Provenance Representation for the National Climate Assessment in the Global Change Information System

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Abstract—The important topic of global climate change builds on a huge collection of scientific research. It is common for agencies releasing climate change information to be served with requests for all supporting materials resulting in a particular conclusion. Capturing and presenting global change provenance, linking to the research papers, data sets, models, analyses, observations, satellites, etc., that support the key research findings in this domain can increase understanding and aid in reproducibility of results and conclusions. The U.S. Global Change Research Program is now coordinating the production of a national climate assessment (NCA) that presents our best understanding of global change. We are now developing a global change information system that will present the content of that report and its provenance, including the scientific support for the findings of the assessment. We are using an approach that will present this information both through a human accessible Web site as well as a machine-readable interface for automated mining of the provenance graph. We plan to use the developing World Wide Web Consortium (W3C) PROV data model and ontology for this system. This paper will describe an overview of the process of developing the NCA and how the provenance trail of the report and each of the technical inputs can be captured and represented using the W3C PROV ontology. This will improve the visibility into the assessment process, increase understanding and possibility of reproducibility, and ultimately increase the credibility and trust of the resulting report.

Index Terms—Data management, government information systems, knowledge representation.

I. BACKGROUND

A. USGCRP

THE U.S. Global Change Research Program (USGCRP) coordinates and integrates federal research on changes in

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the global environment and their implications for society. The USGCRP began as a presidential initiative in 1989 and was mandated by Congress in the Global Change Research Act (GCRA) of 1990 [1], which called for "a comprehensive and integrated United States research program which will assist the Nation and the world to understand, assess, predict, and respond to human-induced and natural processes of global change."

The USGCRP is developing a global change information system (GCIS) that will link to global change information throughout the 13 federal agencies of the program. That information and a depiction of the provenance information and relationships will be presented through the USGCRP Web presence http:// globalchange.gov. The first implementation will support the national climate assessment (NCA).

B. NCA

The GCRA requires a report to the President and the Congress at least every four years that integrates, evaluates, and interprets the findings of the USGCRP; analyzes the effects of global change on the natural environment, agriculture, energy production and use, land and water resources, transportation, human health and welfare, human social systems, and biological diversity; and analyzes current trends in global change, both human-induced and natural, and projects major trends for the subsequent 25 to 100 years.

A federal advisory committee of experts is now producing a report that will become the 2013 NCA and has defined 30 chapters, which are being developed by 62 "convening lead authors" and 180 additional authors. Those designated contributing authors and their institutional affiliations are a critical part of the provenance of the NCA that will be captured. All of that information will not only be part of the printed and Web-based text of the document but also expressed in a formal structured machine-readable format.

Through an open public process, the NCA has received over 500 distinct official technical inputs to the 2013 NCA report, many of which are reports distilling and synthesizing even more information, coming from thousands of individuals around the federal government, nongovernmental organizations, academic institutions, etc. In additional to the official technical inputs, authors are free to use any other sources of relevant information. The inputs used in the 2013 NCA report include peer-reviewed scientific publications, model data, observational data (physical, societal, and economic), historical data, sectoral and regional assessments, and data at a variety of scales and resolutions. Most original data are archived in long-term agency data centers responsible for long-term stewardship of the items, but some includes "unconventional" information collected from public health departments, states and tribes, nongovernmental organizations, and data collected but not yet reviewed. Where the data are transformed into new graphics, graphs, or charts, the process and methods used must be clearly and reproducibly documented.

This poses a tremendous challenge (and opportunity) for provenance capture, archive, and presentation. We plan to make information about the NCA process itself, as well as the inputs to the process available through a publicly accessible Web site and SPARQL end point. The GCIS will provide links from the content and findings of the NCA back to their antecedent artifacts.

C. IQA

As a highly influential scientific assessment, the NCA report is subject to the highest standards of the Information Quality Act (IQA) [2]. A scientific assessment is considered "highly influential" if its dissemination could have a potential impact of more than \$500 million in any one year on either the public or private sector; if the dissemination is novel, controversial, or precedent-setting; or if it has significant interagency interest. One of the ways that information can exert economic impact is through the costs or benefits of a regulation based on the disseminated information.

The IQA directed the White House Office of Budget and Management (OMB) to issue government-wide guidelines that "provide policy and procedural guidance to federal agencies for ensuring and maximizing the *quality*, *objectivity*, *utility* and *integrity* of information (including statistical information) disseminated by federal agencies" [2]. In those guidelines, OMB defines "quality" as the encompassing term, of which "utility," "objectivity," and "integrity" are the constituents.

In order to provide *objectivity* and *integrity* of content, a strict peer review process has been adopted for the NCA reports. All narrative and images included in a report will be subject to a detailed review process by experts in the scientific community (the National Research Council, among others), by the individual federal agencies involved in the process, by the NCA Development and Advisory Council, and by the public in general. The USGCRP Review and Comment System will be used to accommodate expert and public participation in this process by capturing and organizing comments for the authors and the responses to those comments.

The IQA requirement for *utility* can be better accomplished by creating a transparent system that provides access to information about the processes, analyses, and data sources. A commitment by the NCA to transparency is revealed at different levels: 1) Information sources are captured with full references; 2) quality and provenance of data are clearly described and peer reviewed; 3) data and image details are represented with standardized metadata (ISO 19115); 4) data, documents, and code are version controlled and managed in an accessible configuration management system; 5) narrative assessment and graphics link to source data and information; and 6) the rationale underlying the key messages of the report is captured in *traceable accounts*.

