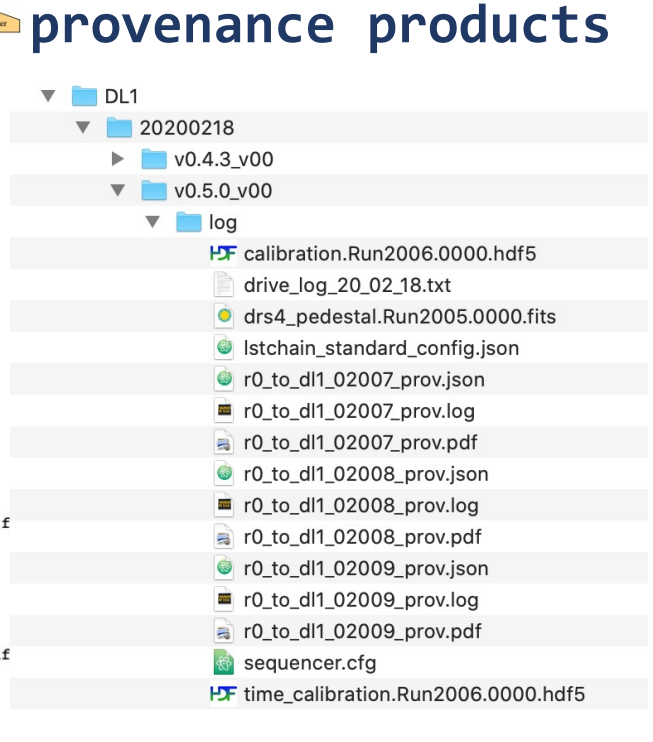
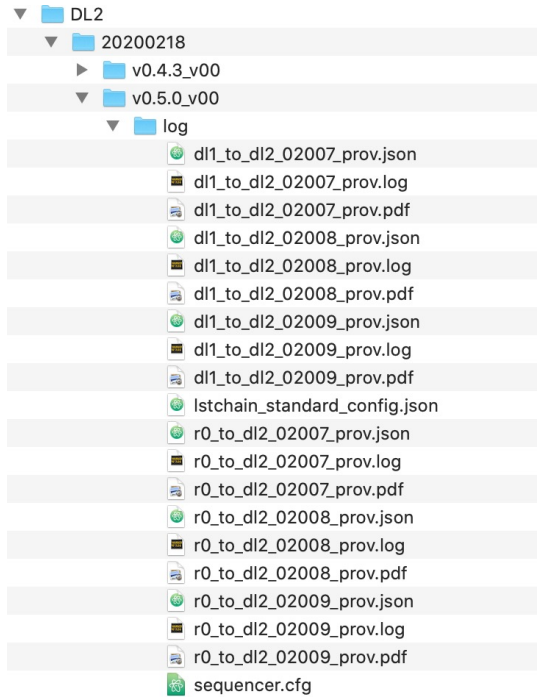


provenance products





lstosa

Full provenance

- provides a graph view of the whole process
- chain of commands datasets parameters/values

