NASA ROSES ACCESS

Advancing Collaborative Connections for Earth System Science

Provenance Services for Tracking Production of Multi-Sensor Merged Climate Data Record

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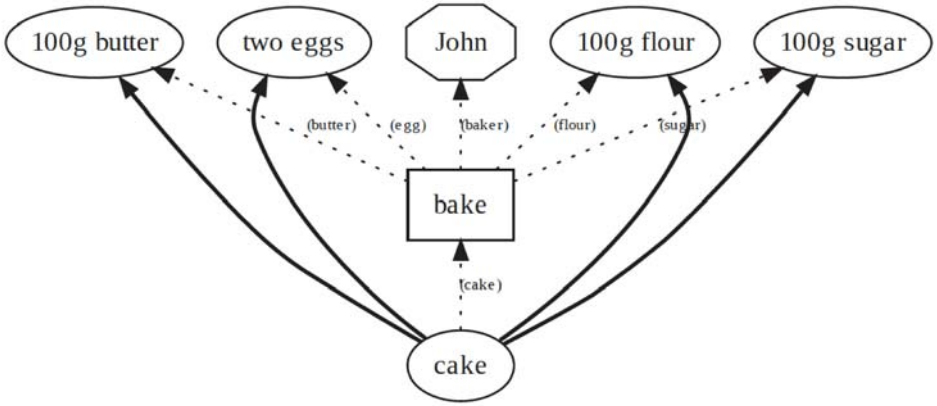
Transparency

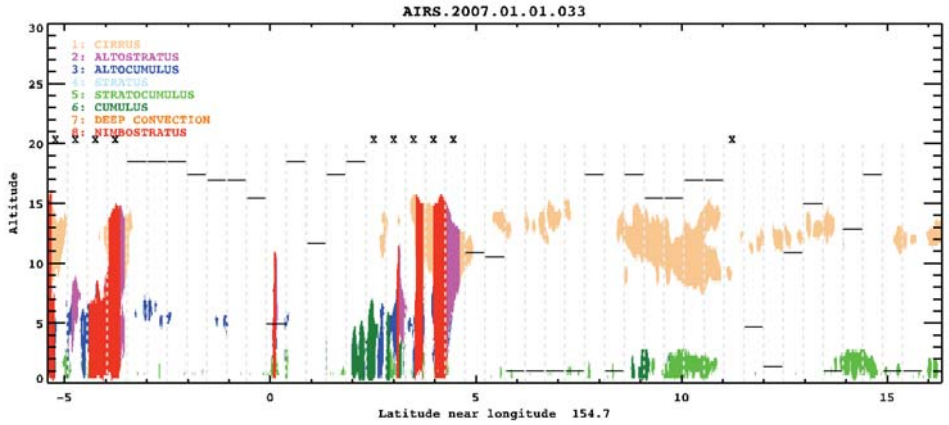
- *"We have a baked cake, but we don't know the recipe."*



- Climategate
  - Perception of lack of transparency.
  - Common scientific practice (ad-hoc)
  - Outcome: *there should be greater openness and information sharing*

MEaSUREs Project: A Multi-Sensor Water Vapor Climate Data Record Using Cloud Classification

- Create a complete and consistent record of water vapor from the **A-Train satellite constellation**.
- **Merge** with water vapor observations obtained prior to the A-Train period, and with observations obtained from non-A-Train sensors.
- **Quantify** the effects of cloud variability on water vapor changes over years to decades.

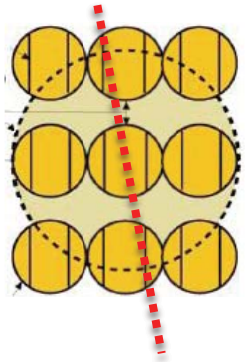


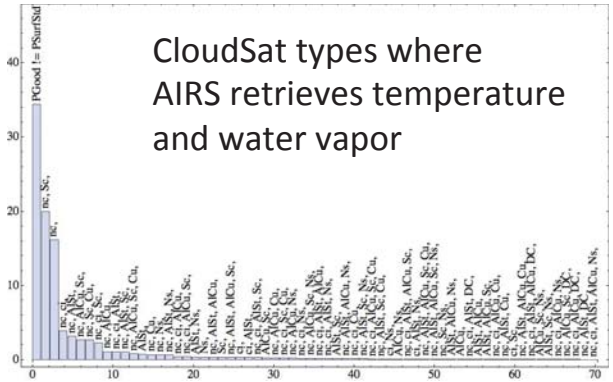
AIRS Preferentially Samples Some Cloud Types

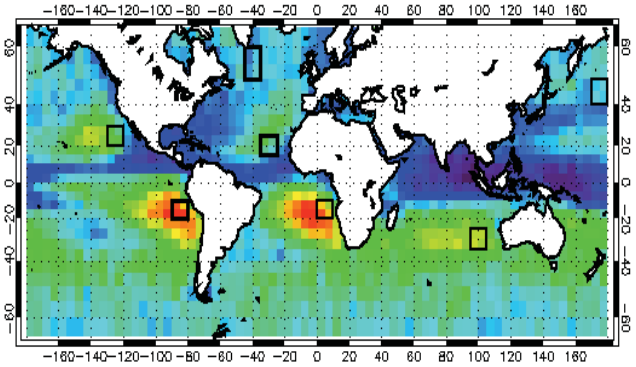
MEaSUREs WVCC PI: Eric Fetzer, Jet Propulsion Laboratory

MEaSUREs WVCC Data Products

- Level 2 data sets matched to CloudSat
  - AIRS, MLS, AMSR-E
- Cloud occurrence within water vapor scenes.
- Level 3 data sets
  - Summaries based on CloudSat-identified cloud types.
  - Use of MODIS cloud types.





