CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY

DATA MANAGEMENT BEST PRACTICES WEBINAR

Data management practices to improve usability of data sets – now and forever

CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY

Workshop Information

Part –1 : Planning Data collection (Today's Webinar)

- Data Management Overview
- Best Practices for data collection
  - Site data
  - Field Data Collection
  - Model data

Part –2 : Data Tools for Exploratory Data Analysis (EDA) (Future)

- Best Practices for getting most out of the data
- Tools for
  - Data Search
  - Visualization
  - Data Analysis

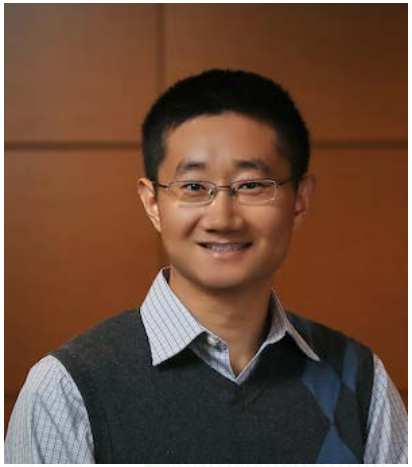
Speakers

Suresh Vannan is the manager of the Distributed Active Archive Center for Biogeochemistry at ORNL Suresh has extensive experience with building data management plans and in handling data workflows from collection to archival.

Giri Prakash is the Architecture and Services Strategy Team Manager for the Atmospheric Radiation Measurement (ARM) Archive. Giri's expertise include building end-to-end data management capabilities for climate and biodiversity projects.

Terri S. Killeffer is the Scientific Data Curator on the Data Team for the Next-Generation Ecosystem Experiments - Arctic (NGEE Arctic) project interacting with investigators to obtain data, assign metadata, and develop documentation.

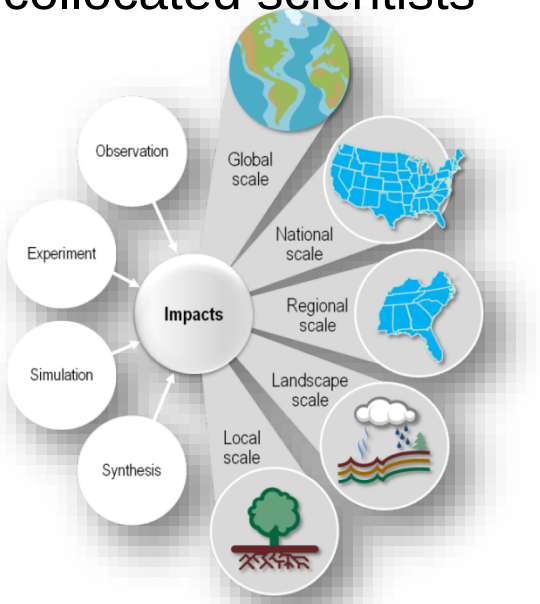
Yaxing Wei is a scientist at the ORNL Distributed Active Archive Center. Wei has been working on several research projects to provide geospatial information management, analysis, visualization, and sharing.



About the Climate Change Science Institute

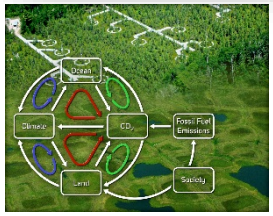
Advancing the Knowledge of Climate Change and Understanding its Consequences

- Formed in 2009 to integrate ORNL's climate research programs
- 130 collocated scientists



- https://ccsi.ornl.gov
- Facebook, Twitter, YouTube

Earth System Modeling



Integrative Ecosystem Science

Data Integration, Dissemination and Informatics

Impacts, Adaptation, and Vulnerability Science

CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY

Webinar Notes

- Please fill out the survey at the beginning of this webinar
- Towards the end, there will be another quick survey
- Please mute your microphones
- Please send your questions via the Q&A box on your screen
  - Questions will be answered at the end of the webinar
- Slides will be made available on the CCSI website; link will be forwarded to your email address

Data Management Best Practices - Part 1

Workshop Goals and

Data Management Overview

Suresh Vannan

Data Theme Lead, CCSI

santhanavans@ornl.gov

OAK RIDGE National Laboratory

Workshop Goal

Provide data management practices that investigators should perform during the course of data collection to improve the usability of their data sets

Data Management – What?

20-year rule

The data set and accompanying documentation should be prepared for a user 20 years into the future

Prepare the data and documentation for a user who is unfamiliar with your project, methods, and observations

Data Management – Why?

- **Protection:** About 32 percent of computer users experience data loss each year.
- **Publication:** Agencies are now required to manage the digital data resulting from federally funded scientific research
- **Provenance:** To support research findings we need to preserve data and its provenance to be able to trace and record the origins of the data
- **Author Credit:** Recognize data creators for the value of their data

The Washington Post

Hackers post scientists' e-mails

Climate change skeptics say content proves data rigged to pin cause of global warming on humans.

» Juliet Eilperin

CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY

Fundamentals of Data Management – Project Level

1. Define data workflow – Collection to Archive
2. Train staff for data/metadata handling
3. Communicate standards and metadata needs
4. Define Data Quality criteria
5. Establish a long-term data steward
6. Establish and communicate a Data use/Submission policy

Fundamentals of Data Management – Data Set Level

1. Define the contents of your data files
2. Define the variables
3. Use consistent data organization
4. Use stable file formats
5. Assign descriptive file names
6. Preserve processing information
7. Perform basic quality assurance
8. Provide documentation
9. Protect your data
10. Preserve your data

Data Management Plan

- Information about the data
  - Description of data to be produced
  - How will it be managed in short-term?
- Description of Data
  - Format, number of files, approx. volume
  - Processing and quality
- Metadata Content & Format
  - Documentation about the data
- Policies for Access, Sharing, & Reuse
- Long-term Storage & Data Managemen
  - Where will data be archived?

Research Data Management: An introductory Webinar from OpenAIRE and EUDAT:
https://goo.gl/OX6dAc

Remember to include data management costs in Proposal Budget

Costs

At least **10% of total funding** is suggested to be devoted towards managing the data used and produced by a project. Cost will be relative to the size, complexity, length, and access needs for a project.

Another way to interpret this is that at least **10% of investigators time** should be spent on actively managing their data.

Data collection vs Data Management

The 1990 census:

- $2.6 billion for data Collection
- $433 million for data Processing
- $114 million for data Dissemination

Source: http://www.nap.edu/read/4805/chapter/5

Staffing and Training

- Establish a Data Management plan
- Communicate plan
- Establish standards and conventions
- Embedded data management in the research costs
- Cultivate culture of data management to be done alongside research
- For large projects (multi-organization, multi-year, multi-levels of data) recruit a data officer
- Specialized technicians are needed for advanced tiers of services.
- Regularly communicate about data and metadata needs within the project

Standards - Metadata

Type	Standard
GIS data? Raster/vector or point data	FGDC Content Standard
Data retrieved from instruments such as monitoring stations or satellites	ISO 19115
Ecological data	Ecological Markup Language
Specimen occurrence and observational records	Darwin Core

Most importantly …

Document… Document…Document

- Data characteristics and description
  - When and how frequently the data were collected
  - Where and with what spatial resolution the data were collected
  - The name(s) of the data file(s) in the data set
  - Example data file records for each data type file
  - Special codes used, including those for missing values
  - Date the data set was last modified
  - English language translation of any data values and descriptors in another language
  - How each parameter was measured or produced (methods), units of measure, format, precision and accuracy, and relationship to other data in the data se
- Data acquisition
- Quality assessment
- Supplemental information

http://goo.gl/MJjXmt

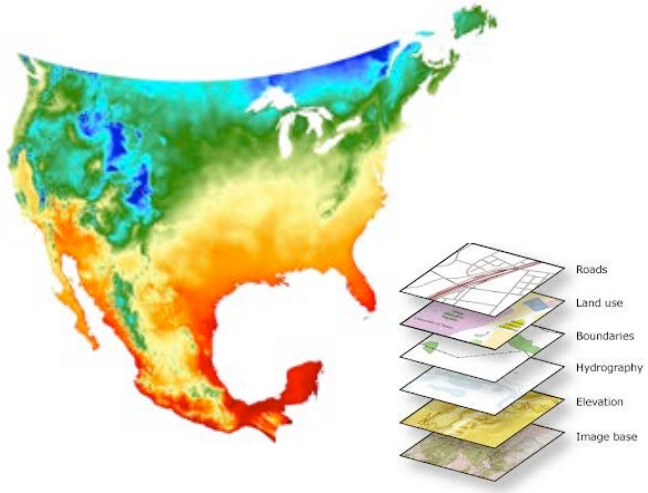
Standards – File formats

Raster

- Geotiff
- netCDF
  - with Climate and Forecast convention preferred

Vector

- Shapefile
- KML



Tabular

- CSV

Resources

USGS data management web site: http://www.usgs.gov/datamanagement/index.php

ORNL DAAC Data Management for Data Providers: http://daac.ornl.gov/PI/manage.shtml

ORNL DAAC Best Practices for Preparing Environmental Data Sets to Share and Archive: http://daac.ornl.gov/PI/BestPractices-2010.pdf

OSU Libraries Research Data Services: http://guides.library.oregonstate.edu/managing-data

DataONE Best Practices: https://www.dataone.org/sites/all/documents/DataONE_BP_Primer_020212.pdf

Agency Specific Data Management

DOE: http://science.energy.gov/funding-opportunities/digital-data-management/

DOE-BER: http://science.energy.gov/ber/funding-opportunities/digital-data-management/

NSF: http://www.nsf.gov/news/special_reports/public_access/index.jsp?WT.mc_id=USNSF_51

Open access plans for all agencies: http://guides.library.oregonstate.edu/federaloa

NASA: http://science.nasa.gov/earth-science/earth-science-data/data-management-plan-guidance

Data Management Best Practices - Part 1

Site Data Management

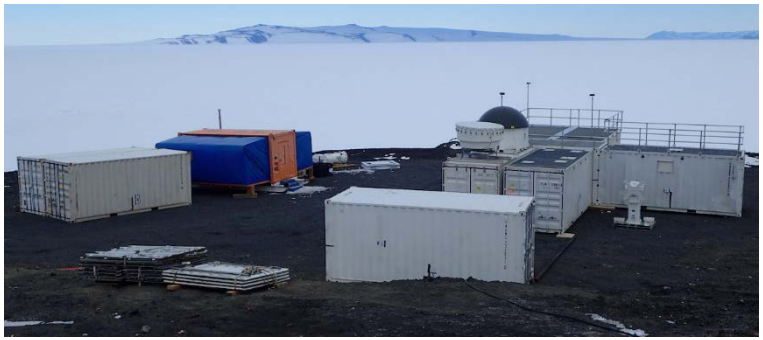
Giri Prakash
Architecture and Services Strategy Team Manager for the Atmospheric Radiation Measurement (ARM) Archive.

Palanisamyg@ornl.gov

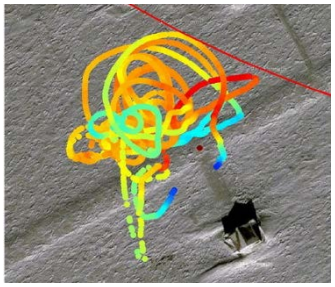
Topics

- Instrument deployment
- Site data collection
- Data retention & transfer
- Data ingest & data flow monitoring
- Preparing and communicating data quality
- Data security and archival
- Metadata management

Site Data



This view shows the location of the Manacapuru, Brazil, ARM Mobile Facility.