cta cherenkov telescope array

Improvements on provenance tracking #34

Open **Bultako** wants to merge 14 commits into `main` from `prov`

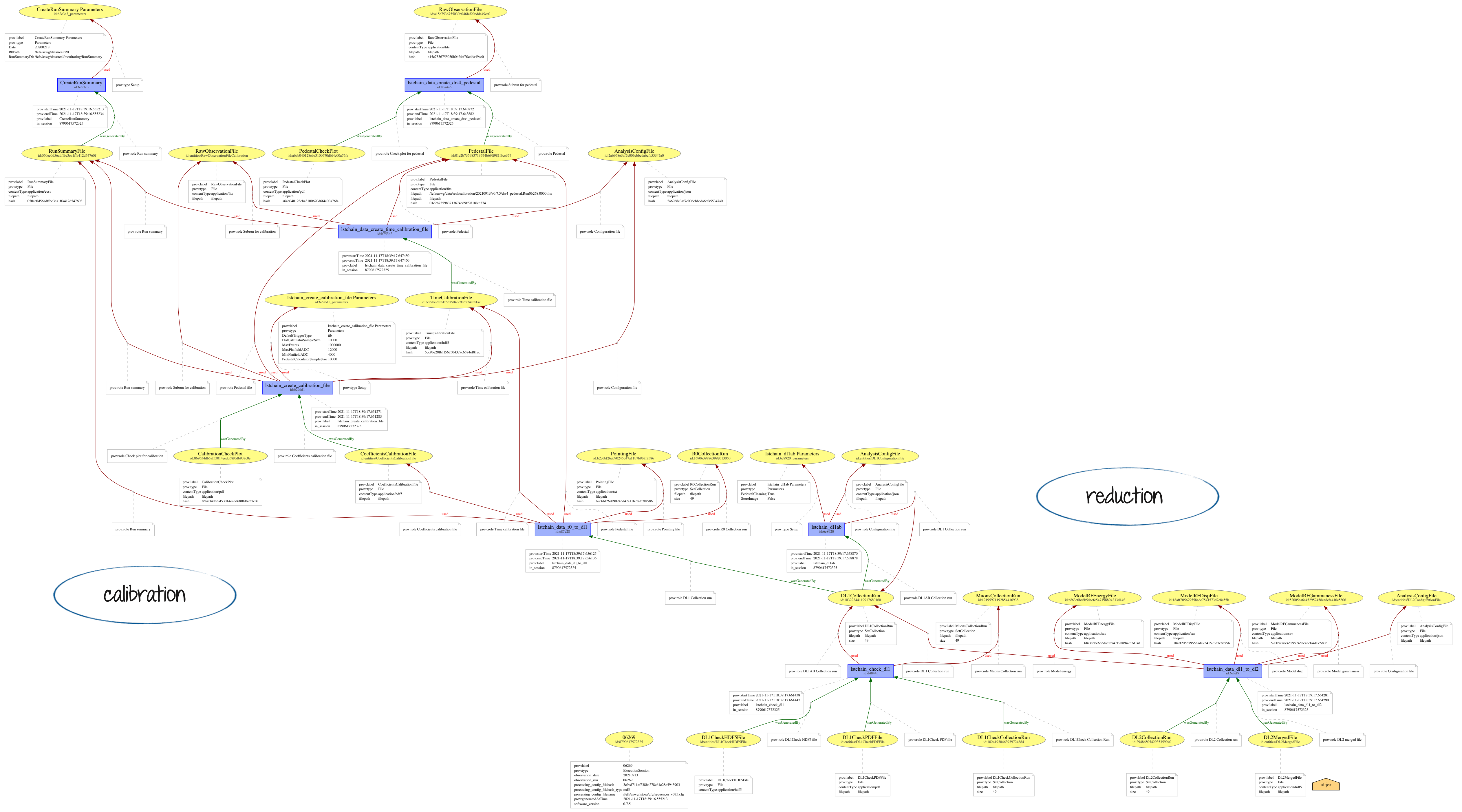
Conversation 0 | Commits 14 | Checks 1 | Files changed 8

Bultako commented 1 hour ago — Collaborator

The content of this PR is the following:

- fixes some issues derived from changes in the data processing steps that have not been translated into the model up to now.
- adds calibration processes to the simulate processing script
- tracks and saves python packages dependencies of the conda environment
- adds `lstchain_dl1ab` process into the data sequence provenance
- adds `dl1_datacheck` process into the data sequence provenance
- adds missing DL2 merged file to the provenance
- adds lstosa config file used (i.e. `sequencer.cfg`) as a session parameter