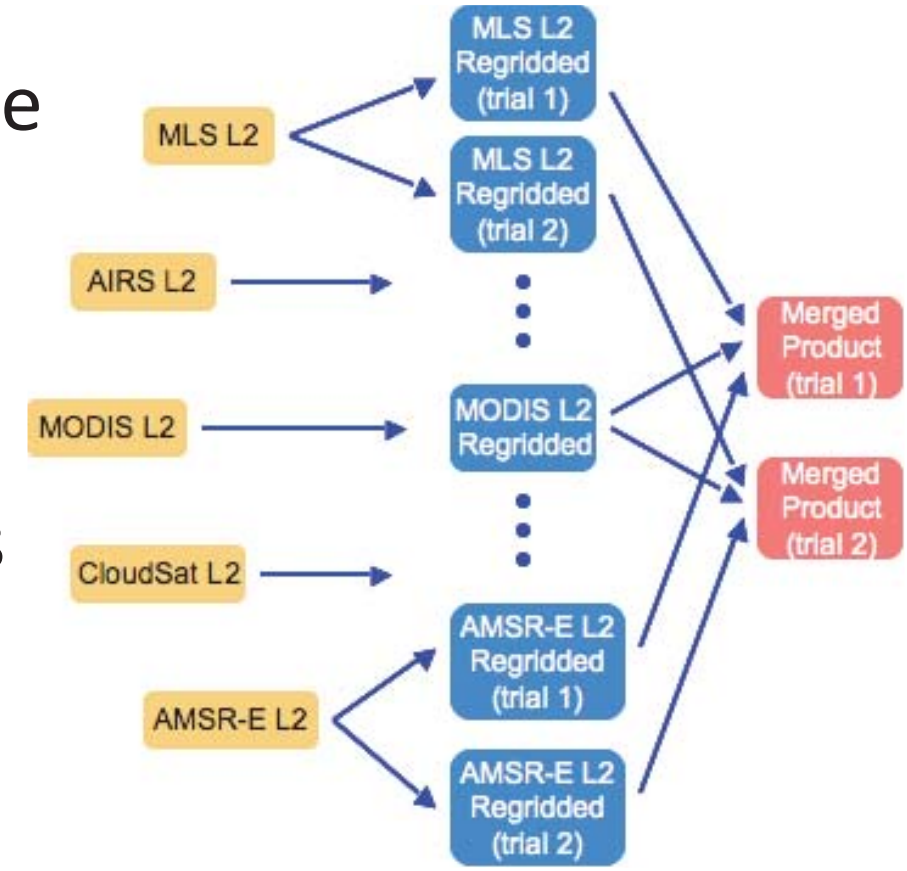


Production Legacy Challenges

- *Multi-sensor merged data products is difficult*
  - *Heterogeneous data handling*
  - *Coherent fusing of measurements*
- *Reproducibility is a basic tenet of science. However…*
- Reproducibility is difficult with existing satellite data Level 2 data sets.
  - Processing algorithms are complex.
  - Cross-platform calibration is challenges.
- Multi-parameter, multi-sensor analyses are particularly difficult.
  - Sensor are rarely designed to work together.
  - Science analysis is usually very '*free form*'.

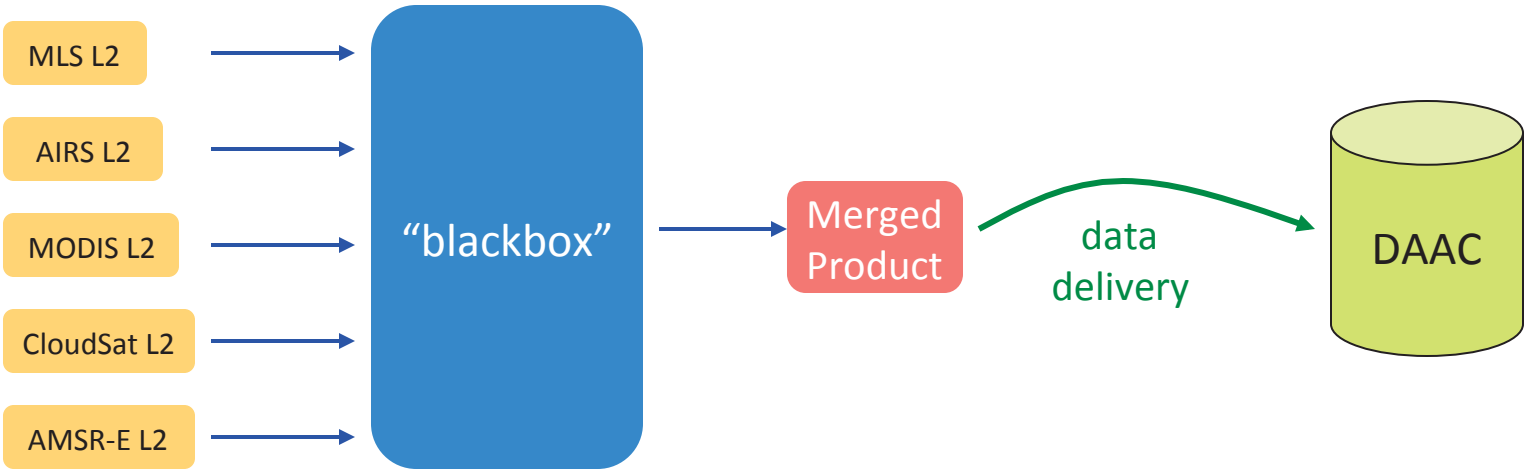
Exploratory Analysis

- Incredibly informal
- Automatically capture "what if" scenario runs
- Have an incredibly *unstructured* process
- How to create a *structured* data record