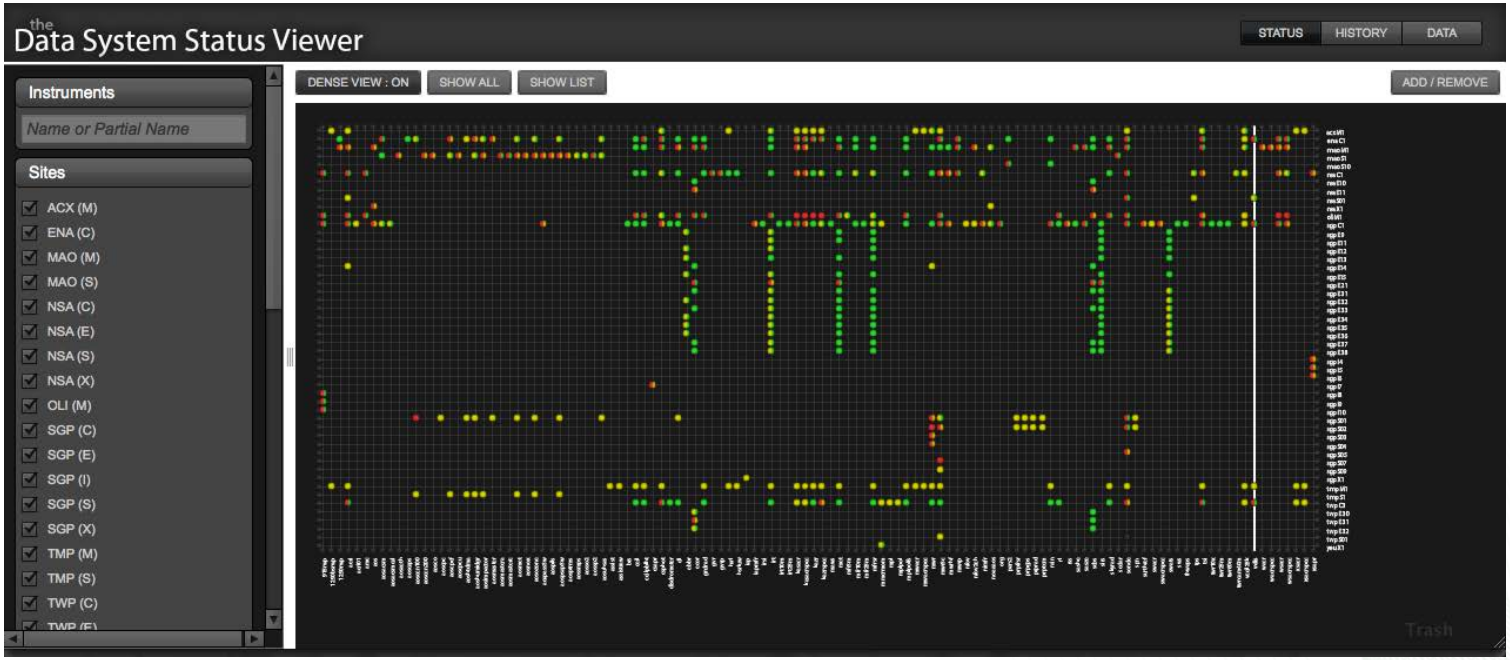


Deployment of Site Instruments/Sensors

- Site visit & logistics
- Plan for a pre-operational period
  - Deployment and initial calibration
- Assign instrument experts
- Assess quality of pre-operational data and calibrate as necessary.

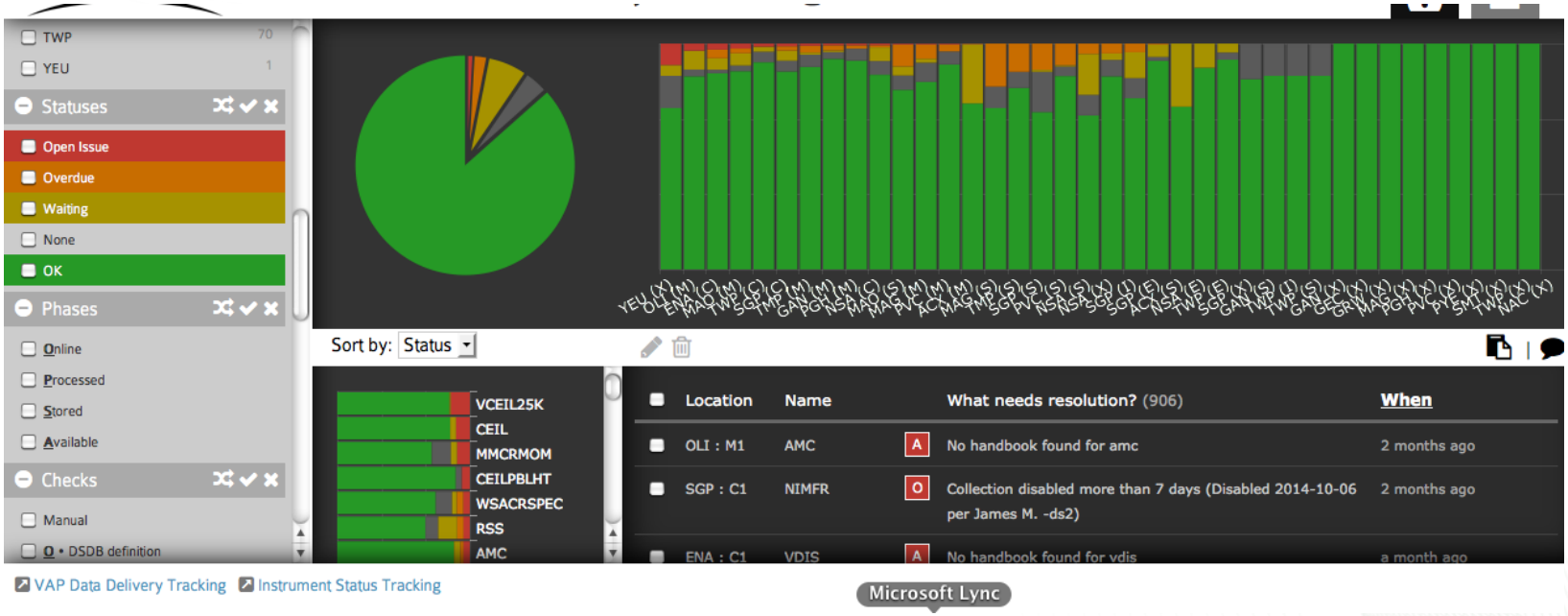
Data Collection

- Set up a site data system
- Establish network from instrument – data system – data center
- Train and mentor the site technician to manage the data system
- Establish instrument monitoring



Data Flow and Tracking

- Track the data through various phases – online, processed, stored and available
- Each phase has various checks to enable operations teams to monitor any data issues



Data Transfer

- Secured network-based access to the site data systems
- Data transfer from site to data center
  - Network based transfer
  - Disk shipments
- Confirmation of successful data transformation using checksums
- Setting up enough disk space until the data transfer is fully complete and verified

Data Processing

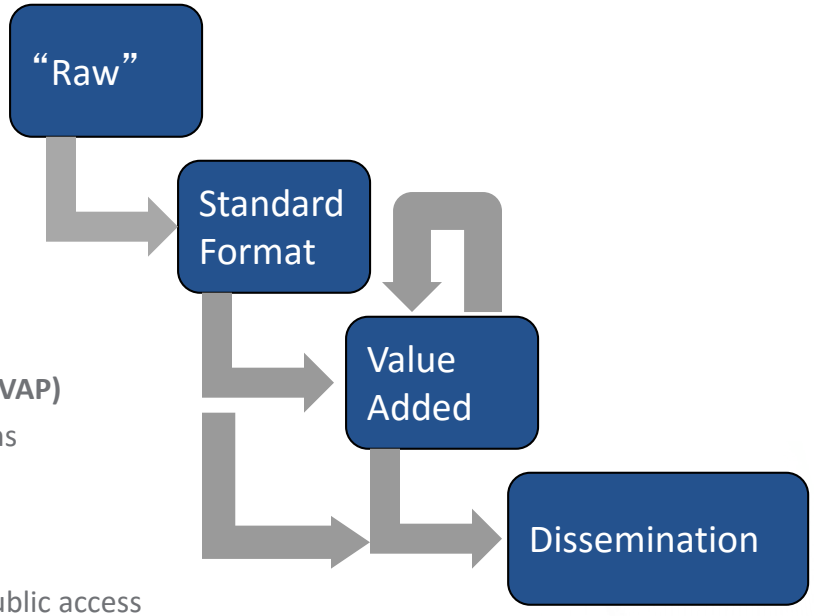
- Unmodified from instrument

Ingests

- Engineering units
- Quality flags
- Updated hourly

Value-added Products (VAP)

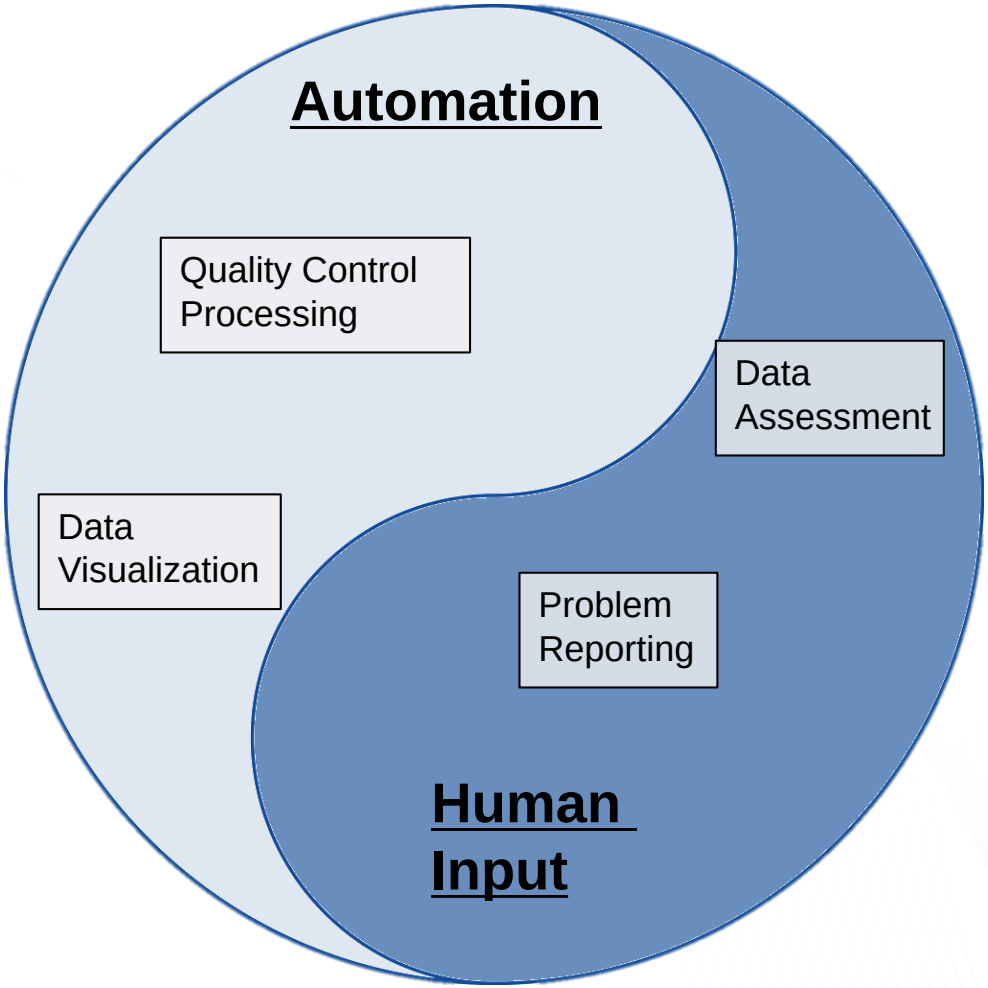
- Advanced algorithms
- Multiple inputs
  - Principal investigators/Public access



