ONE APPROACH TO ENSURING THAT DATA ANALYSIS PROJECTS AND RESEARCH REPORTS ARE REPRODUCIBLE

UCAR Software Engineering Assembly (SEA) conference
Tuesday, April 5th, 2016 9:30AM

Janine Aquino, Bill Brown, Teresa Campos, Al Cooper, Mike Daniels

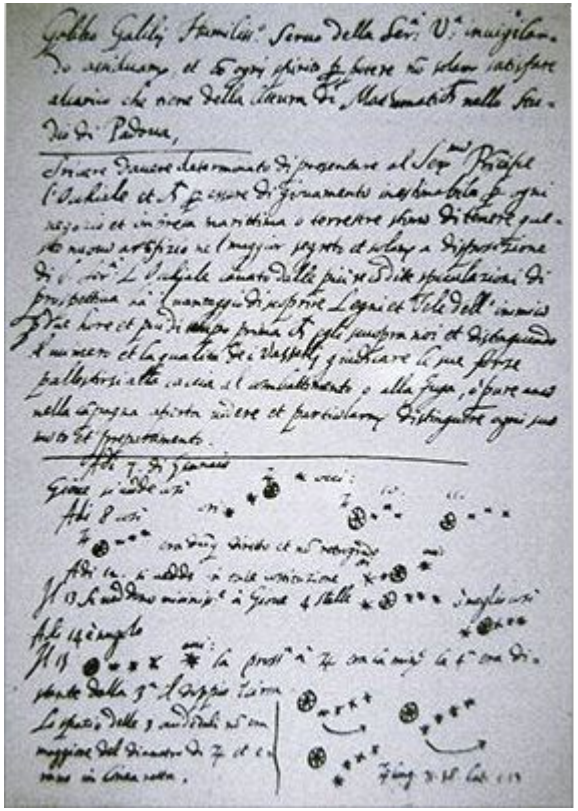
NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

EARTH SYSTEM LABORATORY

Importance - initiatives, funding and journal requirements

"To promote transparency and reproducibility, papers should reference the Data, Software and Scientific Workflow used to produce results"

NCAR OntoSoft GPF Training, The Geoscience Paper of the Future, Sept 28, 2015[1]



A page from Galileo's journal

Importance - initiatives, funding and journal requirements

"Major takeaway: Users rely on PI/project support for understanding nuances of the science and supporting data…

Priority #1 (EOSDIS, High Value): … a data usage guidelines document with examples [to] capture what is needed for users when the PIs are gone and only DAACs are supporting the products."

- DRAFT - Report of ESDSWG Airborne Data Working Group Study, October 2015[4]

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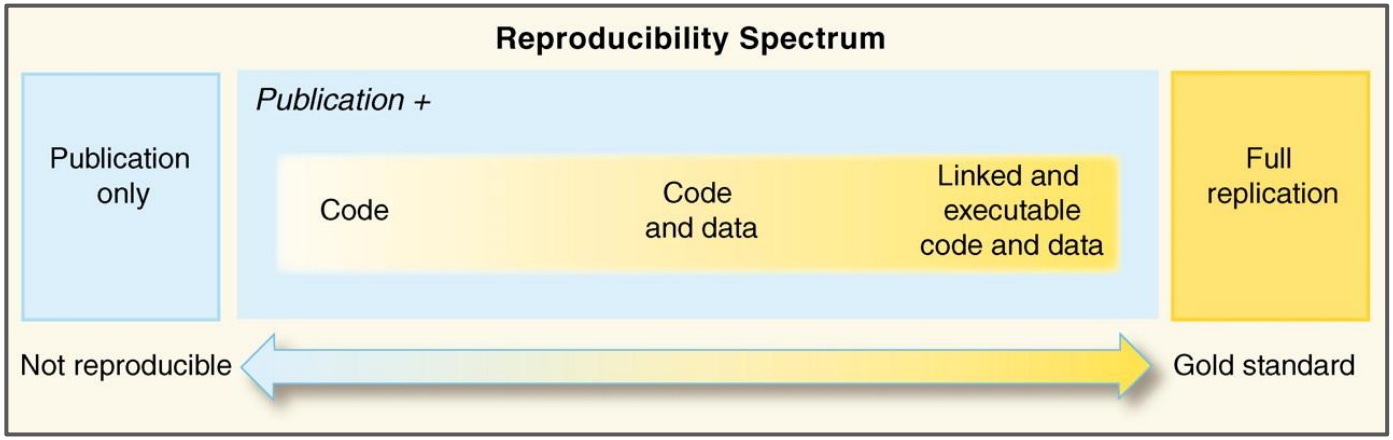
Contrast physical science with computer science...

2011

Peng, Roger D., Reproducible Research in **Computational Science**[9]

1. **Data sources** should be available in public repositories, with assigned DOIs, and there should be sufficient provenance to trace their origins and those responsible for their collection and curation.
2. **Analysis software** should similarly be preserved and where possible assigned identifiers that ensure their preservation and public access.
3. **Workflow and/or provenance descriptions** should accompany the work. It is not sufficient to preserve the software, which depends on a reproducer being able to understand the program and run it in a suitable environment. A workflow description can include the requisite conditions (software packages, version numbers of commercial packages, the computing environment) and can also describe parts of the investigation pursued and found unproductive, how choices were made and figures constructed, etc. These descriptions need to be archived with the analysis programs so that others might duplicate or extend the work.



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Importance - initiatives, funding and journal requirements

"...the results of unclassified research that are published in peer-reviewed publications directly arising from Federal funding should be stored for long-term preservation and publicly accessible to search, retrieve, and analyze in ways that maximize the impact and accountability of the Federal research investment."

John P. Holdren, Increasing Access to the Results of Federally Funded Scientific Research, OSTP Memorandum February 22, 2013[3]

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Importance - initiatives, funding and journal requirements

"Scientific research products, whether data or software or articles, are not only of great interest to scientists in other fields but have well recognized societal value. Open science practices are crucial to the dissemination of scientific knowledge, including digital scholarship, data and software stewardship, and routine reproducibility."

Farzad Kamalabadi, Basil Gomez, Yolanda Gil, David Arctur, Steve Richard, Jay Pearlman, EarthCube Strategic Vision, May 22, 2015[2]

EarthCube:
Developing a Community-Driven Data and Knowledge Environment for the Geosciences

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Importance - initiatives, funding and journal requirements

The ESIP committee on Preservation and Stewardship

“ develops and fosters practices and standards that ensure continued and reliable information content, quality, access to, and usability of Earth system science data for as long as they are deemed to be of value. ”[5]

ESIP
The Federation of Earth Science Information Partners
Fostering connections to make data matter

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Importance - reproducibility (defend our findings)

Defend our findings

Thomas Karl's testimony to the House Committee on the IPCC report, addressing "*increasing demands for authoritative information and products to inform climate adaptation and mitigation activities*"[6]

Legal Harassment of Climate Scientist Michael Mann "*demanding all internal notes, emails and correspondence concerning a study its scientists published in the journal Science. The study found that the "rate of global warming during the last 15 years has been as fast as or faster than what was seen during the latter half of the 20th century.*"[7,8]

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Importance - reproducibility

Save ourselves the hassle

EOL aircraft group - 2016 Summer intern to determine binary format, by deconstructing Fortran IV code that no longer runs, because the format was never documented.