Want to Avoid "Blackbox" Operations

- ATBD describes approach
- But may still want traceability for each granule

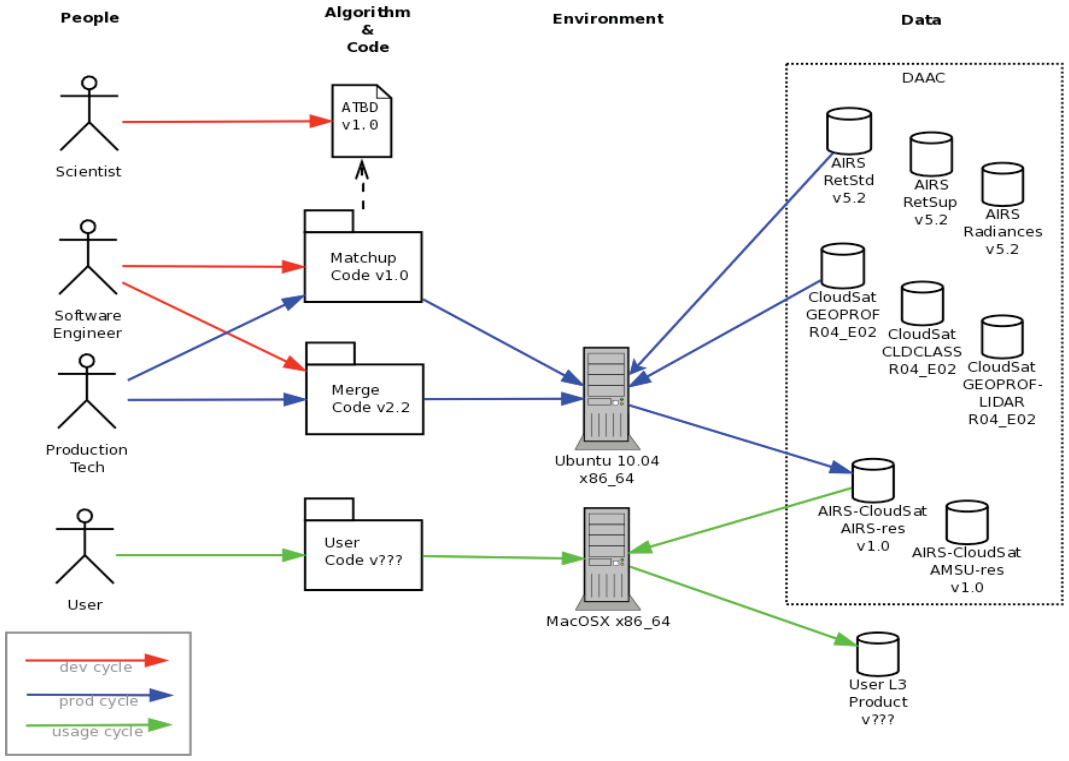


Web Services and Tools for Provenance Capture

PROVENANCE SERVICES

Provenance and Context in MEaUREs Data Production

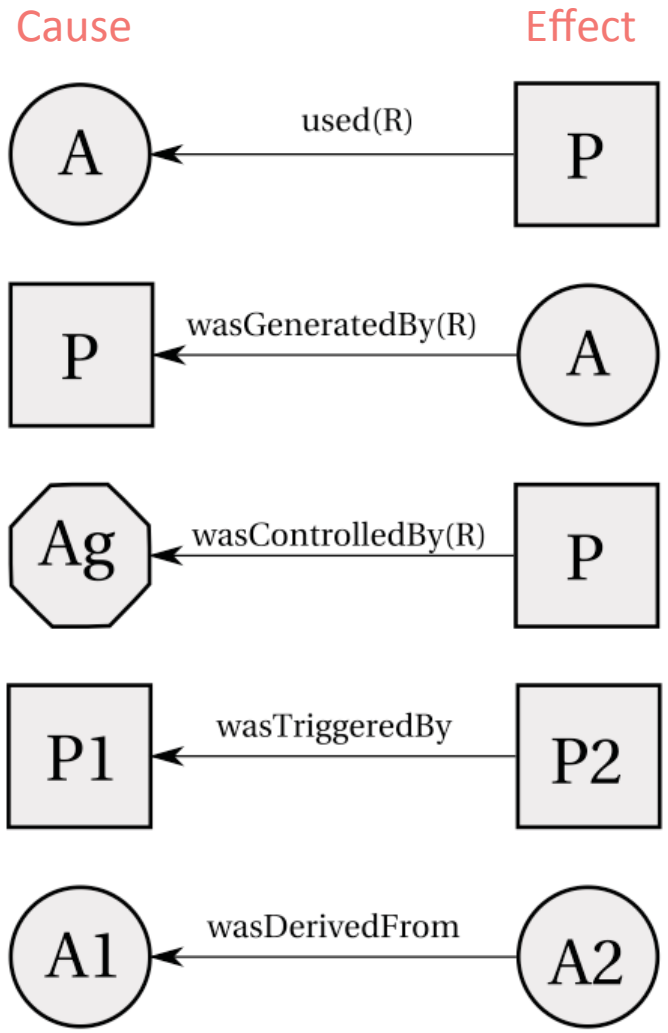
- Track data pedigree
  - Upstream data, executables, algorithms, parameters, instrument sources, environment, and users



- Provenance can be used to enable reproducibility
- Context allows the use of the information for something else.