Fills some of the unmet measurement needs

Improves the quality of existing measurements

Data Quality



Data Quality

- Quality Control (QC) Processing
  - Automated Mentor QC (Included in data files)
    - MIN/MAX/DELTA; Many include additional QC tests
    - Library of functions to make these tests easily adaptable from one instrument to the next
  - Summarized into Easy to Read Metrics Tables

```
float precip(time) ;
        precip:long_name = "Total precipitation over one minute sampling period" ;
        precip:units = "mm" ;
        precip:valid_min = 0.f ;
        precip:valid_max = 100.f ;
        precip:missing_value = -9999.f ;
        precip:comment = "Sum of the 20 3-second observations during the sampling period." ;
int qc_precip(time) ;
        qc_precip:long_name = "Quality check results on field: Total precipitation over one minute sampling period" ;
        qc_precip:units = "unitless" ;
        qc_precip:description = "This field contains bit packed values which should be interpreted as listed. No bits set (zero) represents good data." ;
        qc_precip:bit_1_description = "Value is equal to missing_value." ;
        qc_precip:bit_1_assessment = "Bad" ;
        qc_precip:bit_2_description = "Value is less than the valid_min." ;
        qc_precip:bit_2_assessment = "Bad" ;
        qc_precip:bit_3_description = "Value is greater than the valid_max." ;
        qc_precip:bit_3_assessment = "Bad" ;
        qc_precip:bit_4_description = "Difference between current and previous values exceeds valid_delta." ;
        qc_precip:bit_4_assessment = "Indeterminate" ;
        qc_precip:bit_5_description = "Scans per min does not equal to 20. data set to -9999." ;
        qc_precip:bit_5_assessment = "Bad" ;
        qc_precip:bit_6_description = "Error latch does not equal to 0, data set to -9999." ;
```

Data Quality

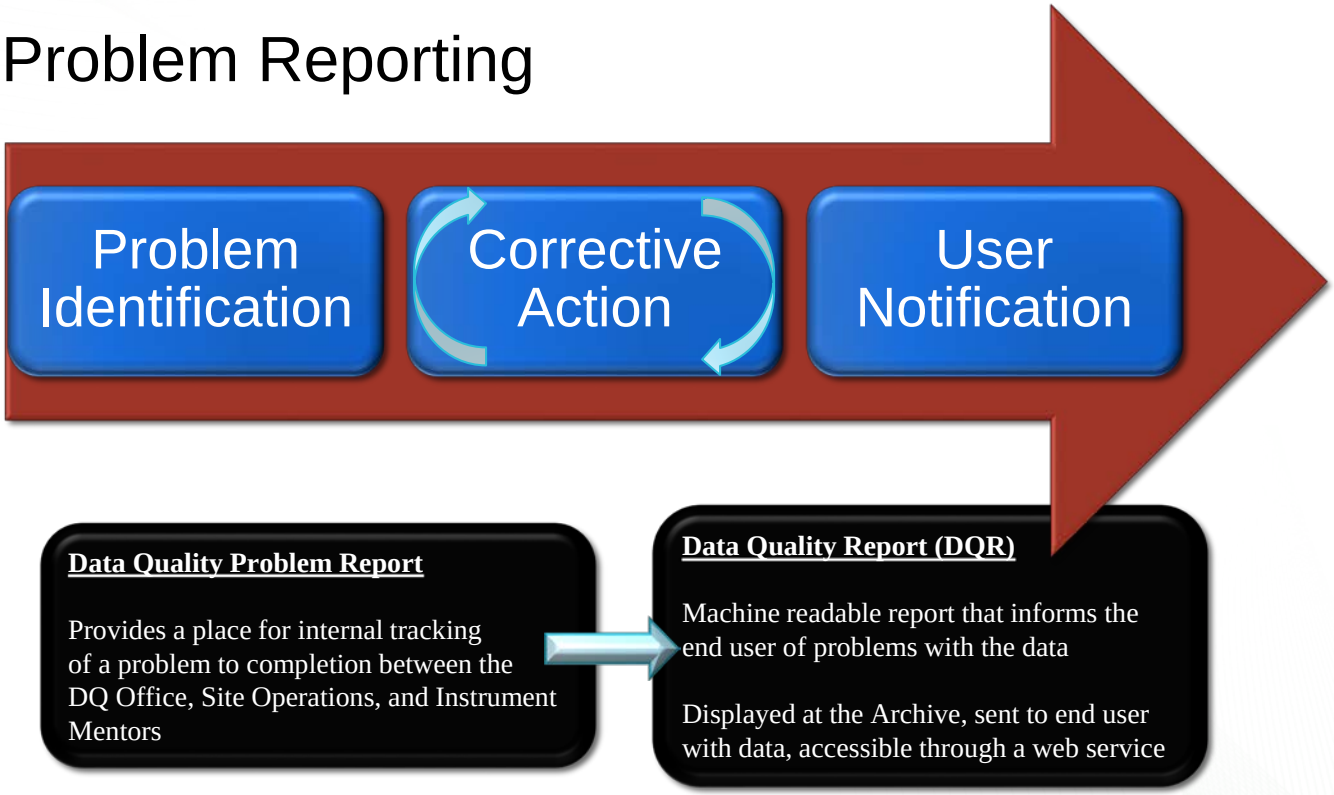
- Quality Control Tests/Metrics
  - Some QC Tests:

- Persistence (Flatlined data)
- Grubbs Statistical Test for Outliers
- Instrument Comparison
- Derived Quantity Comparison
- Time Drift
- Power Outage Flagging
- Probability Density Function
  - Cross Instrument and Cross Site Comparisons
- Time Varying Limits
- Specialized QC developed in conjunction with the Instrument Mentors

Data Quality

- Data Assessment
  - Review the data on a daily or weekly basis
  - Report findings to the infrastructure through a Data Quality Assessment Report
  - Make use of undergraduate student analysts

Data Quality



Data Security and Archival

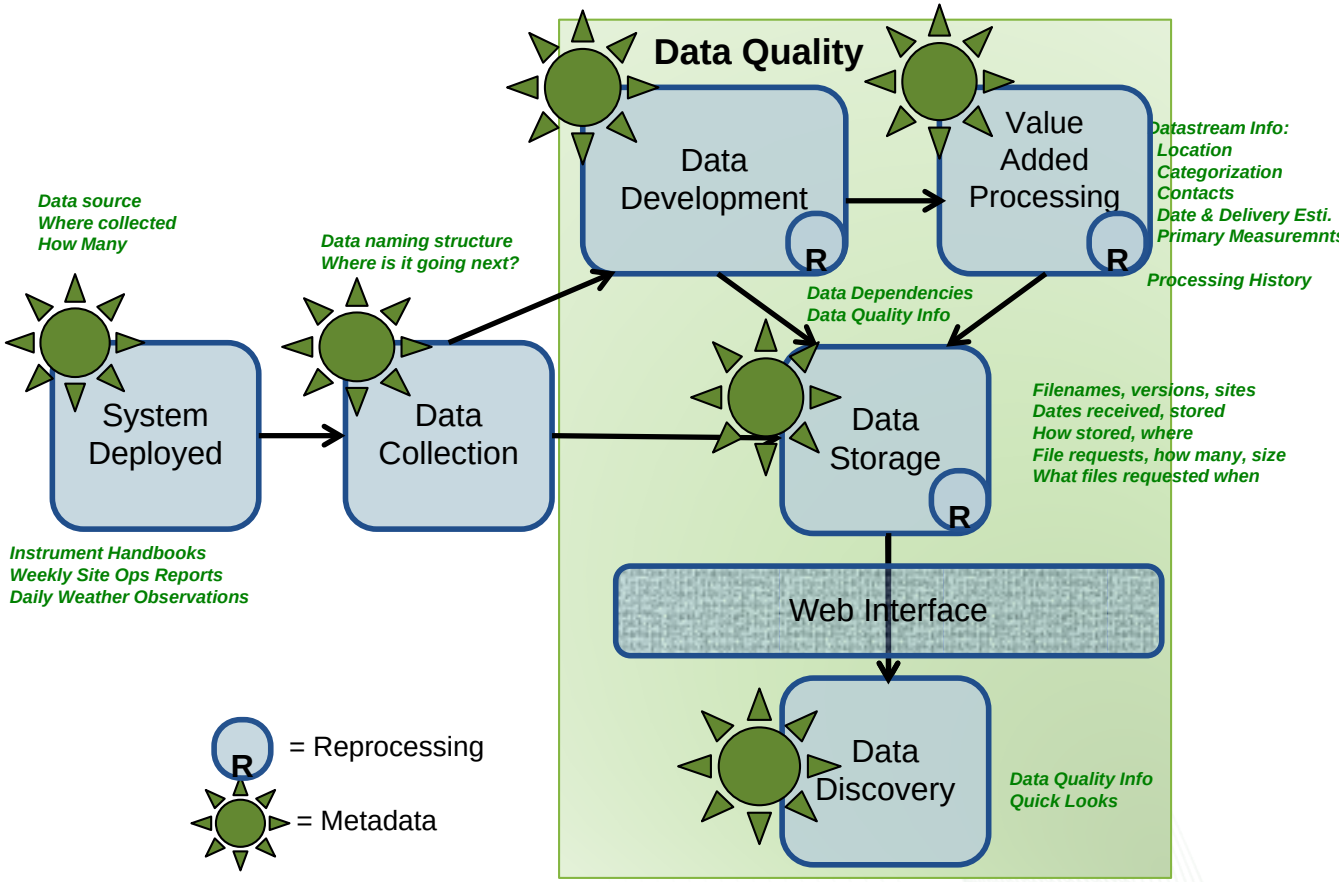
- Verify data integrity during data transfer
- Archive every version of data files that are released from upstream process:
  - Rule of thumb: if you can't reproduce, then it should be archived
- Archival needs to include backup strategy, both onsite (for immediate data recovery) and offsite (disaster recovery)

Reprocessing and Communications

- Changes to the published datasets
- Communicating users about any change in data quality and resulting new version of data
  - Archiving user order details

Metadata – Captured Throughout the Data Lifecycle

- Metadata Management
  - Define term
  - Example: Aerosol Observing System
  - Why, what, who, where, how
- Processing data to add value
  - Data products
  - VAP processing
  - Reprocessing
  - Data lifecycle and metadata overlay



Source: Alice Cialella, ARM

Data Management Best Practices - Part 1

Field Data Collection

Terri Killeffer

NGEE-Arctic Data Curator

killefferts@ornl.gov

OAK RIDGE National Laboratory

What is Field Data?

Examples of Field Data Collections

- Organism observation/collection
- Soil samples
- Geophysics
- Sap flow
- Mineralization rates
- Soil incubation studies
- Geochemical and isotopic analyses
- Biodiversity inventory
- Images

Electrical Resistivity Methods Used to Explore Subsurface Properties in Ice-Rich Tundra. Stan Wullschleger. 2012-08-24. CC BY-NC 2.0
Proteus aircraft (426 004 001). Energy.gov.
USGS Hawaiian Volcano Observatory at Kilauea Volcano. Michael Poland, USGS. 2008-09-03..
Modeling climate change. Argonne National Laboratory. 2013-07-25. CC BY-NC-SA 2.0.
Ice Core. Kris McCraken. 2013-03-23. CC BY-NC-SA 2.0
Procambarus clarkii. Ryan Hagerty, USFWS. 2016-05-12
Two Instrument Arrays Monitor Geomechanical Properties of Permafrost Soils. Stan Wullschleger. 2012-09-22. CC BY-NC-SA 2.0

CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY


Before Collecting Data
While Collecting Data
After Collecting Data

Image:
Research Data Management.
Janneke Staaks. 2013-11-10. CC BY-NC 2.0)

Don't Work in Isolation

- Data will be less interoperable
- Potential duplication of effort
- Possibly miss collecting important data

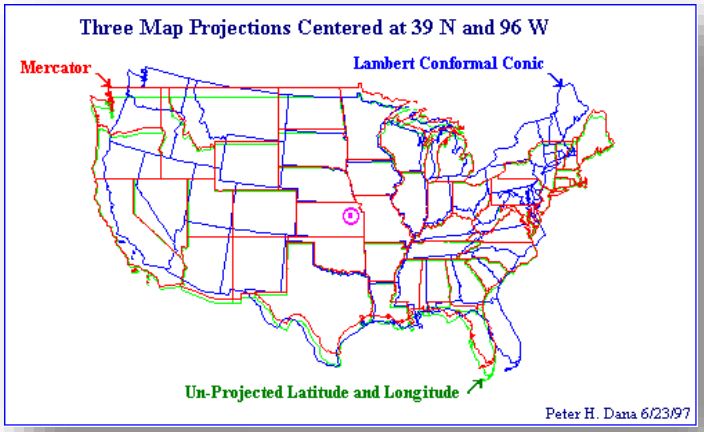
Cooperate, Coordinate, and Collaborate

- Work within and across teams/disciplines
- Work across related projects
- Review and refine the Data Management Plan