EOL surface group - found an error and are working back through 10 years of data

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Importance - reproducibility

Usability into the future

The ATD/RDP group created a DVD containing data and a GUI tool to use it (executable that doesn't require IDL - cross-platform: linux, windows, mac)

- turned out to be more system dependent that it was supposed to be, and no longer runs.

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Importance - reproducibility

Look like a rock star

Al Cooper was able to describe to a researcher how he obtained his results, years after the paper was published, by referring to a complete documentation package.

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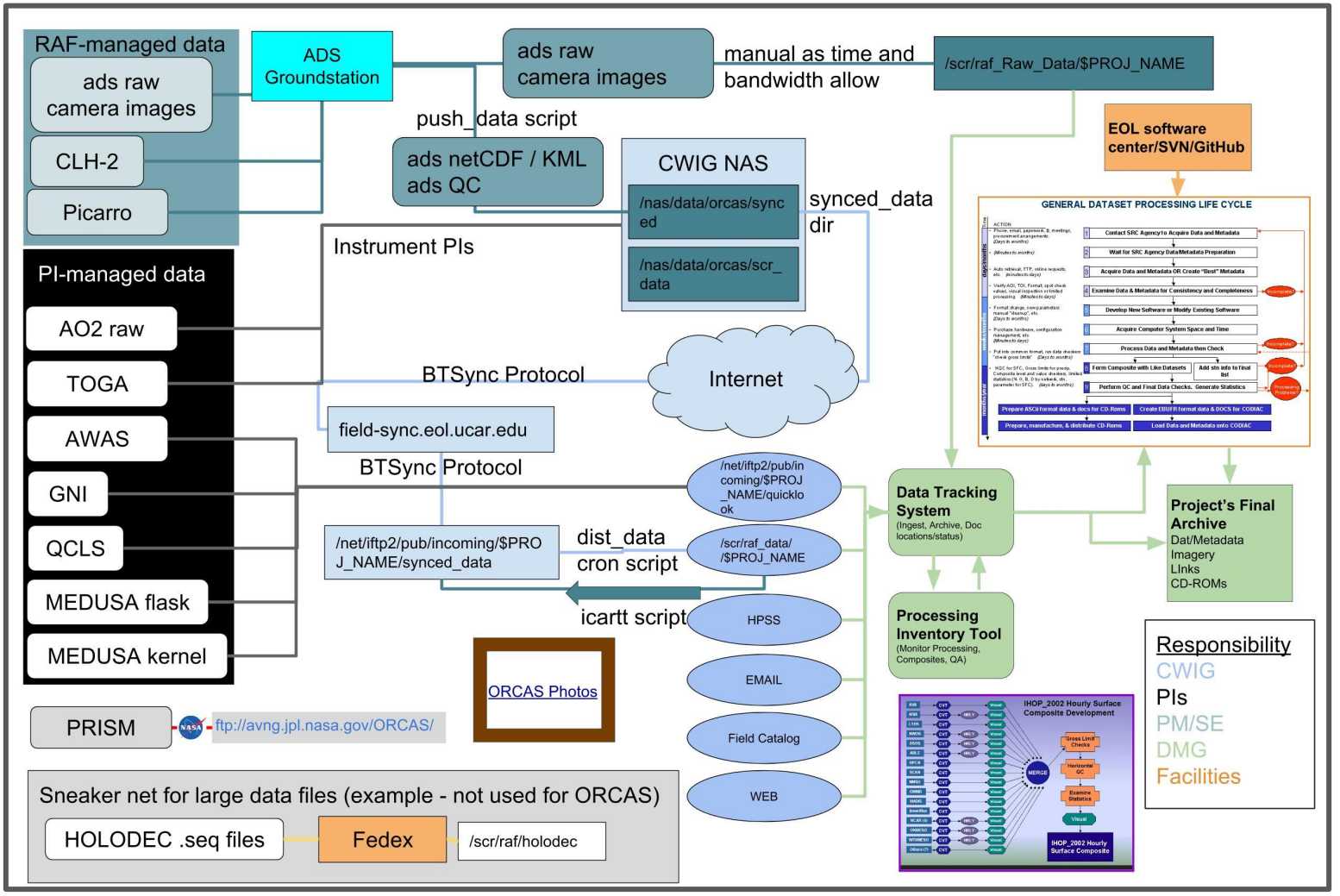
Traceability - Where we go wrong?