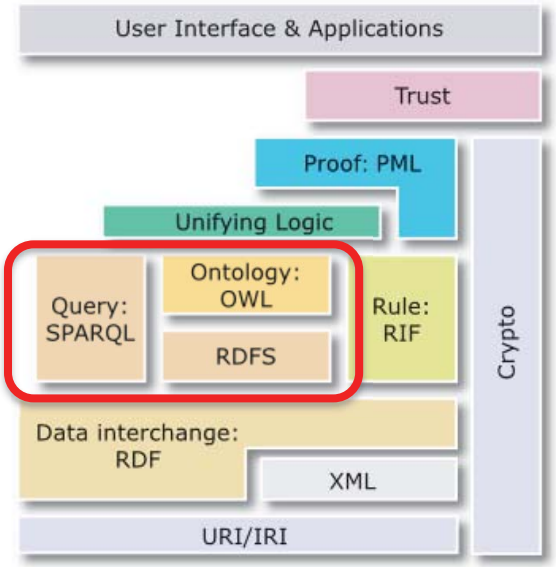
Open Provenance Model: Abstract Model

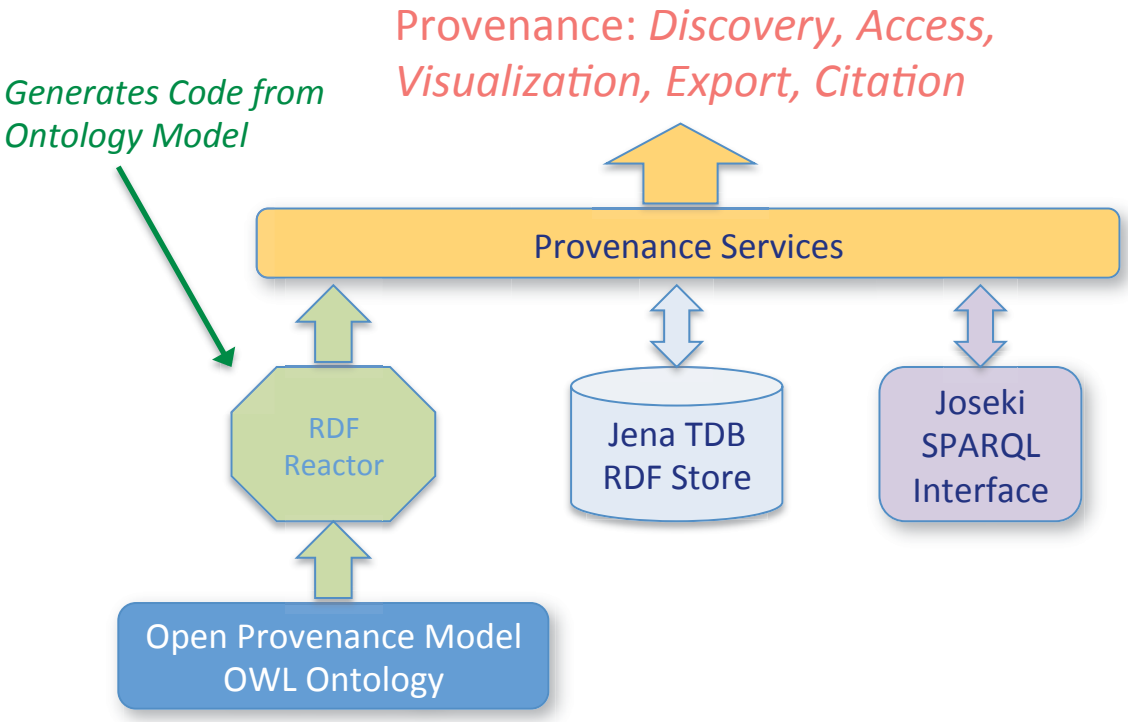
- Allows for process-oriented and dataflow oriented views
- Nodes
  - **A**rtifacts, **P**rocesses, **Ag**ents
- Edges (Dependencies)
  - Causal dependencies between the artifacts, processes, and agents
- A model of artifacts in the past, explaining how they were derived
  - Invert edge direction for present tense