Project Goals
Final Products
Data Goals

Items to Address Across the Project

- Naming of sampling locations
- Base maps
- Spatial Reference System and spatial coordinates
- Reporting time and date
- Identify data and sample archives
- Standardize variable names
- Instruments
- Collection techniques
- Sample and subsample labeling and tracking



http://www.colorado.edu/geography/gcraft/notes/mapproj/gif/threepro.gif

Plan to Capture Metadata at Every Stage

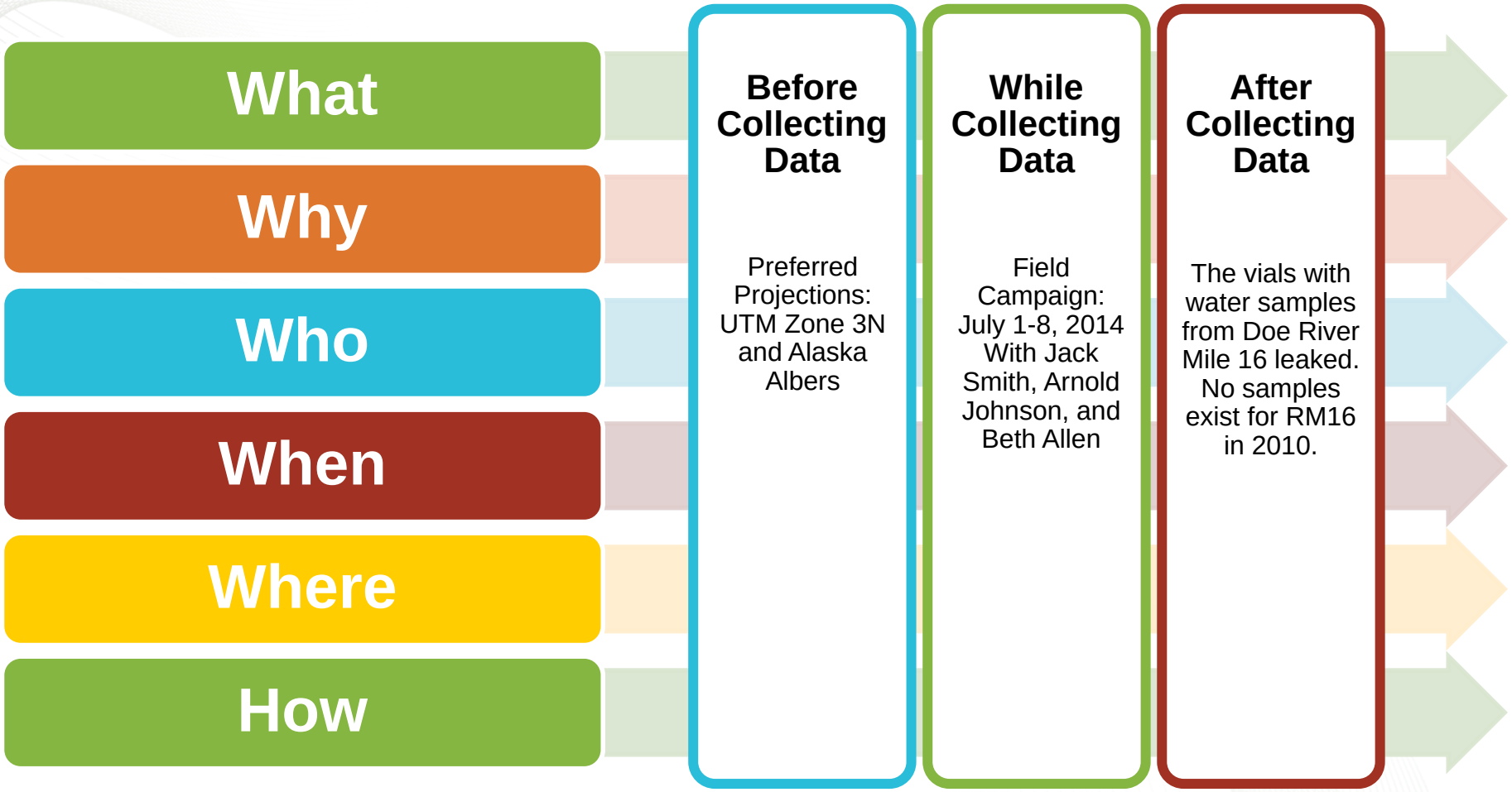


Image:
Research Data Management.
Janneke Staaks. 2013/11/10. CC BY-NC 2.0)

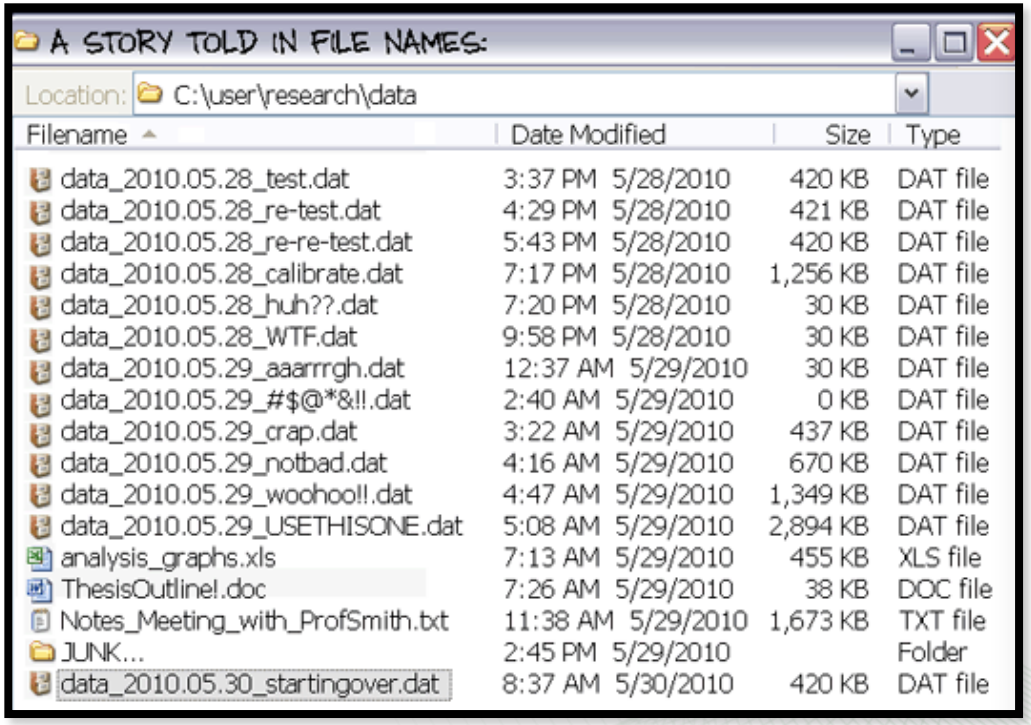
Data in Development

- Record the names of people participating in the field collection or laboratory analysis
- Take pictures and videos
- Follow best practices and record methodology
- Record method/instrument for capturing data and geolocation

Data in Development

- Label samples
- Note issues, lost samples/data, defective instruments, reason no data collected, etc.
- Develop well organized data files
- Record all data processing steps
- Backup data