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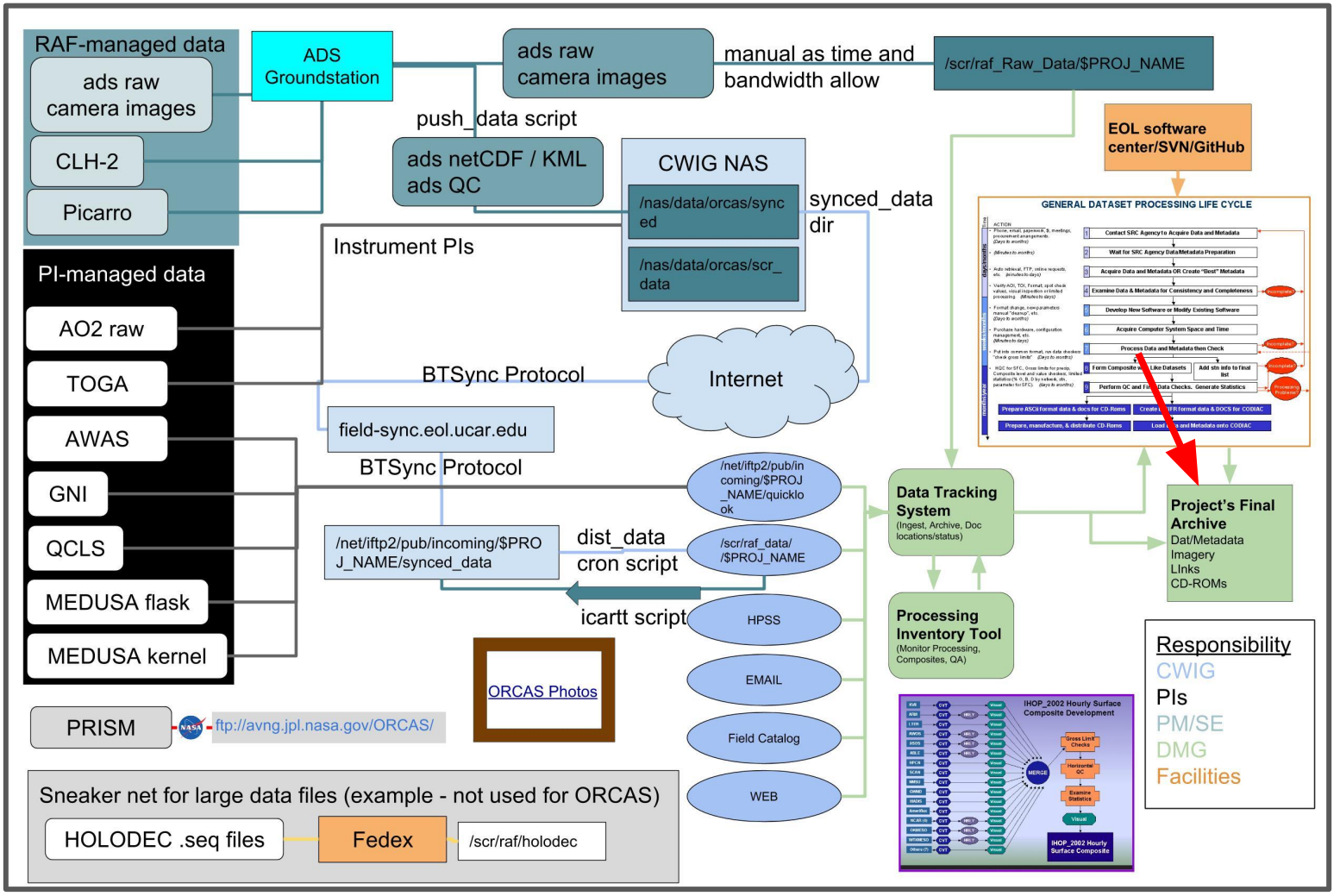
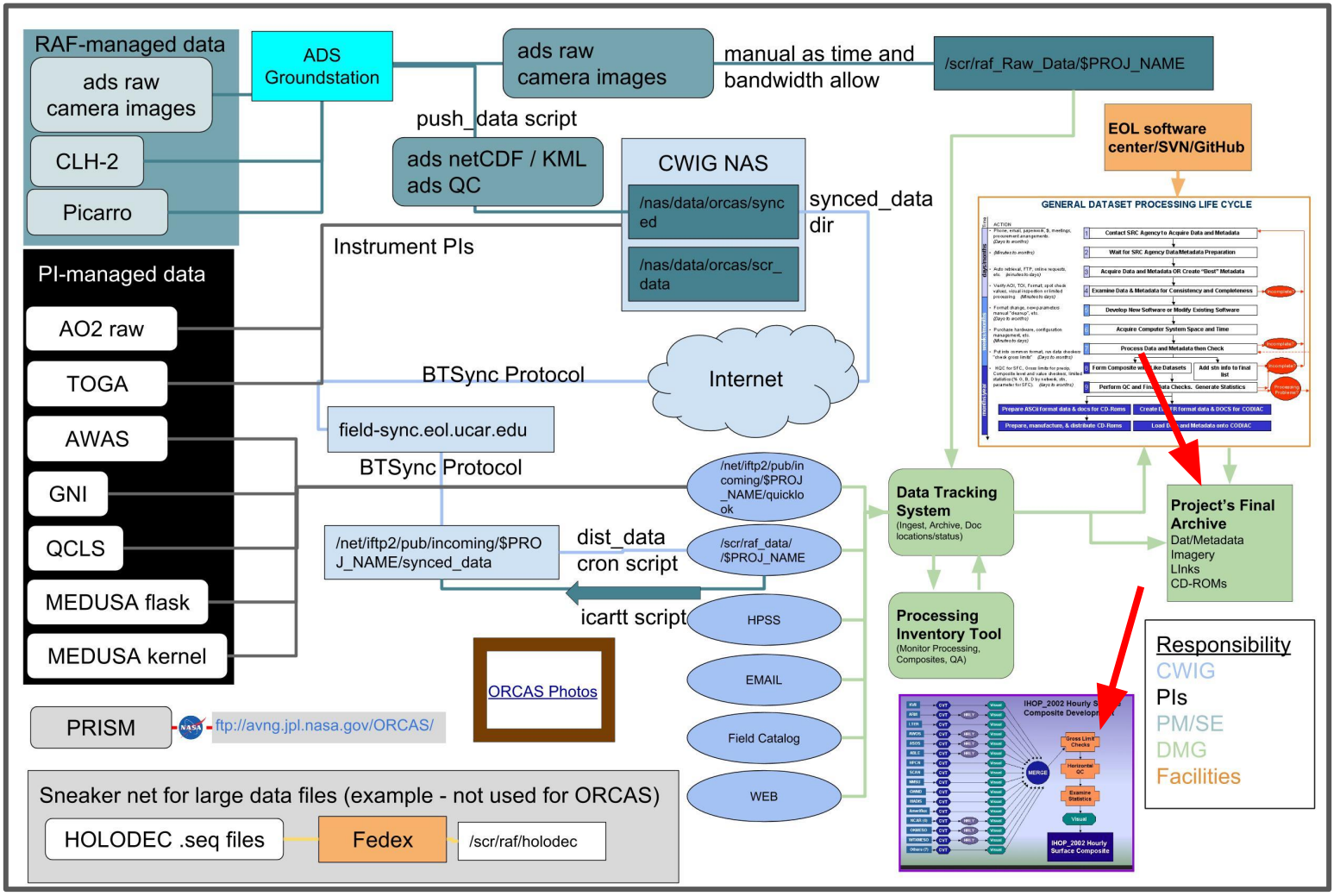
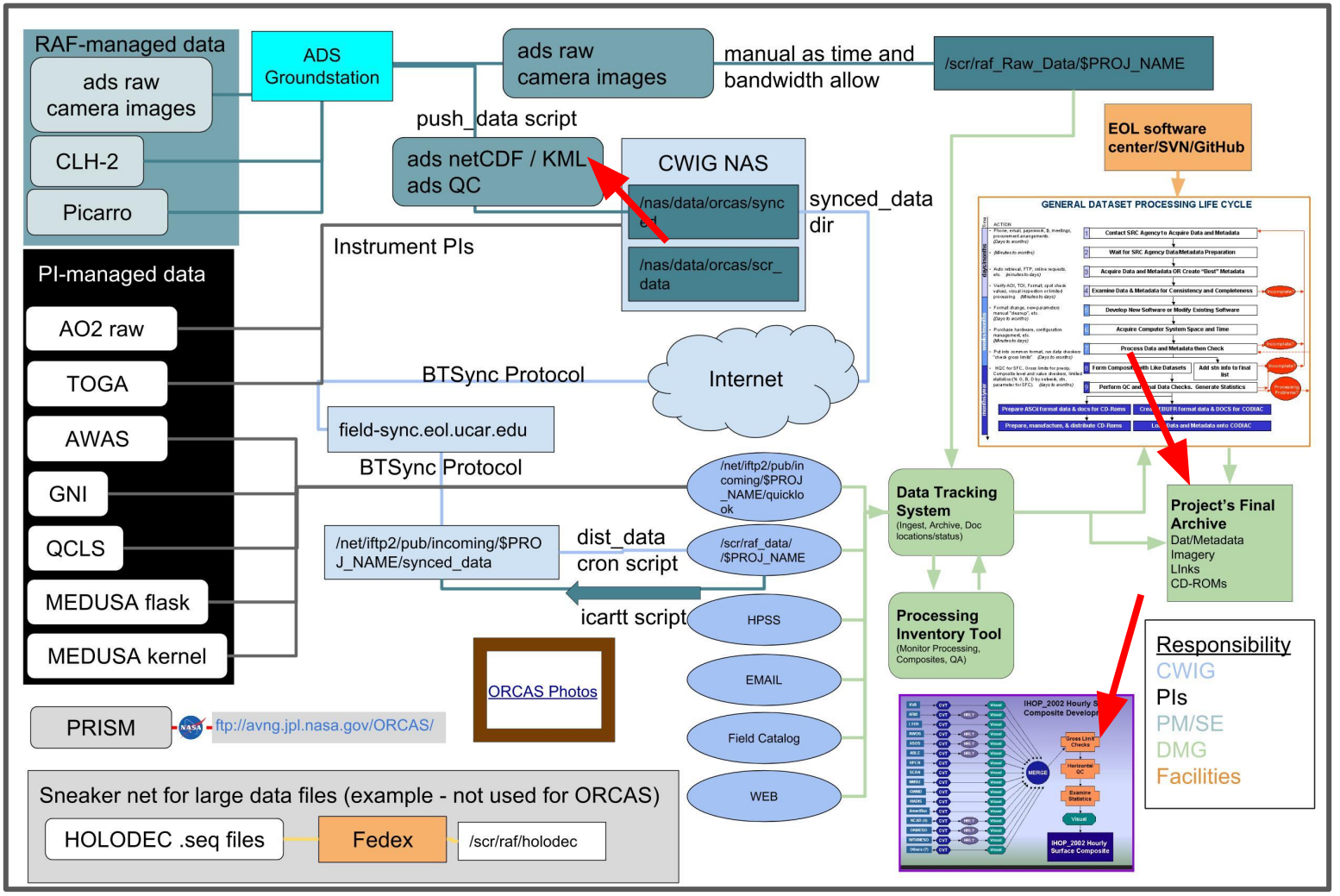
Traceability - Where we go wrong?