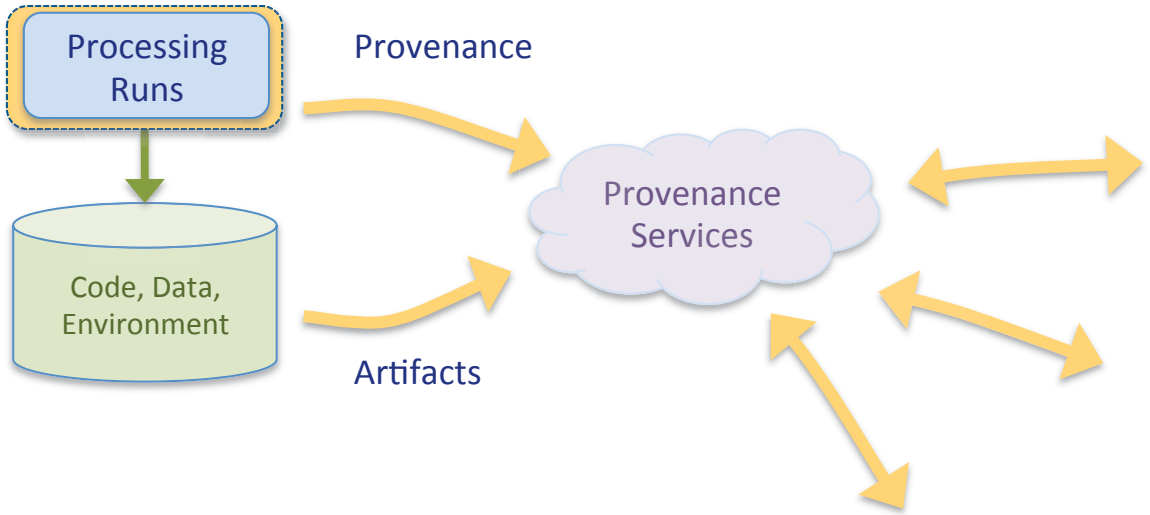
Semantic Web

- Reuse open source semantic web tools

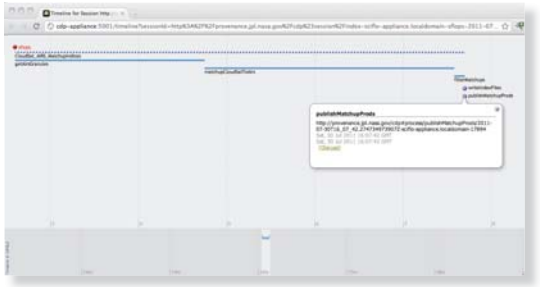




Provenance Services



Lineage Graph



Processing Timeline

Faceted Search

Enable:

1. Capture
2. Exploration
3. Transparency
4. “Reproducibility”

Provenance Capture Approaches

- *"One size does not fit all"*
- Support multiple client-side approaches
  1. Simple REST web service calls to provide real-time provenance
  2. Instrument processing code. Buffering provenance to log file for deferred single upload
  3. Provenance from workflow engine
  4. Automatic capture of runs

Approach #1: REST Web Service Invocations

- Simple REST web services for "real-time" provenance capture
- Example calls using "*one-liner commands*":
  - Process controlled by agent

```
curl -f "http://provenance.jpl.nasa.gov:8099/services/process/was_controlled_by_agent?process=process/
generateMatchupIndices/2010-12-16T22_03_59.842924-node1-9813&agent=agent/gmanipon/node1"
```

  - Process was triggered by another process

```
curl -f "http://provenance.jpl.nasa.gov:8099/services/process/was_triggered_by_process?
triggered_process=process/getMatchupIndices/2010-12-16T22_03_59.843623-gerald-
manipon.jpl.nasa.gov-9813&process=process/generateMatchupIndices/2010-12-16T22_03_59.842924-node1-9813"
```

  - Process used an artifact

```
curl -f "http://provenance.jpl.nasa.gov:8099/services/process/used_artifact?process=process/
getMatchupIndices/2010-12-16T22_03_59.843623-node1-9813&artifact=file://node1/data/sensors/atrain/airs.aqua/
L2/v5/2006/07/15/airx2ret/AIRS.2006.07.15.091.L2.RetStd.v5.0.14.0.G07294185430.hdf/20100804T150641.273418"
```

  - Artifact was generated by process

```
curl -f "http://provenance.jpl.nasa.gov:8099/services/process/was_generated_by_process?artifact=file://
node1/data/measures/pickles/airs.aqua_cloudsat/v2.1/2006/07/15/index-cloudsat_airs.aqua-
v2.1-2006.07.15.082803.pkl/2010-12-16T22_13_02.403408&process=process/getMatchupIndices/
2010-12-16T22_03_59.843623-node1-9813"
```

  - Artifact was derived from another artifact

```
curl -f "http://provenance.jpl.nasa.gov:8099/services/process/was_derived_from_artifact?
derived_artifact=file://node1/data/measures/pickles/airs.aqua_cloudsat/v2.1/2006/07/15/index-
cloudsat_airs.aqua-v2.1-2006.07.15.082803.pkl/2010-12-16T22_13_02.403408&artifact=file://node1/data/sensors/
atrain/airs.aqua/L2/v5/2006/07/15/airx2ret/AIRS.2006.07.15.091.L2.RetStd.v5.0.14.0.G07294185430.hdf/
2010-08-04T15_06_41.273418"
```

Approach #2: Instrumentation Functions

Python

```
processStart('generateMatchupIndices', '/home/sflops/runMatchups.py', 'v0.1')
processUsedArtifacts('data:AIRS:RetStd', ['/home/sflops/AIRS.
2009.06.23.031.L2.RetStd.v5.2.2.0.G09175065058.hdf'], 'input')
processGeneratedArtifacts('indexFiles', ['/home/sflops/index-001.txt'], 'output')
processEnd('generateMatchupIndices')
```

Matlab

```
processStart('generateMatchupIndices', EXECUTABLE_PATH, VERSION, PROJECT_NAME, SESSION_NAME);
processUsedArtifacts(AIRS_COL, AIRS_GRANULES, 'input');
processGeneratedArtifacts(INDEX_COL, INDEX_FILES, 'output');
processEnd('generateMatchupIndices');
```