Courtesy of PhD Comics



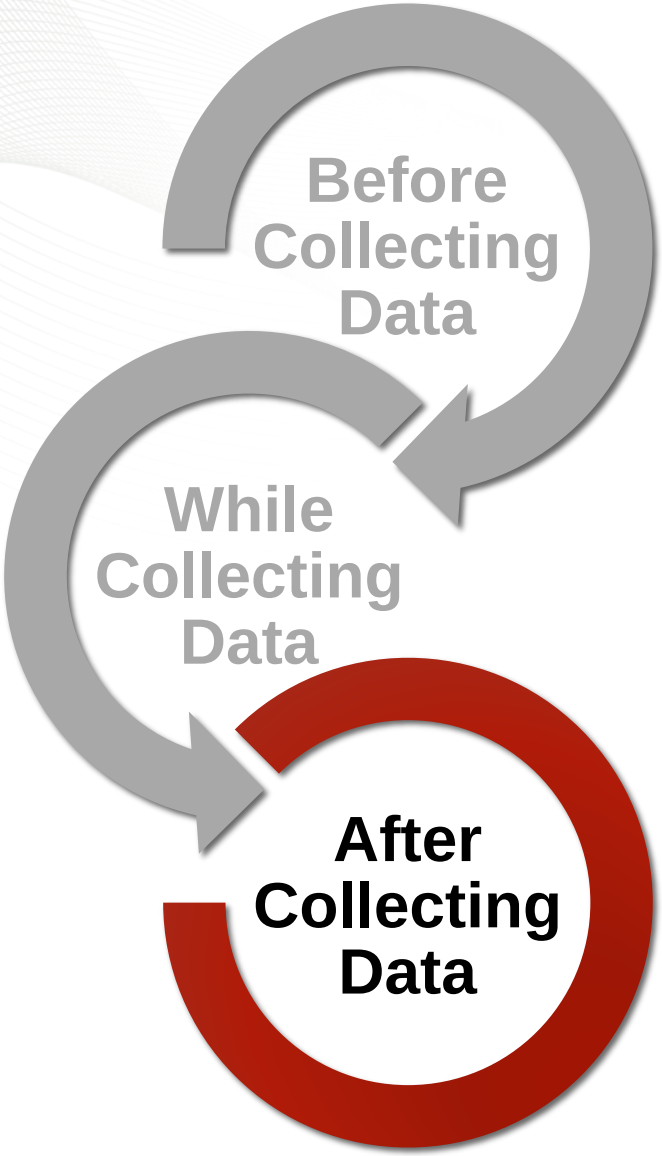
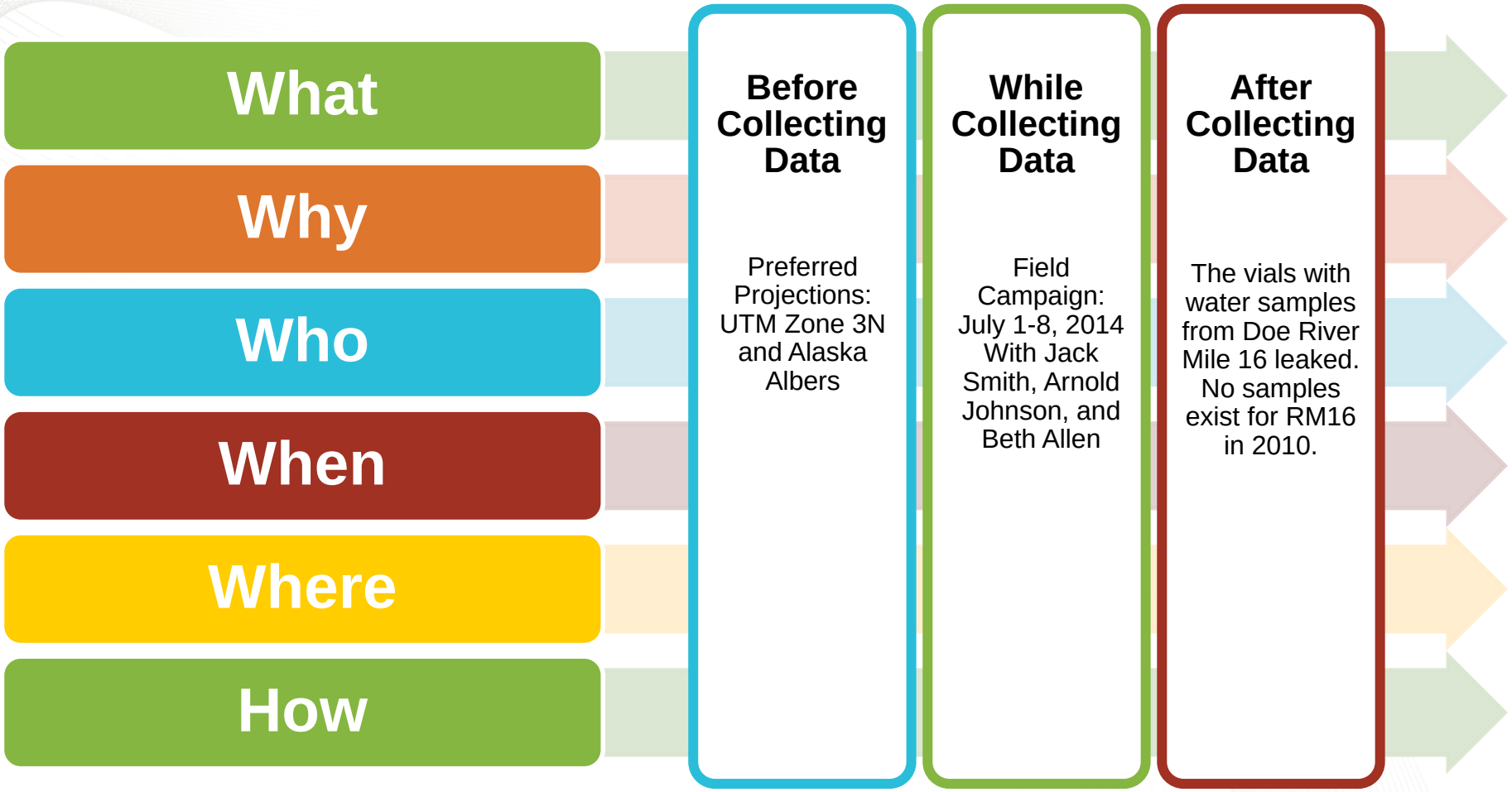
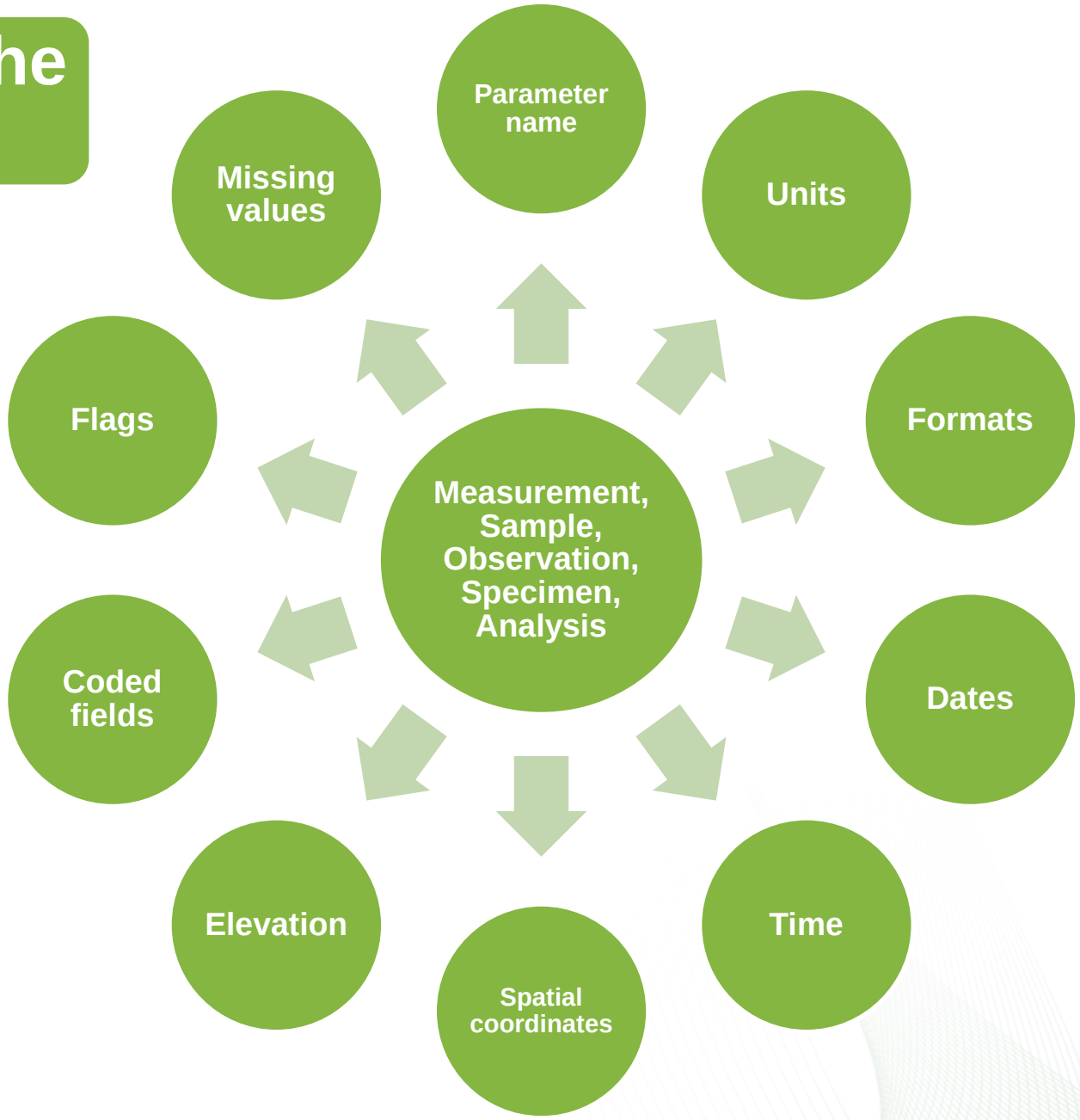


Image:
Research Data Management.
Janneke Staaks. 2013-11-10. CC BY-NC 2.0)

Metadata Collected



Content of the Data Files



ORNL DAAC, Define the contents of your data files

Data Dictionary Example

column_name	units/format	description
Core_ID		Core collection: Hydraulic drill (Big Beaver) with a fitted liner was used to collect intact frozen soil cores to a maximum depth of 1m. See footnote 1.
Date_sampled	YYYY-MM-DD	Date core was collected.
Lab_processed		ORNL core processing: Soil cores were shipped frozen and returned to -20°C freezer and stored until further processing.
Date_processed	YYYY-MM-DD	Date core was processed at ORNL.
Region		Possible values: North Slope, Seward Peninsula
Locale		Possible values: Barrow, Council
Site		Possible values: Intensive Site 0, Intensive Site 1
Area		Possible values: A,B,C,D
Northing_UTM	meters	Core collection location. NGEE Arctic is working in the Universal Transverse Mercator (UTM) coordinate system. All coordinates are in northing and easting meters. We are using NAD 83 datum and UTM Zone 4North.
Easting_UTM	meters	Core collection location. NGEE Arctic is working in the Universal Transverse Mercator (UTM) coordinate system. All coordinates are in northing and easting meters. We are using NAD 83 datum and UTM Zone 4North.
Elevation	meters	Core collection location elevation.

Data Dictionary from dataset: http://dx.doi.org/10.5440/1109232

Data Dictionary Example

Column_name	Units/format	Description
Moisture_content_of_soil_layer	percent	Percent soil moisture during incubation.
pH_of_soil_layer	pH units	Initial pH of soils before incubation; Conducted on 2:1 distilled water to soil slurry (for mineral soil) or 4:1 distilled water to soil slurry (for organic soil).
Incubation_length	Days	Length of the incubation study in days.
Target_Incubation_Temperature	Degrees Celsius	Incubation temperature set on incubators (Thermo Scientific Precision Model 815 Incubator, Marietta, OH).
Anaerob_treat		Soil incubations - aerobic or anaerobic
Day_of_Incubation		Measurement day (if multiple measurements over incubation period).
CO_2_per_g_dry_weight	mg C/ g dry weight	Cumulative CO_2 production per g dry soil over a given period of the incubation (e.g., between days 1 and 3). A value of "-9999" indicates missing data – see data quality flag column.
CO_2_per_g_dry_weight_fl		Data quality flag for cumulative CO_2 production per g dry soil to indicate missing data. V0 is valid value, M1 is missing value because no value is available (a bad injection on the gas chromatograph).

Data Quality Flag Table Example

Flag Value	Description
V0	Valid value
V1	Valid value but comprised wholly or partially of below detection limit data
V2	Valid estimated value
V3	Valid interpolated value
V4	Valid value despite failing to meet some QC or statistical criteria
V5	Valid value but qualified because of possible contamination (e.g., pollution source, laboratory contamination source)
V6	Valid value but qualified due to non-standard sampling conditions (e.g., instrument malfunction, sample handling)
V7	Valid value but set equal to the detection limit (DL) because the measured value was below the DL
M1	Missing value because no value is available
M2	Missing value because invalidated by data originator
H1	Historical data that have not been assessed or validated

Filename :	mercury_methylation_in_tundra_soils.csv
Contact:	Richard Murphy murphy@murphy.com
Data modified:	2016-04-13
Modified by:	Bob Lane
DOI:	1234567
Data citation:	Mercury Methyla Barrow, Alaska. Charlie Brown, Chris Sn

Header for the File

Location Coordinates

CORE_ID	Date_sampled	Longitude	Latitude	Region	Locale	Site
	YYYY-MM-DD	decimal degrees	decimal degrees			
NGADG0071	2012-04-16	-156.6046	71.2793	North Slc	Barrow	Intensive
NGADG0071	2012-04-16	-156.6046	71.2793	North Slc	Barrow	Intensive
NGAD						

METHYL_MERCURY	METHYL_MERCURY_SD	METHYL_MERCURY_DL	METHYL_MERCURY_FL
ng/g dwt	ng/g dwt	ng/g dwt	
0.079	0.014	0.004	V0
-9999	-9999	0.004	M1
0.256	0.023	0.004	V0
-9999	-9999	0.004	M1
0.42	0.051	0.004	V0
-9999	-9999	0.004	M1

Missing Values

Quality Flag Column

Modified dataset from: http://dx.doi.org/10.5440/1235032

Standardizing the File Formats

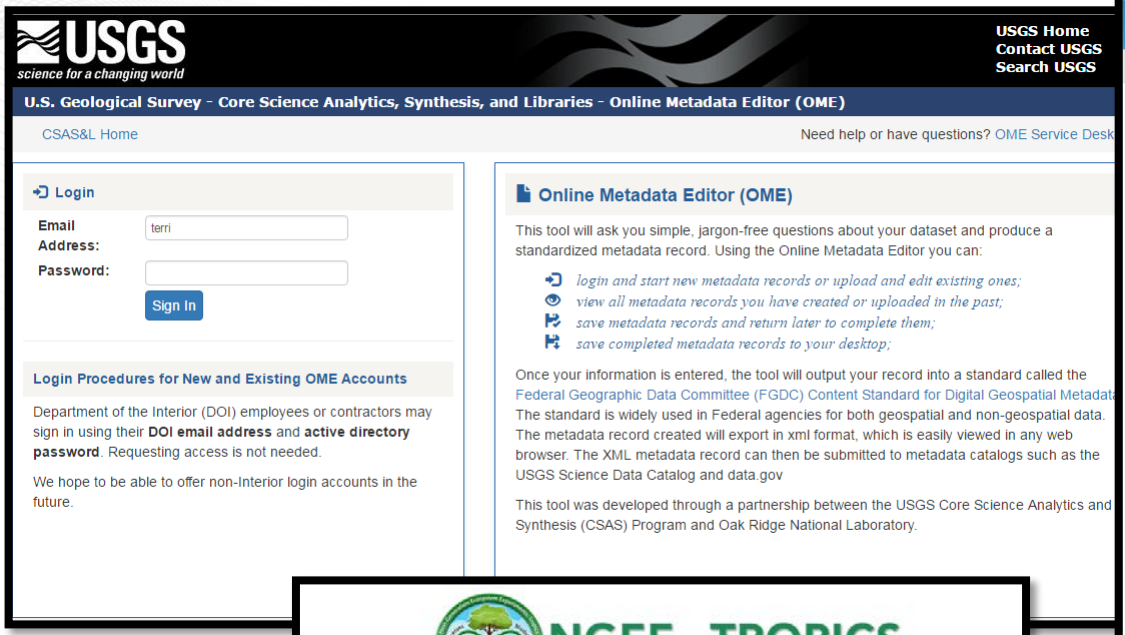
- Save files in open software or open file format
- Proprietary software will most likely become obsolete or not back compatible
- Use text (ASCII) file formats for tabular data
  - e.g., .txt or .csv (comma-separated values)
- Utilize the standard formats established in the Data Management Plan