The final graph produced is as below.
provDLshort.pdf



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RawObservationFile
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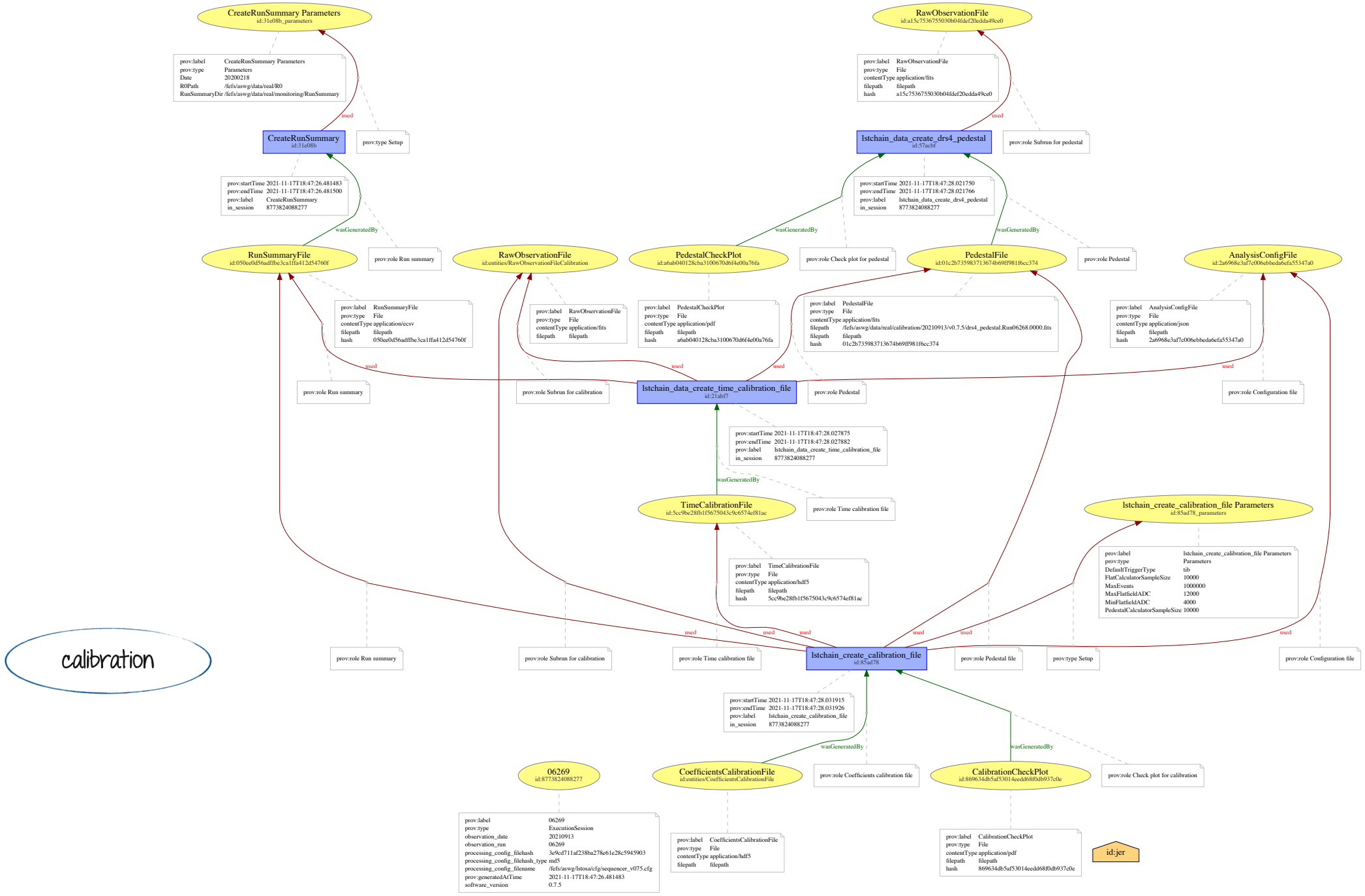
RunSummaryFile
RawObservationFile
PedestalCheckPlot
PedestalFile
AnalysisConfigFile
lstchain_data_create_time_calibration_file
lstchain_create_calibration_file Parameters
TimeCalibrationFile
lstchain_create_calibration_file
CalibrationCheckPlot
CoefficientsCalibrationFile
PointingFile
R0CollectionRun
lstchain_dl1ab Parameters
AnalysisConfigFile
lstchain_data_r0_to_dl1
lstchain_dl1ab
reduction
calibration
DL1CollectionRun
MuonsCollectionRun
ModelRFEnergyFile
ModelRFDispFile
ModelRFGammanessFile
AnalysisConfigFile
lstchain_check_dl1
lstchain_data_dl1_to_dl2
06269
DL1CheckHDF5File
DL1CheckPDFFile
DL1CheckCollectionRun
DL2CollectionRun
DL2MergedFile
id:jer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prov:role Subrun for calibration
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MaxEvents 1000000
MaxFlatfieldADC 12000
MinFlatfieldADC 4000
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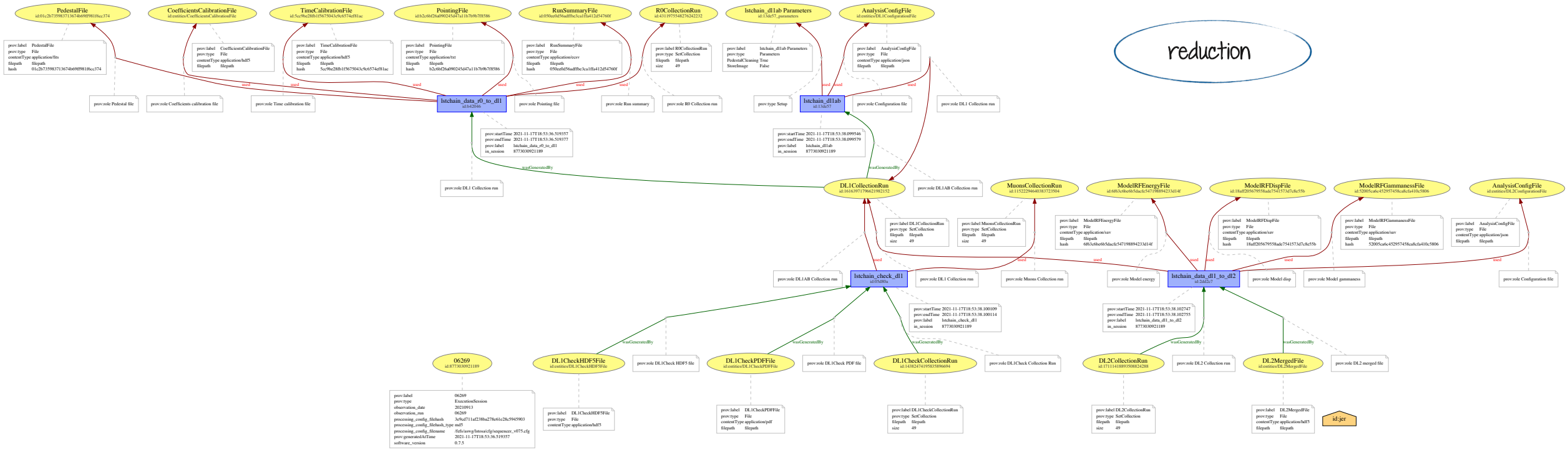
calibration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ModelRFGammanessFile
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prov:label MuonsCollectionRun
prov:type SetCollection
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size 49
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contentType application/sav
filepath filepath
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size 49
prov:label DL2CollectionRun
prov:type SetCollection
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size 49
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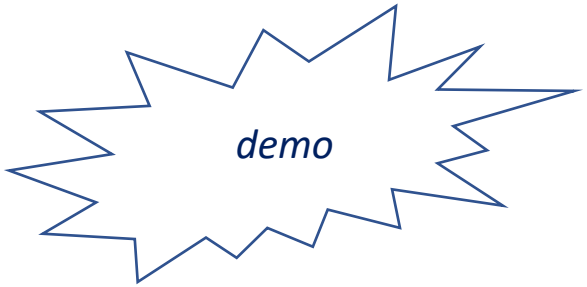
wasGeneratedBy
used