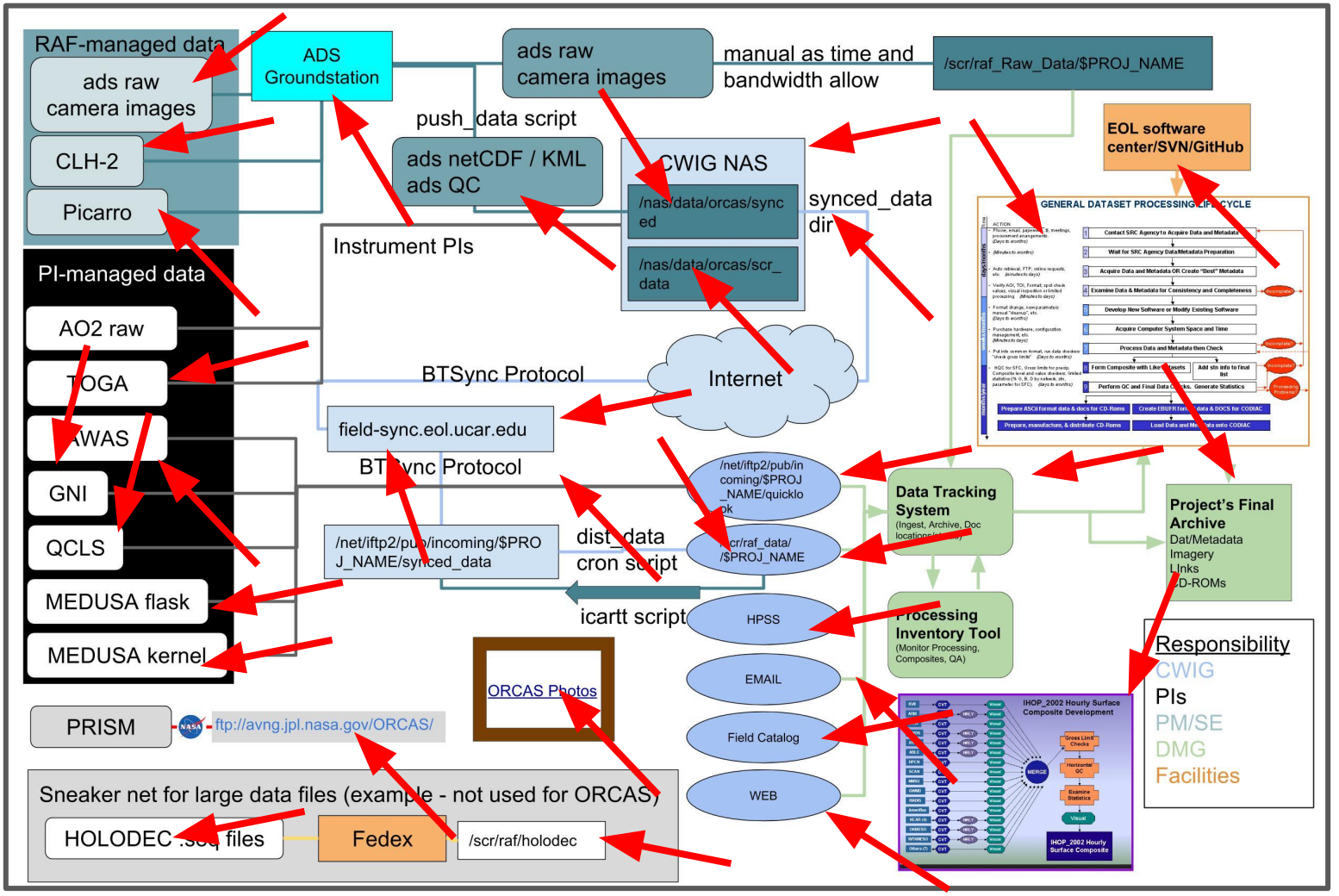
Traceability - Where we go wrong?