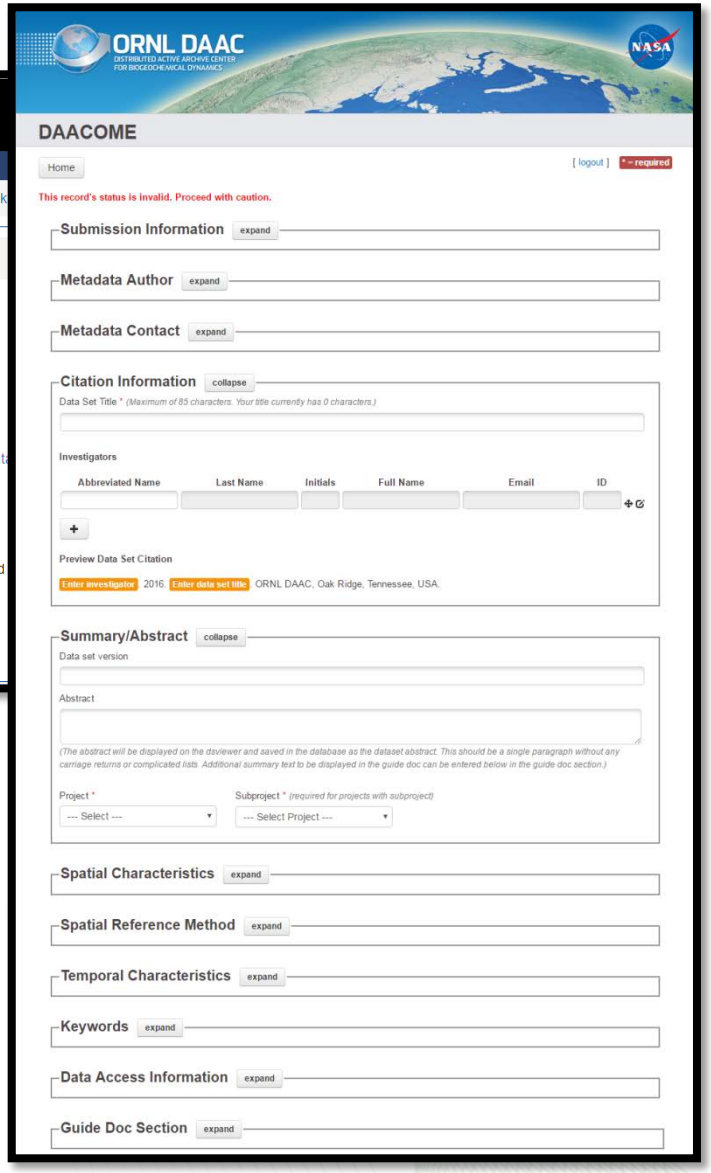
http://news.bbc.co.uk/2/hi/6265976.stm

```
Core_ID,Date_sampled,Lab_processed,Date_processed,Region,Locale,Site,Area,Soil_type,upper_depth_of_soil_layer,lower_depth_of_soil_layer,Incubation_condition,Incubation_temp,Length_of_incubation,Microcosm_Replicate,Respiration_rate,Methane_production_rate
,yyyy-mm-dd,,yyyy-mm-dd,,,,,cm,cm,,degree Celsius,days,,umoles CO2 g dwt-1,umoles CO2 g dwt-1
NGADG0017,2012-04-12,ORNL,2013-01-24,North Slope,Barrow,Intensive Site 1,A,organic,0,21.5,anoxic,-2,2,1,0,0
NGADG0017,2012-04-12,ORNL,2013-01-24,North Slope,Barrow,Intensive Site 1,A,organic,0,21.5,anoxic,-2,2,2,0,0
NGADG0017,2012-04-12,ORNL,2013-01-24,North Slope,Barrow,Intensive Site 1,A,organic,0,21.5,anoxic,-2,2,3,0,0
```

CSV example from dataset: http://dx.doi.org/10.5440/1109232

Help with Metadata Development





CLIMATE CHANGE SCIENCE INSTITUTE
OAK RIDGE NATIONAL LABORATORY

You've Reached the Summit

- ✓Determined what data to archive
- ✓Described the content of the data
- ✓Performed validation and quality control
- ✓Saved in correct file formats
- ✓Obtained a Digital Object Identifier (DOI)
- ✓Submitted to an archive
- ✓Shared with the public

Data Management Best Practices – Part I

Model Outputs

Yaxing Wei

Data Scientist

weiy@ornl.gov

OAK RIDGE National Laboratory

Why Model Outputs Management Matters?

- Consistency and Interoperability
  - To facilitate analysis, integration, and re-use

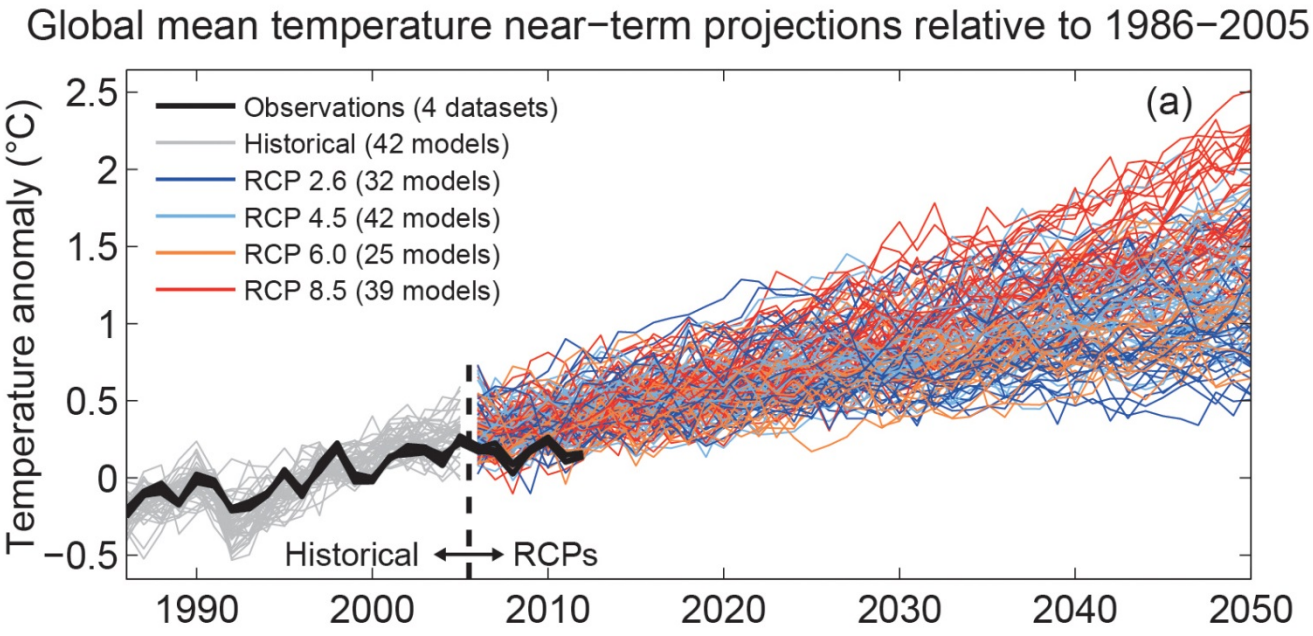


Figure TS.14 in Intergovernmental Panel on Climate Change (IPCC) Assessment Report (AR5) WG1 Report

What Makes Model Outputs Management Hard?

- Spatial
  - Site → Local → Regional → Global
  - Coarse resolution → Fine resolution
- Temporal
  - Paleo → Recent past → Future projections
  - Decadal → Annual → Monthly → Daily → Hourly
- Voluminous
  - 36 TB (CMIP3) x 50 → 1.8 PB (CMIP5) x 50 → 90 PB (CMIP6)*
- Various Formats
  - ASCII, Binary, netCDF, …

CMIP: Coupled Model Intercomparison Project
** Source: Michael Lautenschlager, CMIP5 Data Management, 2013*

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and beyond

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and beyond

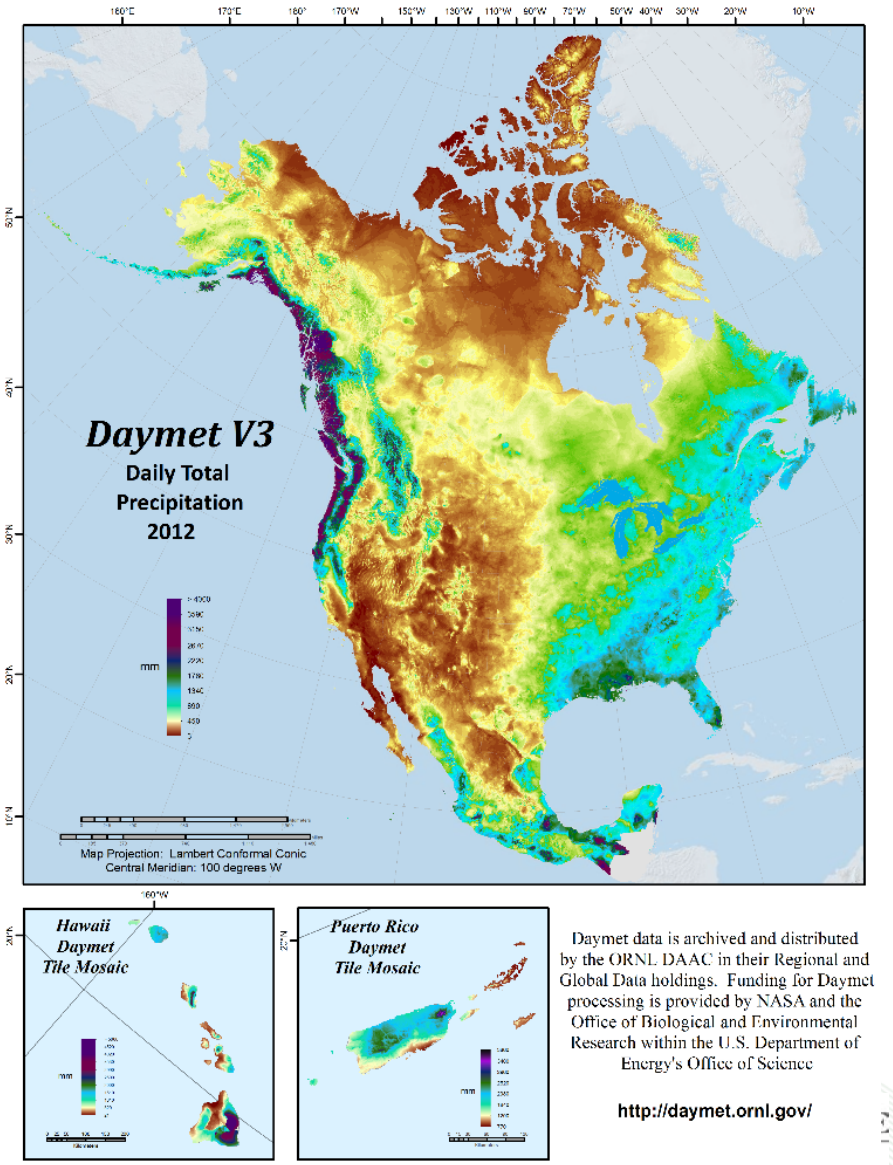
Organize Model Outputs Properly

- Balance the way you divide model outputs into files
  - Avoid too many small files
  - Avoid lumping everything together into huge files
  - Consider needs of target communities
- If your gridded model outputs are too big and need to split them into multiple files
  - First, consider separating independent variables
  - Then, consider splitting based on time, e.g. per year or decade
  - Splitting data spatially will always be your last choice
- Organize data files in hierarchical directory structure
  - e.g. project / model / simulation / variable / …