demo

Lessons learnt and next steps

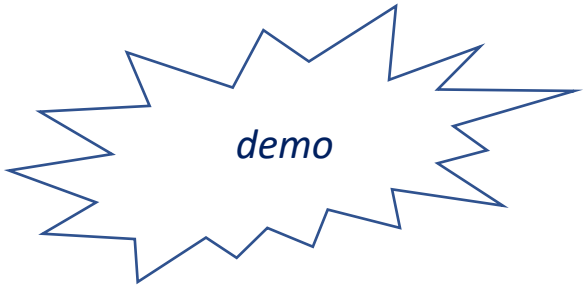
- Continuous update and addition of captured info – **flexible model and implementation**
- **Configuration** may be stored as metadata attached to datasets (***fits headers***/*hdf5 attributes*)
- **Capturing relationships** among activities and entities (*datasets*) needs a provenance model
- **Independent capture for the different dependent software** packages is possible

  lstosa requires lstchain requires ctapipe

- Massive logging subrun-wise makes a very poor performance because of **huge usage of disk**
- **Post-processing** of prov info is needed to produce run-wise info and different **levels of granularity**
- **Structured logging** in text files may be a solution for storage of small sessions provenance
- Considering storing provenance in a RDBMS or *better* in a noSQL **database** (i.e. *mongo + json*)

- Development of a **provenance query mechanism** for detailed analysis and inspection is needed

  *…considering using url query params to produce on-the-fly **SVG graphs with access-links in a browser***


demo