IDL

```
LOG_PROCESS_START, 'generateMatchupIndices', '/home/sflops/runMatchups.pro', 'v0.1'
LOG_PROCESS_USED_ARTIFACTS, 'data:AIRS:RetStd', '/home/sflops/AIRS.
2009.06.23.031.L2.RetStd.v5.2.2.0.G09175065058.hdf', 'input'
LOG_PROCESS_GENERATED_ARTIFACTS, 'data:indexFiles', '/home/sflops/index-001.txt', 'output'
LOG_PROCESS_END, 'generateMatchupIndices'
```

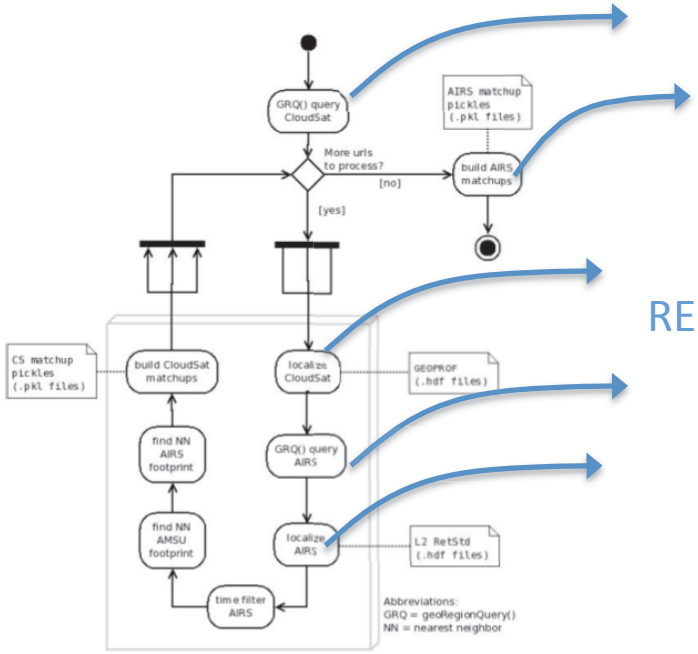
Command Line

```
curl -f -v -X POST --data-binary @generateMatchupIndices_provenance.log http://
provenance.jpl.nasa.gov:8099/services/logfile/upload
```

Approach #3: Workflows

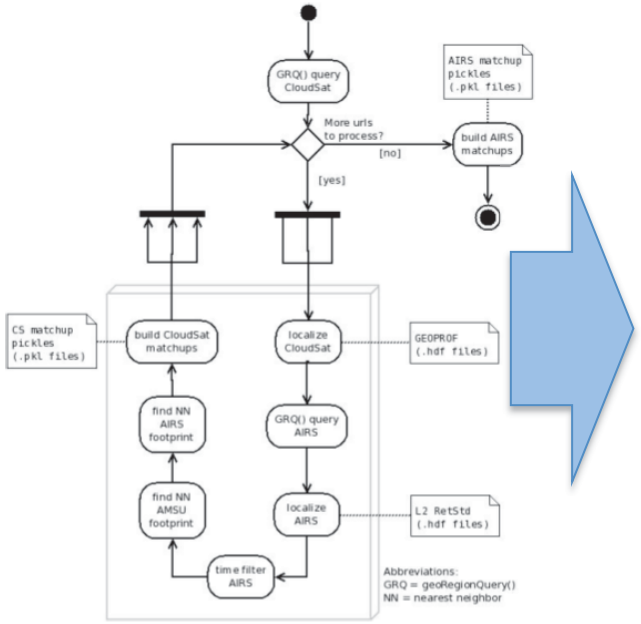
- Two ways to capture provenance from workflows

(a) Instrument workflow tasks to make REST service calls



REST calls

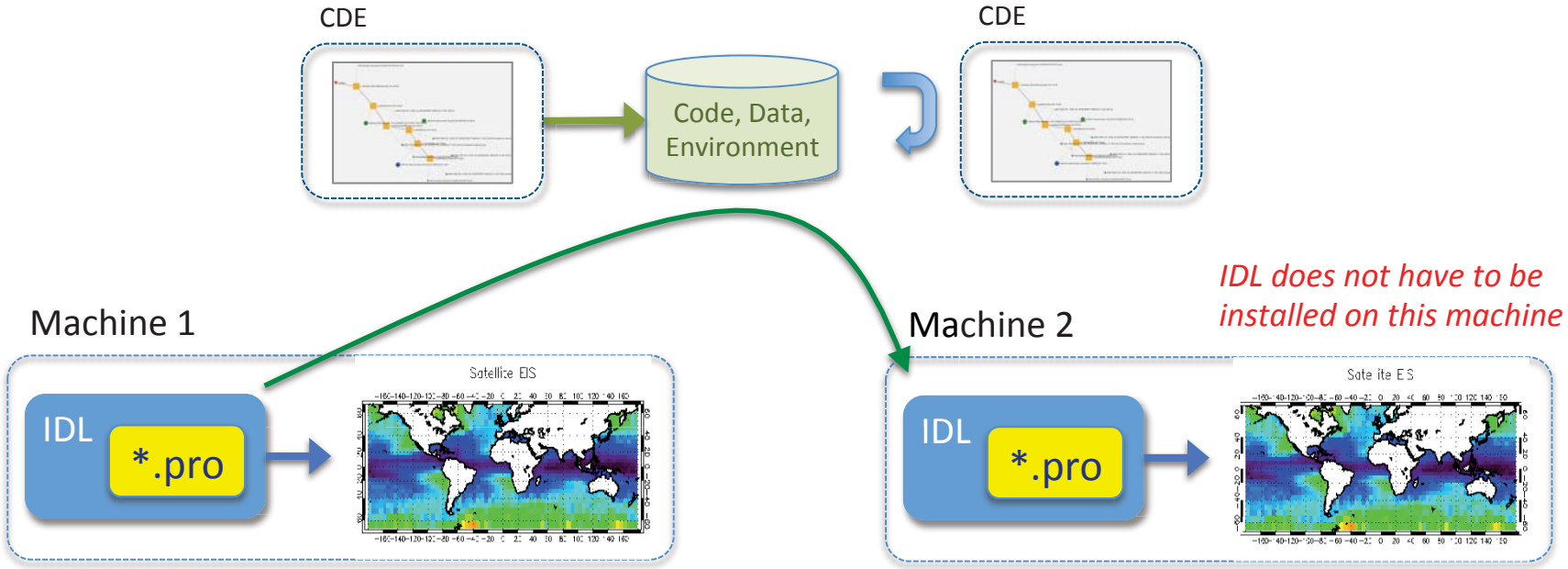
(b) Workflow to produce provenance records