Traceability - Where we go wrong?



Traceability - Where we go wrong?



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What can we do?

Assign identifiers to observational data, software, platforms, physical samples, model output and cite them in research papers

Datasets:

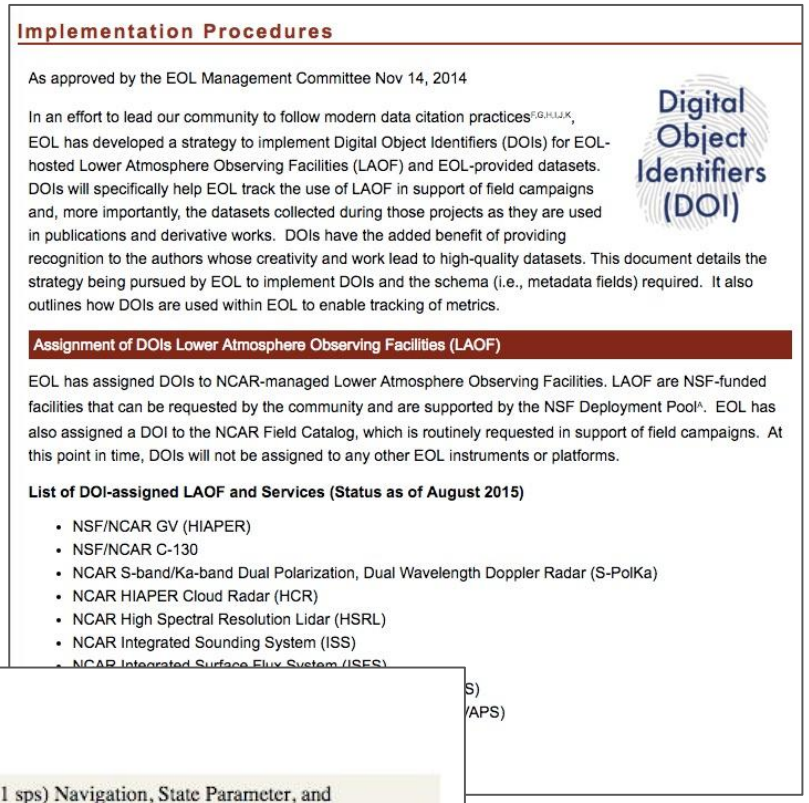
- DEEPWAVE G-V Low Rate (LRT - 1 sps) Navigation, State Parameter, and Microphysics Flight-Level Data [(NCAR-EOL-RAF)], http://dx.doi.org/10.5065/D6J964D9
- DEEPWAVE 449 MHz Profiler data, http://dx.doi.org/10.5065/D67D2S66

Software:

- The NCAR Command Language (Version 6.3.0) [Software]. (2015). Boulder, Colorado: UCAR/NCAR/CISL/TDD. http://dx.doi.org/10.5065/D6WD3XH5

Platforms:

- HIAPER G-V aircraft: http://dx.doi.org/10.5065/D6DR2SJP
- 449 MHz Profiler (as part of ISS): http://dx.doi.org/10.5065/D6348HF9
- S-Pol: http://dx.doi.org/10.5065/D6RV0KR8



Implementation Procedures

As approved by the EOL Management Committee Nov 14, 2014

Digital Object Identifiers (DOI)

In an effort to lead our community to follow modern data citation practices[F,G,H,I,J,K], EOL has developed a strategy to implement Digital Object Identifiers (DOIs) for EOL-hosted Lower Atmosphere Observing Facilities (LAOF) and EOL-provided datasets. DOIs will specifically help EOL track the use of LAOF in support of field campaigns and, more importantly, the datasets collected during those projects as they are used in publications and derivative works. DOIs have the added benefit of providing recognition to the authors whose creativity and work lead to high-quality datasets. This document details the strategy being pursued by EOL to implement DOIs and the schema (i.e., metadata fields) required. It also outlines how DOIs are used within EOL to enable tracking of metrics.

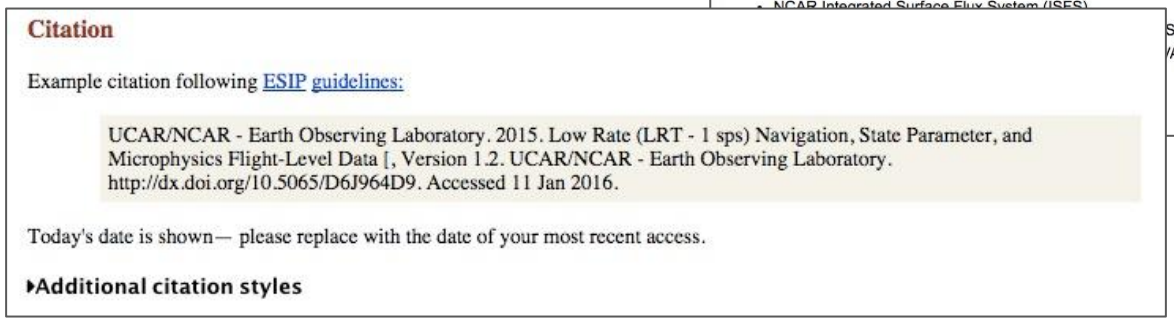
Assignment of DOIs Lower Atmosphere Observing Facilities (LAOF)

EOL has assigned DOIs to NCAR-managed Lower Atmosphere Observing Facilities. LAOF are NSF-funded facilities that can be requested by the community and are supported by the NSF Deployment Pool[A]. EOL has also assigned a DOI to the NCAR Field Catalog, which is routinely requested in support of field campaigns. At this point in time, DOIs will not be assigned to any other EOL instruments or platforms.

List of DOI-assigned LAOF and Services (Status as of August 2015)

- NSF/NCAR GV (HIAPER)
- NSF/NCAR C-130
- NCAR S-band/Ka-band Dual Polarization, Dual Wavelength Doppler Radar (S-PolKa)
- NCAR HIAPER Cloud Radar (HCR)
- NCAR High Spectral Resolution Lidar (HSRL)
- NCAR Integrated Sounding System (ISS)
- NCAR Integrated Surface Flux System (ISFS)

S)
/APS)



Citation

Example citation following ESIP guidelines:

UCAR/NCAR - Earth Observing Laboratory. 2015. Low Rate (LRT - 1 sps) Navigation, State Parameter, and Microphysics Flight-Level Data [, Version 1.2. UCAR/NCAR - Earth Observing Laboratory. http://dx.doi.org/10.5065/D6J964D9. Accessed 11 Jan 2016.

Today's date is shown— please replace with the date of your most recent access.

▸Additional citation styles

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What can we do?