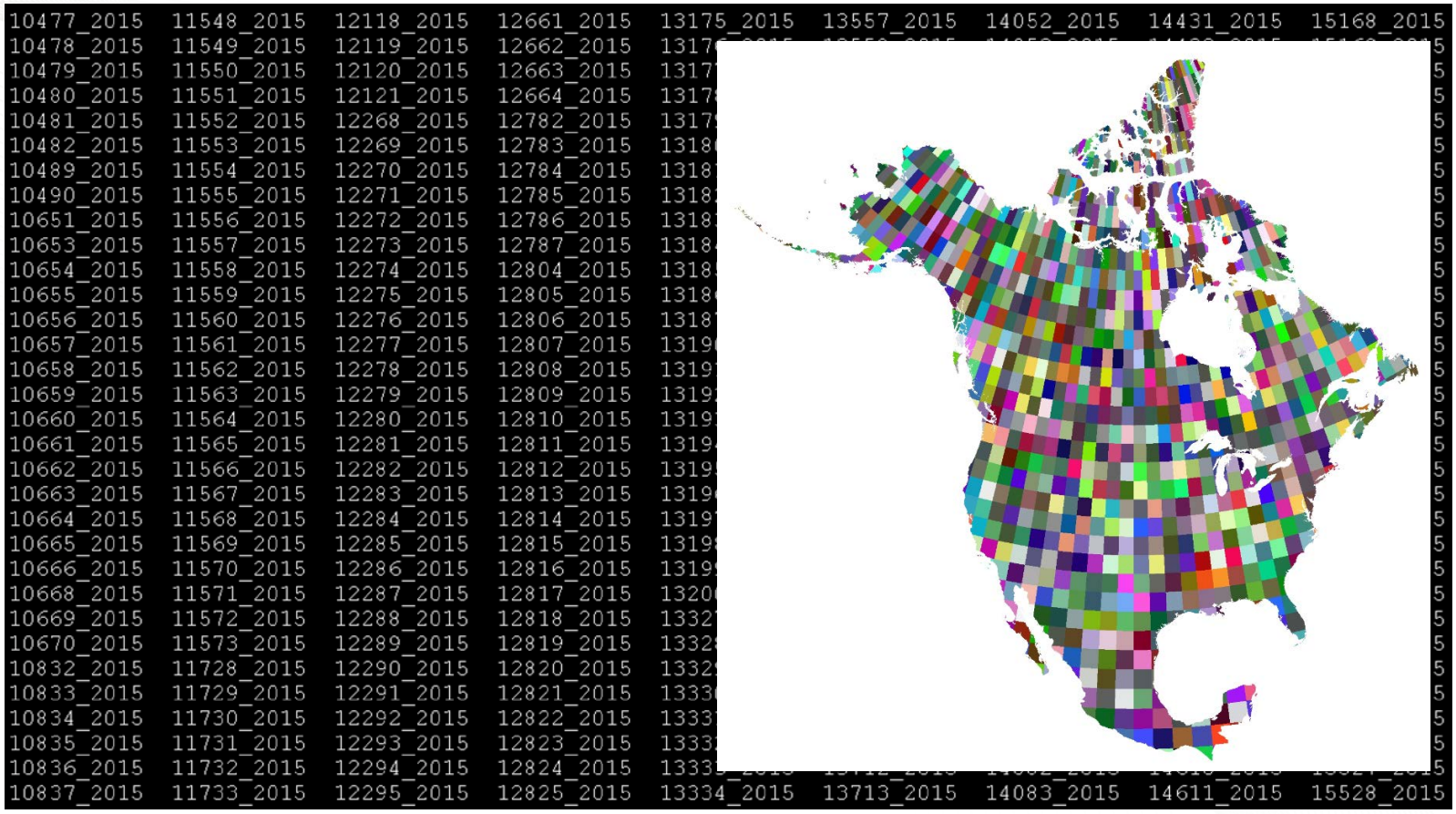
Model Outputs Split by Space

- Daymet V3
  - Provide gridded estimates of daily weather parameters for North America (including Puerto Rico) and Hawaii, on a 1-km grid, from 1980 to 2015.
  - Website:

    https://daymet.ornl.gov



Model Outputs Split by Space



Original outputs of Daymet V3 were split onto 1060 2-deg x 2-deg tiles. There were 267120 individual files with this file organization scheme.

A Better Way for Daymet Outputs Organization

```
2012:
daymet_v3_dayl_2012_hawaii.nc4      daymet_v3_srad_2012_na.nc4          daymet_v3_tmax_2012_puertorico.nc4
daymet_v3_dayl_2012_na.nc4          daymet_v3_srad_2012_puertorico.nc4  daymet_v3_tmin_2012_hawaii.nc4
daymet_v3_dayl_2012_puertorico.nc4  daymet_v3_swe_2012_hawaii.nc4       daymet_v3_tmin_2012_na.nc4
daymet_v3_prcp_2012_hawaii.nc4      daymet_v3_swe_2012_na.nc4           daymet_v3_tmin_2012_puertorico.nc4
daymet_v3_prcp_2012_na.nc4          daymet_v3_swe_2012_puertorico.nc4   daymet_v3_vp_2012_hawaii.nc4
daymet_v3_prcp_2012_puertorico.nc4  daymet_v3_tmax_2012_hawaii.nc4      daymet_v3_vp_2012_na.nc4
daymet_v3_srad_2012_hawaii.nc4      daymet_v3_tmax_2012_na.nc4          daymet_v3_vp_2012_puertorico.nc4

2013:
daymet_v3_dayl_2013_hawaii.nc4      daymet_v3_srad_2013_na.nc4          daymet_v3_tmax_2013_puertorico.nc4
daymet_v3_dayl_2013_na.nc4          daymet_v3_srad_2013_puertorico.nc4  daymet_v3_tmin_2013_hawaii.nc4
daymet_v3_dayl_2013_puertorico.nc4  daymet_v3_swe_2013_hawaii.nc4       daymet_v3_tmin_2013_na.nc4
daymet_v3_prcp_2013_hawaii.nc4      daymet_v3_swe_2013_na.nc4           daymet_v3_tmin_2013_puertorico.nc4
daymet_v3_prcp_2013_na.nc4          daymet_v3_swe_2013_puertorico.nc4   daymet_v3_vp_2013_hawaii.nc4
daymet_v3_prcp_2013_puertorico.nc4  daymet_v3_tmax_2013_hawaii.nc4      daymet_v3_vp_2013_na.nc4
daymet_v3_srad_2013_hawaii.nc4      daymet_v3_tmax_2013_na.nc4          daymet_v3_vp_2013_puertorico.nc4

2014:
daymet_v3_dayl_2014_hawaii.nc4      daymet_v3_srad_2014_na.nc4          daymet_v3_tmax_2014_puertorico.nc4
daymet_v3_dayl_2014_na.nc4          daymet_v3_srad_2014_puertorico.nc4  daymet_v3_tmin_2014_hawaii.nc4
daymet_v3_dayl_2014_puertorico.nc4  daymet_v3_swe_2014_hawaii.nc4       daymet_v3_tmin_2014_na.nc4
daymet_v3_prcp_2014_hawaii.nc4      daymet_v3_swe_2014_na.nc4           daymet_v3_tmin_2014_puertorico.nc4
daymet_v3_prcp_2014_na.nc4          daymet_v3_swe_2014_puertorico.nc4   daymet_v3_vp_2014_hawaii.nc4
daymet_v3_prcp_2014_puertorico.nc4  daymet_v3_tmax_2014_hawaii.nc4      daymet_v3_vp_2014_na.nc4
daymet_v3_srad_2014_hawaii.nc4      daymet_v3_tmax_2014_na.nc4          daymet_v3_vp_2014_puertorico.nc4

2015:
daymet_v3_dayl_2015_hawaii.nc4      daymet_v3_srad_2015_na.nc4          daymet_v3_tmax_2015_puertorico.nc4
daymet_v3_dayl_2015_na.nc4          daymet_v3_srad_2015_puertorico.nc4  daymet_v3_tmin_2015_hawaii.nc4
daymet_v3_dayl_2015_puertorico.nc4  daymet_v3_swe_2015_hawaii.nc4       daymet_v3_tmin_2015_na.nc4
daymet_v3_prcp_2015_hawaii.nc4      daymet_v3_swe_2015_na.nc4           daymet_v3_tmin_2015_puertorico.nc4
```

Daymet V3 outputs were reorganized by merging all tiles in each of the 3 regions together (Continental NA, Hawaii, and Puerto Rico), then split by year. This scheme yielded 756 individual files, with each of them under 5GB in size.

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and with public

Name Data Files and Variables Properly

- Use descriptive file names
  - Model name
  - Simulation code
  - Version number
  - Variable name
  - Space info (e.g. place name and/or resolution)
  - Time info (e.g. range and/or resolution)

Example good filenames:

```
BIOME-BGC_BG1_Monthly_GPP_V2.nc4

rlds_Amon_CESM1-CAM5_historical_r1i1p1_185001-200512.nc

daymet_v3_srad_2012_na.nc4
```

Name Data Files and Variables Properly

- Use unambiguous and “interoperable” variable names
  - Build a table that defines the “short name”→“full name” pairs for variables in your project

```
tmax → land_surface_air__daily_time_max_of__temperature
srad → atmosphere_radiation~incoming~shortwave__transmitted_energy_flux
```

  - Consider “standard names” or common vocabularies used in the community
    - CMIP6 Variable Definitions (https://earthsystemcog.org/projects/wip/CMIP6DataRequest)
    - Climate & Forecast (CF) Standard Names (http://cfconventions.org/standard-names.html)
    - Community Surface Dynamics Modeling System (CSDMS) Standard Names (https://csdms.colorado.edu/wiki/CSDMS_Standard_Names)
  - Use standard data units
    - International System of Units (SI)
    - UDUNITS-2

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and with public

Accurately Define Spatial Information

- Specify the grid space your model is running in
  - Type of grid space
    - Geographic lat/lon grid
    - Projected grid
  - Centers and borders of grid cells
  - Spatial Reference System (SRS)

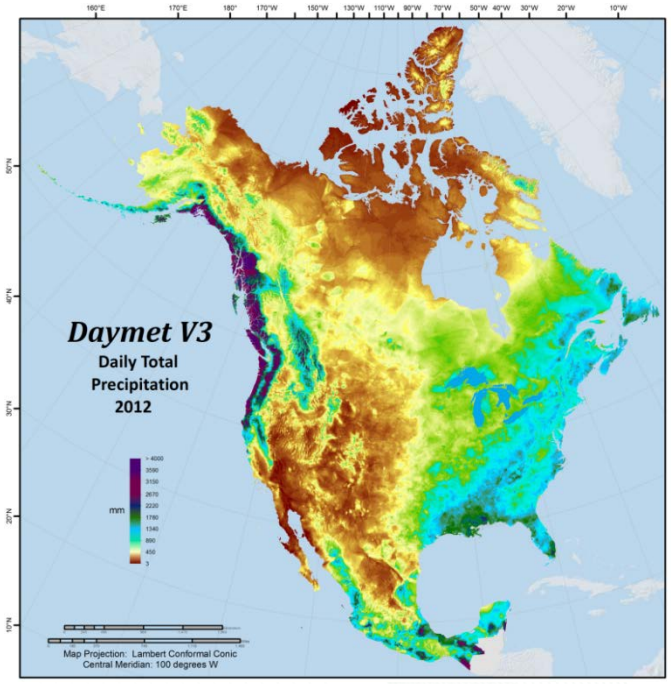
Define the Grid Space For Model Outputs (1)

- NACP regional TBM output
  - Extent
    - West: -170.0
    - South: 10.0
    - East: -50.0
    - North: 84.0
  - Resolution
    - X-resolution: 1-degree
    - Y-resolution: 1-degree
  - SRS
    - Spherical Geographic Lat/Lon (R=6370997m)

Define the Grid Space For Model Outputs (2)