OPM Export, annotated workflow documents, provenance logs

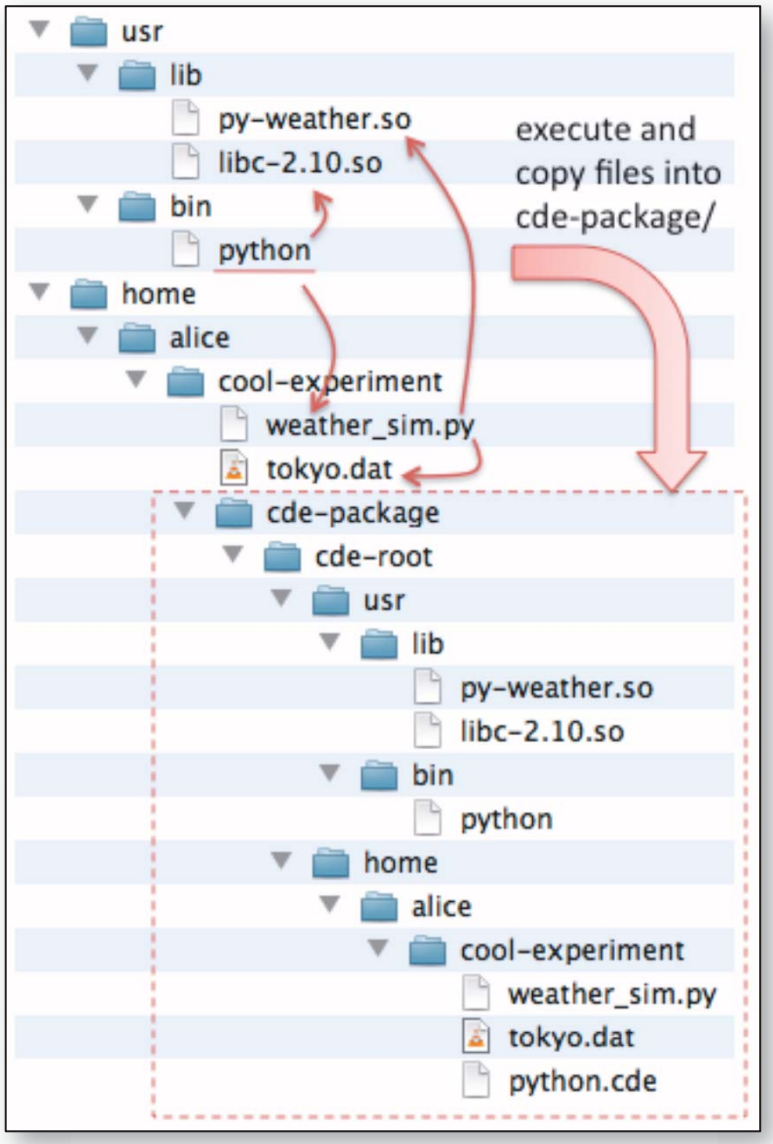
Approach #4: Automatic Capture of Runs

- Leveraged *open source* tool **CDE**: Automatic packaging of Code, Data, and Environment
  - *Philip Guo pg@cs.stanford.edu*
- **No modifications needed to processing code.**
  - High-level interaction recorded. Built upon *strace* tool.



Some Reproducible Research

- CDE creates a complete record of what was run
- Works well for *"incredibly informally"* research approaches
- Perform reproducible research
  - **Records** high-level process spawning, all input files used, and all output files generated.
  - **Packages** up all files and information needed to reproduce a run *(with some limitations)*
- Collaborate with colleagues who can **rerun on different machines**