Attend training sessions or workshops associated with best practices in software and data provenance

- Geosciences Paper of the Future (GPF) training session, see http://www.ontosoft.org/gpf/training-sessions. The group is willing to come to NCAR again to give an abbreviated (2 hour) course
- Software Carpentry training sessions, see http://software-carpentry.org/
  - NCAR is a software carpentry affiliate. Local training capability is being developed. Contact: SEA (Davide Del Vento)
- Data Carpentry training sessions, see http://datacarpentry.org
  - Reproducible Research Hack-a-thon [http://www.datacarpentry.org/blog/reproducible-research-curriculum/]
- Learn about containerization (Docker)
  - Hopefully you saw Erik Johnson's excellent talk yesterday "Whales On A Plane: Deploying Software To NSF / NCAR Research Aircraft w/ Docker"

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What can we do?

Develop tools to make this easier, and get involved in groups developing standards

- ESIP-Drupal group creating a Drupal Module to link EZID metadata with citation display on a webpage.
- ESIP group creating an “Identify Everything” paper
- NASA/ESDSWG evaluating usage of identifiers at the DAACs and has proposed a 2016 working group on software citation. Meeting is tomorrow (April 6, 2016) thru Friday at Goddard Space Flight Center in Greenbelt, MD.
- An EarthCube proposal was submitted in March 2016 to involve NCAR in future training and workshop opportunities, NCAR PI: Mike Barlage (barlage@ucar.edu)

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What can we do?

Document versions, algorithms, calibrations, configurations, assumptions, constraints.

One possible solution:

Steps Toward Reproducibility[10]

Journal Articles, Tech Notes, Data Analysis

Al Cooper
EOL Science Group
20 Jan 2016

with a few mods….

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Making Research and Data Analysis Reproducible

The model:

1. **Construct the text**-generating and analysis programs that create the research paper.

2. **Annotate the text** with references to data, and save specific data sets used.

3. Construct a **workflow document and diagram** to help someone else reproduce the work.

4. **Archive** the text/analysis program and the workflow document along with any other needed program packages and data subsets.

5. **Reference** the data sources.

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1. Construct the text-generating and analysis programs, so far as possible, in a single file

Could create separate files and archive them together, but the advantage of a combined file is that the program output goes directly into the text.

Good options: ipython notebook and R with knitr.

Al's preference: knitr

- Can embed R code into a LaTeX document and reference results from the R code 'chunks' in the document. Alternately, can use HTML for the text part.

- Very useful tool: 'lyx' is integrated with knitr so you can construct the document in a word-processor-like environment.

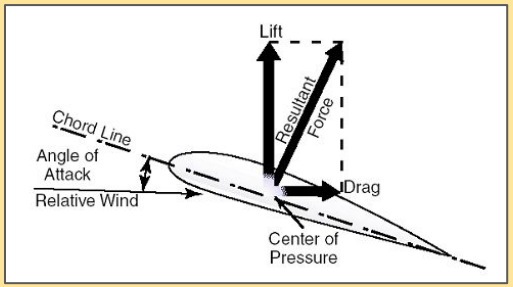
Structure of an '.Rnw' file using 'knitr'

- Easiest using RStudio, which provides a starting LaTeX skeleton
- Options to using LaTeX directly:
  a. Use LibreOffice and export to LaTeX. (I presume Word does this too.)
  b. Use the '.Rmd' format instead, which works with HTML.
  c. Use 'lyx' which generates LaTeX while interacting like a word processor.
- Embed 'chunks' of R code in the file using delimiters:
  a. start chunks with specific headers: <<title, other stuff>>=
  b. then insert R code
  c. end R chunk with @
- Reference results using the LaTeX command \Sexpr{R variable}.
- Figures and tables get inserted appropriately into the resulting document, with captions specified in the chunk headers.

Example 1: A data-analysis task

Objective:

Find appropriate empirical coefficients to use with the radome-port pressures to find the angle-of-attack.



EARTH OBSERVING LABORATORY

Memorandum:

14 October 2015

TO: HIPPO reprocessing file
FROM: Al Cooper
SUBJECT: vertical wind for HIPPO-1

1 The problem to address

Review of HIPPO-1 measurements shows that, when the "standard" sensitivity coefficients as given in the Processing Algorithms technical note are used, there is often a significant offset in vertical wind and there is much variability from flight to flight and even within flights. For example, for HIPPO-1 flight 5, Fig. 1 shows the measurements of vertical wind. The blue line shows 1-Hz measurements, and the red line is the result after 60-s smoothing. The mean offset, 1.3 m/s, is significant, and the offset varies during the flight. Other flights show similar problems but with some inconsistency, often showing pronounced correlation between rate-of-climb and WIC. Figure 2 shows the difference between the reference angle given by (1) and the angle of attack determined using the standard formula. There is a significant offset in mean angle and an apparent residual dependence on Mach Number, so it appears appropriate to reconsider the sensitivity coefficients representing angle of attack for this project.

2 The standard fit

The first step here will be to re-fit the measurements to the standard formula used to represent angle of attack α, from the Processing Algorithms technical note:

$$\alpha = c_0 + \frac{\Delta p_\alpha}{q}(c_1 + c_2 M) \qquad (1)$$

where Δp_α is the pressure difference between upward and downward ports on the radome (ADIFR), q is dynamic pressure (QCF), and M is the Mach number calculated using the uncorrected static and dynamic pressure (PSF and QCF). The three coefficients specified in that document, for projects before 2012, are $\{c\} = \{5.516, 19.07, 2.08\}$ and these are the coefficients used in the initial processing.

[The memo (on Google drive)]12

Why this needs to be reproducible:

- Al has been doing this. His retirement means someone else will need to continue this analysis.
- The coefficients vary with the aircraft configuration so this must be done about once per project.

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A segment of the .Rnw file that generated the memo and performed the calculations in R:

Here is the Google-doc link: AKRDforHIPPO1.Rnw[13]

```
\begin{document}
\EOLmemo

\global\addressee={HIPPO reprocessing file} % >>change
"File" to the "To:" name desired

\begin{tabular}{ll}
\textsf{\textsc{\textcolor{blue}{To:}}}  &
\the\addressee\tabularnewline
\textsf{\textsc{\textcolor{blue}{From:}}}  & Al
Cooper\tabularnewline
\textsf{\textsc{\textcolor{blue}{Subject:}}}  & vertical
wind for HIPPO-1\tabularnewline
\end{tabular}

\bigskip{}

<<initialization,echo=FALSE,include=FALSE>>=
require(knitr)
opts_chunk$set(echo=FALSE, include=FALSE, fig.lp="
fig:")
opts_chunk$set(fig.width=6, fig.height=5, fig.pos="
center", digits=4)
options(digits=3)
thisFileName <- "WI-HIPPO1"
require(Ranadu, quietly = TRUE, warn.conflicts=FALSE)
Directory <- DataDirectory ()
Flight <- "rf01"
Project = "HIPPO-1"
…
@
```

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\textsf{\textsc{\textcolor{blue}{Subject:}}}  & vertical
wind for HIPPO-1\tabularnewline
\end{tabular}

\bigskip{}
```

TEXT

```
<<initialization,echo=FALSE,include=FALSE>>=
require(knitr)
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fig:")
opts_chunk$set(fig.width=6, fig.height=5, fig.pos="
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\bigskip{}
```

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@
```

SOFTWARE

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2. Annotate the text with references to data, and save specific data sets used.