- SRS for Daymet data
  - Projection: Lambert Conformal Conic

```
projection units: meters
datum (spheroid): WGS_84
1st standard parallel: 25 deg N
2nd standard parallel: 60 deg N
Central meridian: -100 deg (W)
Latitude of origin: 42.5 deg N
false easting: 0
false northing: 0
```



Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and with public

Accurately Define Temporal Information

- Calendar your model is using
- Overall start and end temporal representation of a data variable
- Time point/period that each data value represents
- Temporal frequency of a data variable

Calendar

- Determine how many days in each month/year

julian: one leap year in every 4 years
gregorian: leap year if either (i) it is divisible by 4 but not by 100 or (ii) it is divisible by 400
proleptic_gregorian: gregorian calendar extended to dates before 1582-10-15
365_day: no leap year, Feb. always has 28 days
360_day: 30 days for each month
366_day: all leap years

gregorian is the internationally used civil calendar

Time Point and Period

- **ISO 8601:** *Data elements and interchange formats – Information interchange – Representation of dates and times*
- **Time point:** YYYY-MM-DDThh:mm:ss.sTZD

```
2010-03-22T18:00:00.00-06:00
```

- **Duration:** P[n]Y[n]M[n]DT[n]H[n]M[n]S

```
PT1H20M30S
```

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and with public

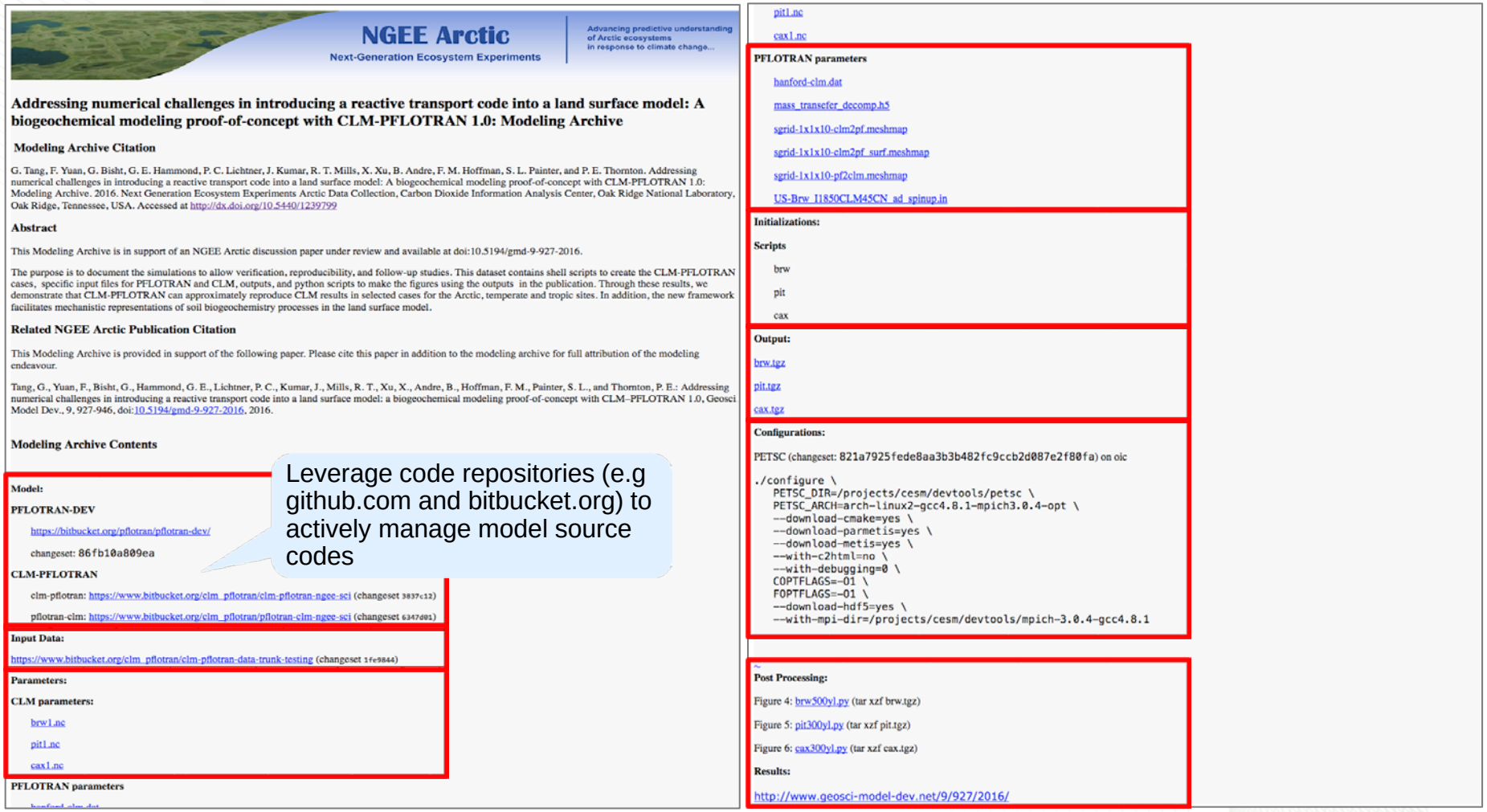
Provide Accurate and Rich Metadata (1)

- Make your model outputs to be easily found, understood, and re-used
- Key elements
  - **What** does the data set describe?
  - **Why** and **how** was the data set created?
  - **Who** produced the data set and **Who** prepared the metadata?
  - **How** reliable are the data?; what is the uncertainty, measurement accuracy?; what problems remain in the data set?
  - **What** assumptions were used to create the data set?
  - **What** is the use and distribution policy of the data set? **How** can someone get a copy of the data set?
  - **Provide** any references to use of data in publication(s)

Provide Accurate and Rich Metadata (2)

- Link your model outputs to the context they were created
  - Model codes
  - Input data (data files, parameters, initializations)
  - Configurations
  - Post-processing/distillation and analysis
  - Publication/presentation results
- Consider archiving the whole model package
  - [NGEE-Arctic Example] Addressing numerical challenges in introducing a reactive transport code into a land surface model: A biogeochemical modeling proof-of-concept with CLM-PFLOTRAN 1.0: Modeling Archive

http://dx.doi.org/10.5440/1239799



NGEE Arctic
Next-Generation Ecosystem Experiments
Advancing predictive understanding of Arctic ecosystems in response to climate change...

Addressing numerical challenges in introducing a reactive transport code into a land surface model: A biogeochemical modeling proof-of-concept with CLM-PFLOTRAN 1.0: Modeling Archive

Modeling Archive Citation

G. Tang, F. Yuan, G. Bisht, G. E. Hammond, P. C. Lichtner, J. Kumar, R. T. Mills, X. Xu, B. Andre, F. M. Hoffman, S. L. Painter, and P. E. Thornton. Addressing numerical challenges in introducing a reactive transport code into a land surface model: A biogeochemical modeling proof-of-concept with CLM-PFLOTRAN 1.0: Modeling Archive. 2016. Next Generation Ecosystem Experiments Arctic Data Collection, Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA. Accessed at http://dx.doi.org/10.5440/1239799

Abstract

This Modeling Archive is in support of an NGEE Arctic discussion paper under review and available at doi:10.5194/gmd-9-927-2016.

The purpose is to document the simulations to allow verification, reproducibility, and follow-up studies. This dataset contains shell scripts to create the CLM-PFLOTRAN cases, specific input files for PFLOTRAN and CLM, outputs, and python scripts to make the figures using the outputs in the publication. Through these results, we demonstrate that CLM-PFLOTRAN can approximately reproduce CLM results in selected cases for the Arctic, temperate and tropic sites. In addition, the new framework facilitates mechanistic representations of soil biogeochemistry processes in the land surface model.

Related NGEE Arctic Publication Citation

This Modeling Archive is provided in support of the following paper. Please cite this paper in addition to the modeling archive for full attribution of the modeling endeavour.

Tang, G., Yuan, F., Bisht, G., Hammond, G. E., Lichtner, P. C., Kumar, J., Mills, R. T., Xu, X., Andre, B., Hoffman, F. M., Painter, S. L., and Thornton, P. E.: Addressing numerical challenges in introducing a reactive transport code into a land surface model: a biogeochemical modeling proof-of-concept with CLM–PFLOTRAN 1.0, Geosci Model Dev., 9, 927-946, doi:10.5194/gmd-9-927-2016, 2016.

Modeling Archive Contents

Model:

PFLOTRAN-DEV

https://bitbucket.org/pflotran/pflotran-dev/

changeset: 86fb10a809ea

CLM-PFLOTRAN

clm-pflotran: https://www.bitbucket.org/clm_pflotran/clm-pflotran-ngee-sci (changeset 3837c12)

pflotran-clm: https://www.bitbucket.org/clm_pflotran/pflotran-clm-ngee-sci (changeset 6347d01)

Input Data:

https://www.bitbucket.org/clm_pflotran/clm-pflotran-data-trunk-testing (changeset 1fe9844)

Parameters:

CLM parameters:

brw1.nc

pit1.nc

cax1.nc

PFLOTRAN parameters

Leverage code repositories (e.g github.com and bitbucket.org) to actively manage model source codes

pit1.nc

cax1.nc

PFLOTRAN parameters

hanford-clm.dat

mass_transefer_decomp.h5

sgrid-1x1x10-clm2pf.meshmap

sgrid-1x1x10-clm2pf_surf.meshmap

sgrid-1x1x10-pf2clm.meshmap

US-Brw_I1850CLM45CN_ad_spinup.in

Initializations:

Scripts

brw

pit

cax

Output:

brw.tgz

pit.tgz

cax.tgz

Configurations:

PETSC (changeset: 821a7925fede8aa3b3b482fc9ccb2d087e2f80fa) on oic

```
./configure \
   PETSC_DIR=/projects/cesm/devtools/petsc \
   PETSC_ARCH=arch-linux2-gcc4.8.1-mpich3.0.4-opt \
   --download-cmake=yes \
   --download-parmetis=yes \
   --download-metis=yes \
   --with-c2html=no \
   --with-debugging=0 \
   COPTFLAGS=-O1 \
   FOPTFLAGS=-O1 \
   --download-hdf5=yes \
   --with-mpi-dir=/projects/cesm/devtools/mpich-3.0.4-gcc4.8.1
```

Post Processing:

Figure 4: brw500yl.py (tar xzf brw.tgz)

Figure 5: pit300yl.py (tar xzf pit.tgz)

Figure 6: cax300yl.py (tar xzf cax.tgz)

Results:

http://www.geosci-model-dev.net/9/927/2016/

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and with public

Leverage Community Conventions

- One step forward for consistency and interoperability
- Choose proper data formats to maximize model outputs re-use
  - netCDF
- Follow conventions to create self-descriptive model output files
  - Climate & Forecast (CF) convention (http://cfconventions.org)

Best Practices for Managing Model Outputs

- Organize model outputs properly
- Name your data files and variables properly
- Accurately define spatial information
- Accurately define temporal information
- Provide accurate and rich metadata
- Leverage community conventions
- Effectively share data within team and beyond

Effectively Share Data Within Team and With Broader User Communities

- Set up team and public data repositories
  - Dedicated data storage and management servers
  - For non-sensitive data, commercial products like Dropbox provide out-of-box features, e.g. access control, version tracking, and backup, for setting up data repositories
- Set up services to support on-demand data access
  - Variable-, spatial-, temporal-subset
    - OPeNDAP: Open-source Project for a Network Data Access Protocol
    - NCSS: NetCDF Subset Service

Leverage Advanced Data Transfer Services

- Multistreaming transfer utilities
  - BBCP
  - GridFTP and Globus Transfer

Summary

- Follow best practices to create self-descriptive and interoperable data, your model outputs will be readily available for visualization, analysis, and re-use in future researches
- Leverage proper tools and services to share data within team and/or with public so research can be conducted collaboratively and effectively within your team and usage of your model outputs can be maximized.

THANK YOU!

- Thanks for participating in this webinar
- Slides and a recording of this webinar will be available
  - Link will be sent to you by e-mail.
- Please fill out the survey at the bottom of your screen
- Send any additional feedback to sanseverinoj@ornl.gov
- Future webinars will be announced by e-mail