THE BIG PICTURE

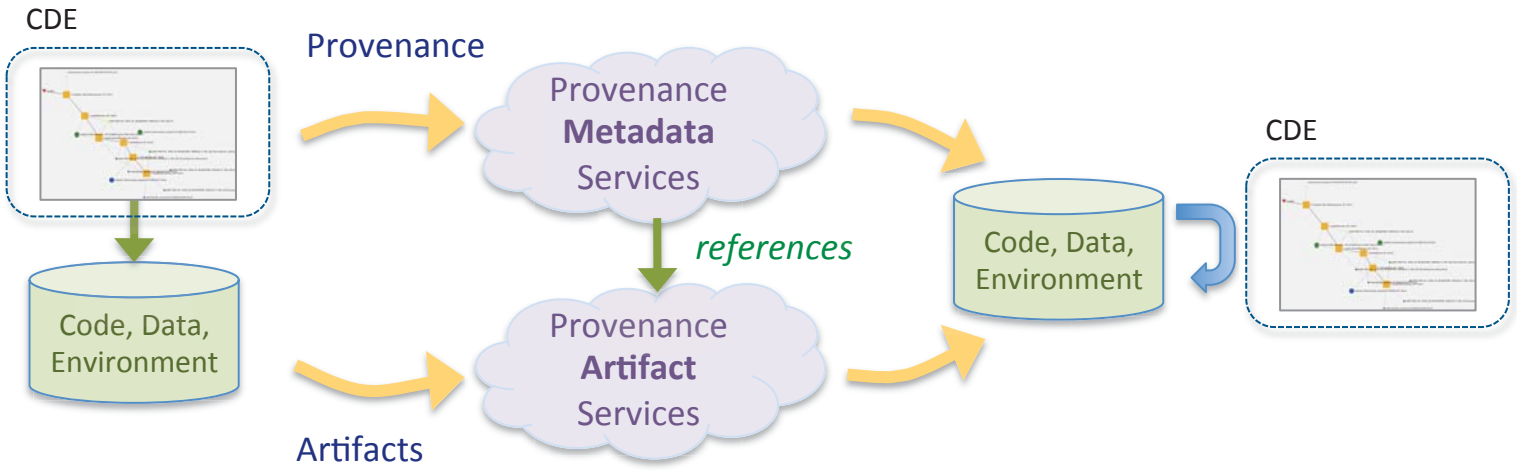
NASA Earth Science Data Preservation Content Specification

- *"…identify all the content items that need to be preserved to ensure their availability to support future investigations in long-term global change research."*

- These provenance services can support preservation of:
  - Data
  - Product software used in processing
  - Algorithm inputs (e.g. ancillary data)
  - Software tools used in processing and analysis

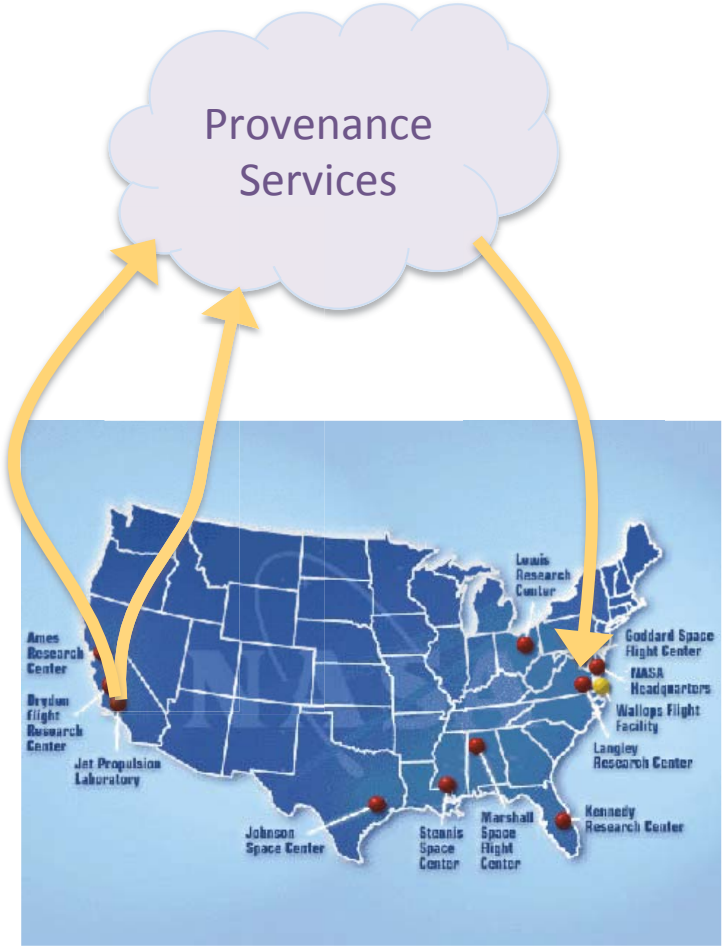
A Portable Runnable Preservation Record

- Provenance services addressing **preservation** of data product generation and analysis
- Provenance services enabling *some* **reproducibility** of results
- Provenance services facilitating **collaboration**



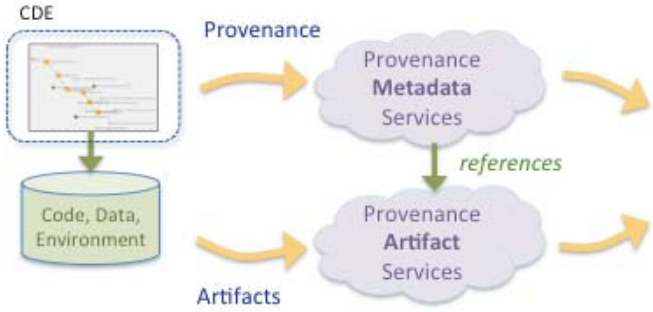
Provenance Collection for an "Earth Science Collaboratory" (ESC)

Provenance Collection



Provenance, Preservation, Discovery, Access, Visualization, Export, Reproducibility

Improving the Understanding of Production Legacy



- Improve understanding of data and processing lineage
- Near instant
  - Faceted search
  - Lineage graph
  - Lineage Timeline