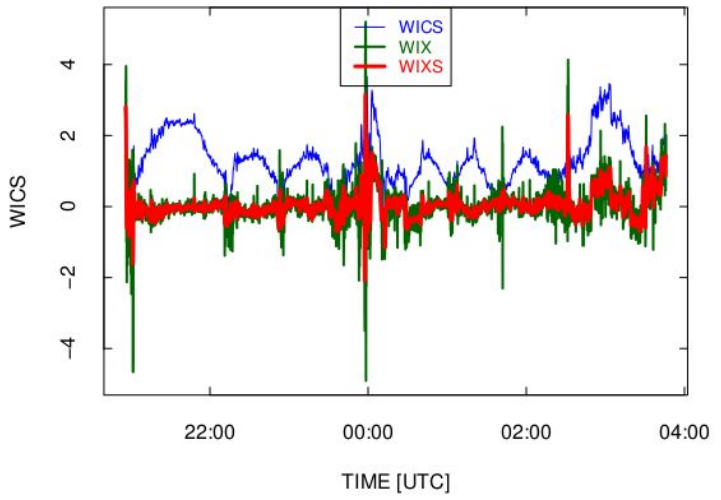

Figure 4: As for Fig. 1 but adding the new variable WIX for the vertical wind.

5 New values of the vertical wind

The revised vertical wind based on the new coefficients can be estmated from the previous value (WIC) modified to be WIX=WIC+(α-AKRD)πV/180 where α is given by (1), V is the airspeed and $\pi/180$ is needed to convert from degrees to radians. Figure 4 repeats Fig. 1 for flight 3 with the addition of this new measurement of the vertical wind. The red trace (WIXS, WIX with 60-s smoothing) represents the new variable, which shows mean values close to zero for most of the flight and is a significant improvement over WIC.

– End of Memo –

Reproducibility:

PROJECT:	WI-HIPPO1
ARCHIVE PACKAGE:	WI-HIPPO1.zip
CONTAINS:	attachment list below
PROGRAM:	AKRDforHIPPO1.Rnw
THIS DOCUMENT:	AKRDforHIPPO1.pdf
WORKFLOW:	WorkflowFindAKRDcal.pdf
ORIGINAL DATA:	/scr/raf_data/HIPPO/HIPPO-1rf01.nc, etc
DATA ARCHIVE:	NCAR HPSS (not github)
GIT:	https://github.com/WilliamCooper/Reprocessing.git

Attachments: AKRDforHIPPO1.Rnw
AKRDforHIPPO1.pdf
WorkflowFindAKRDcal.pdf
SessionInfo

6 Recommendation

Use the sensitivity coefficients {4.864, 12.429, 9.451} for HIPPO-2.

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3. Construct a workflow document and diagram

EARTH OBSERVING LABORATORY

Memorandum:

14 October 2015

TO: HIPPO reprocessing file
FROM: William Cooper
SUBJECT: Workflow to find sensitivity coefficients

1 Purpose

This memo describes the workflow for finding new sensitivity coefficients characterizing measurements of angle of attack using the radome gust system. The example used is "AKRDforHIPPO1.Rnw", a file containing both text and R code. That file generates the memo "AKRDforHIPPO1.pdf" and the archive file "WI-HIPPO1.zip" that contains the generating file, the document in PDF format, and this workflow memo.

The final authority regarding workflow is the ".Rnw" document itself, but this overview and diagram is intended to help explain the workflow at a general level and so should substitute for reading the R and LaTeX code. The intent is to describe the workflow in sufficient detail to support replication of the analysis and figures presented in "AKRDforHIPPO1.pdf" and also to enable changes based on new data or new analysis approaches.

There are references and citations for the tools used (R, RStudio, knitr) in this technical note: Characterization of Uncertainty in Measurements of Wind from the NSF/NCAR GV Research Aircraft. The workflow document for that technical note also contains some additional explanations of the procedures that are used again in generating the present memo and the steps taken to ensure reproducibility of the results.

2 Acquisition of the primary data

The best measurements for the purpose of this analysis are those obtained during "speed runs," constant-altitude flight maneuvers where the flight speed is varied through the flight envelope of the aircraft,, preferably with modest rates of acceleration and deceleration. Those maneuvers cause the angle of attack to chance with airspeed through the normal range of measurements. Two aspects of the maneuver are crucial, that the vertical wind be near-zero and that the *geometric* altitude be constant.

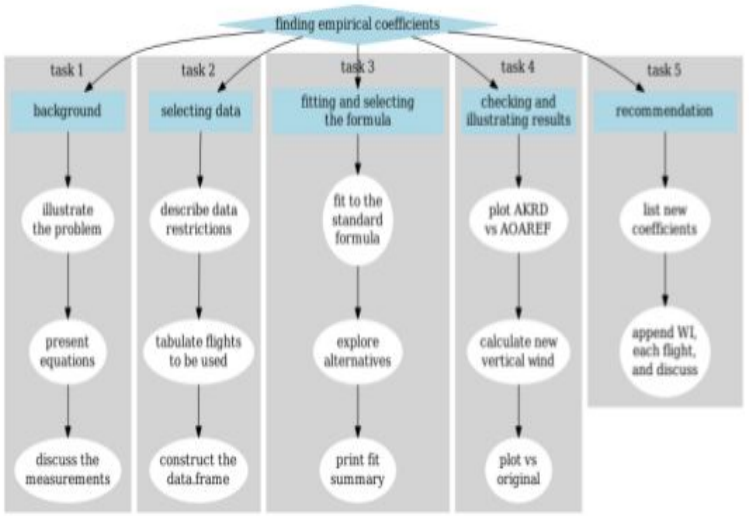

Figure 1: Flow chart describing the workflow.

3 Overview of the workflow

A flow chart describing the workflow is provided by Fig. 1. The workflow is organized into five tasks, each of which is discussed below. Everything in this flow chart, both generating the text document and performing the calculations, is embedded in AKRDforHIPPO1.Rnw. Where particular tasks require calculations using R, the R code is isolated in "chunks" that have header titles, so those titles are referenced below where appropriate. The first chunk is "initialization," which loads some required R packages. An important one is "Ranadu", a set of routines used for accessing, manipulating, and plotting variables in the archived data files. This package is available at this github link and must be installed. Also required is "knitr" so that the text document can be constructed. A list of required variable names is also contained in this chunk; later, when data.frames are constructed for analysis, this list is used to determine the variables to load from the netCDF files.

The workflow document (Google-doc)

3.3 Fitting and selecting the formula to use

1. *Fit to the standard formula.* This task begins by finding the best fit coefficients using the standard formula (1). The R chunk "fits" performs this fit, after the subset data.frame "DF" is defined to apply the data restrictions to the data.frame "Data". The linear-model R function "lm()" is used to find the coefficients, and the resulting coefficients are incorporated into the text via "\Sexpr{ }" expressions included in the LaTeX text so that, if there is any change, the coefficients quoted will be updated automatically.

2. *Explore alternatives.* If the fit does not appear to be adequate, alternative approaches should be explored here. They might involve using different parameters in a formula like (1) or even applying filtering to the resulting vertical wind in cases where no good fit procedure is available. (This was the case, for example, in HIPPO-5.) In the present case, the standard deviation (0.1 °) was quite good in comparison to most cases and the fit provided coefficients with low uncertainty, so this fit seems fully acceptable. If it had been unacceptable, some other alternatives like those explored in the Wind Uncertainty Technical Note. Some of the possibilities explored in connection with the present study are listed in the text, but none led to sufficient improvement to justify the added complexity of the formula.

3. *Print fit summary.* A special function "SummarizeFit()", defined in the chunk "summarize-fit," is used to write a summary of the results into the text file.

etc… Provides detail about alternates considered, what fit routine is used, and other mechanics. This example came to five single-spaced pages -- details are an important part of reproducibility.

4. Archive the text/analysis programs, packages, & workflow document.

Example: Application to a journal article
(status: internal review)

"Algorithms for correcting measurements of attitude angles"

Prepared for Atmospheric Measurement Techniques, where it is acceptable to provide supplementary information. Planned supplement:

- The composite file that generates the manuscript.
- A workflow description.
- Waiting for expiration of the DEEPWAVE data-reservation period because this uses DEEPWAVE data; then include DOI for files used.
- The draft (Google drive)[15]
- All also to GitHub: See https://github.com/WilliamCooper/AMTD-AAC.git[16]

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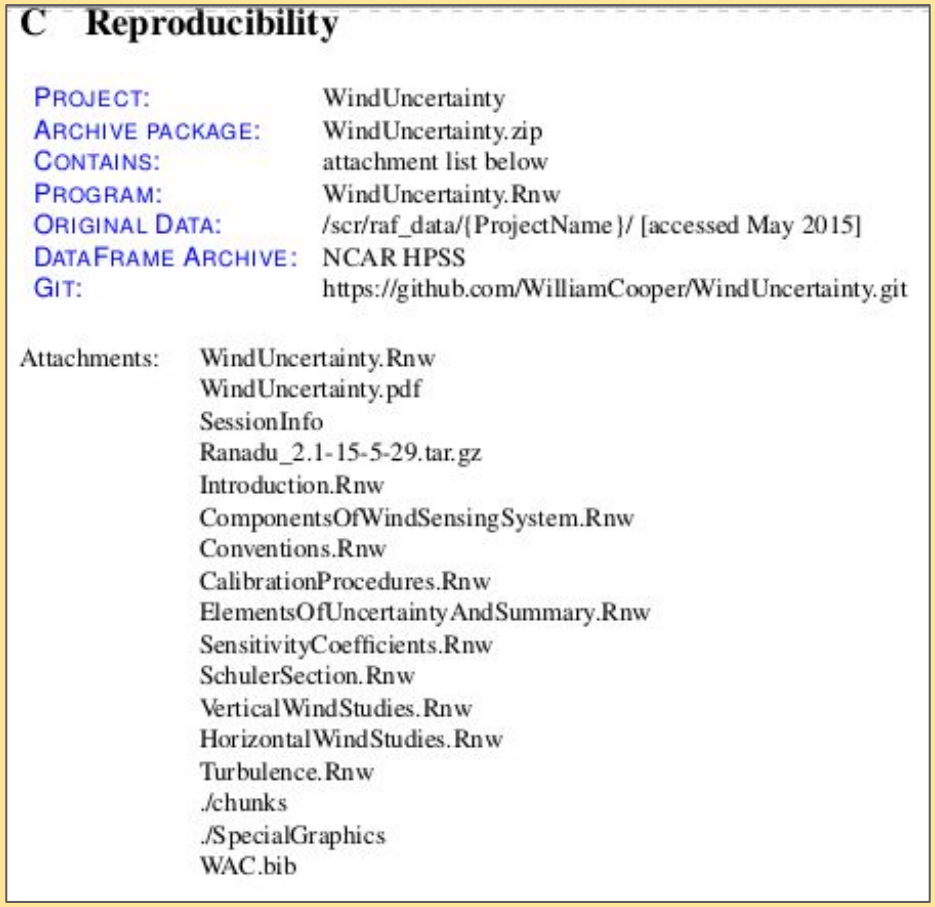
5. Reference the data sources, programs, and workflow documents in your research and data analysis publications.

Example: Application to an NCAR Technical Note

"Characterization of Uncertainty in Measurements of Wind from the NSF/NCAR Gulfstream V Research Aircraft" [status: submitted to EOL for approval]



C Reproducibility

PROJECT:	WindUncertainty
ARCHIVE PACKAGE:	WindUncertainty.zip
CONTAINS:	attachment list below
PROGRAM:	WindUncertainty.Rnw
ORIGINAL DATA:	/scr/raf_data/{ProjectName}/ [accessed May 2015]
DATAFRAME ARCHIVE:	NCAR HPSS
GIT:	https://github.com/WilliamCooper/WindUncertainty.git

Attachments:
WindUncertainty.Rnw
WindUncertainty.pdf
SessionInfo
Ranadu_2.1-15-5-29.tar.gz
Introduction.Rnw
ComponentsOfWindSensingSystem.Rnw
Conventions.Rnw
CalibrationProcedures.Rnw
ElementsOfUncertaintyAndSummary.Rnw
SensitivityCoefficients.Rnw
SchulerSection.Rnw
VerticalWindStudies.Rnw
HorizontalWindStudies.Rnw
Turbulence.Rnw
./chunks
./SpecialGraphics
WAC.bib

The Technical Note (Google drive)[17]

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Next Steps

DAT

A

SOFTWARE

Submit a Geoscience Paper of the Future (GPF)[1]

- GPF papers may be submitted to a special section of the AGU Earth and Space Sciences Journal by July 1, 2016, see: http://onlinelibrary.wiley.com/journal/10.1002/%28ISSN%292333-5084/homepage/call_for_papers.htm

- SCIENCE magazine accepts GPF's

WORKFLOW

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Comments/Questions?