D. Traceable Accounts

Accompanying most key messages emerging from the NCA 2013 Report, there will be a traceable account that summarizes the thought process that leads to a specific narrative. A traceable account describes the evidence base and the major uncertainties of a statement and provides an assessment of the confidence, attributed by the authors, based on evidence of agreement in the related communities of expertise. That level of confidence is a qualitative measure (very high, high, medium, and low) specific to each key message. In addition, authors are asked to provide, when possible, a measure of estimated likelihood of impact or consequence following a scale that ranges from "very likely" (greater than nine in ten) to "very unlikely" (less than one in ten). The use of traceable accounts will provide access to information concerning the sources of information and the justification supporting the key messages for a given report.

For example, a key message might be something like "The length of the frost-free season (and the corresponding growing season) is increasing nationally, with the largest increases occurring in the western U.S., affecting ecosystems and agriculture. Continued lengthening of the growing seasons across the U.S. is projected."

The traceable account for that message would describe the evidence base supporting that message, citing specific technical inputs. It would also describe new information and remaining uncertainties and include an assessment of the confidence in the message based on the evidence analyzed, for example, "Given the evidence base and remaining uncertainties, confidence is **very high** that the length of the frost-free season (also referred to as the growing season) is increasing nationally, with the largest increases occurring in the western U.S, affecting ecosystems, gardening, and agriculture. Confidence is **very high** that there will be continued lengthening of these seasons across the U.S. given the evidence base."

To increase the general credibility and usability of the NCA report and its content, the NCA aims to go beyond the IQA requirements for transparency and traceability, and support reproducibility for all its content. This will be accomplished by keeping accurate records of all processes and collecting metadata on data sources, images, and code. The objective is to make publicly (and easily) available the information required to allow any user to reproduce that same image independently.

NCA goals for providing reproducibility require a strong commitment from the entire community involved in the process of generating the NCA reports, and the level of effort will require a phased approach to its implementation. Fig. 1 depicts the range of the goals for the NCA, ranging from the basic requirements for traceability through those required for full reproducibility.

By documenting all sources underlying the narrative and images of the report and keeping track of the chain of custody

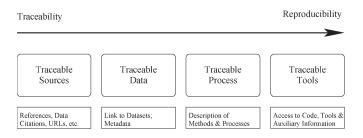


Fig. 1. Transparency goals for the NCA.

for that content, one may ensure compliance with IQA requirements.

II. PRESERVATION CONTENT

In 1998, the National Aeronautics and Space Administration (NASA) and the National Oceanic and Atmospheric Administration (NOAA) sponsored a workshop coordinated through the USGCRP, which produced a report on global change science requirements for long-term archiving [3]. It describes a particular content that future consumers of science might be interested in. Building on that and other efforts, the NASA Earth Science Data and Information System project published the NASA Earth Science Data Preservation Content Specification [4] in 2011. It provides guidance on "specific content items that need to be preserved from each of NASA's missions." As the provenance graph from the NCA is explored, figures to papers to datasets, and so forth, the relationships between those items can be followed. Each of the items recommended for longterm preservation and their relationships could be useful for various classes of readers of the NCA. A later example will describe a particular use case in examining the provenance graph describing a representation of the relationships between some of those preservation content items.

A. Data Citations

One of the major content item relationships of concern is that between a scientific paper and the datasets used by the researcher in producing the conclusions in the paper. New science builds on previous efforts, and citing other papers is a fundamental practice in documenting good science. Documenting data has not always been as rigorously practiced [5]. Recent advances such as the technologies of the World Wide Web have made data easier to obtain and also make it easier to reference and direct others to data that were used. In particular, a study coordinated by Ruth Duerr through the NASA Earth Science Data Systems Working Group and the Federation of Earth Science Information Partners (ESIP) analyzed identification schemes for earth science data and recommended that data centers assign Digital Object Identifiers (DOIs) to datasets just as publishers assign them to journal articles [6]. Guidelines for data citations building on those recommendations were approved by the ESIP Assembly in 2012 [7].

As science journal authors, reviewers and editors start following those guidelines, discovering the relationships between science papers, and their data will become easier not only for direct consumers of their research but also for incorporation of those relationships into citation and provenance graphs in systems such as the GCIS.

For our initial application, the NCA, we have often found data citation practices poor to nonexistent. While some automation can be employed to extract basic information (authors, chapters, key messages, and even reference metadata), a support team is working with the author teams to manually track down input data sources and enter sufficient metadata into the system.

B. Identifiers

Following the general data model for provenance described in the World Wide Web Consortium (W3C) PROV, described in more detail hereinafter, the GCIS assigns globally unique persistent identifiers to all of the entities, activities, and agents relevant to our discussions of provenance. These allow us to reference the items uniquely, both internally to the GCIS and externally to and from other related systems. We link to existing identifiers where possible and appropriate, using journal- or data-center-assigned DOIs for papers and datasets. The Global Change Master Directory of NASA has also assigned standard reusable identifiers for many of the datasets, services, and other keywords that we are referencing [8]. These include their dataset Entry_ID and universally unique identifiers for keywords.

Each identifier is mapped to a uniform resource identifier (URI) in the USGCRP name space rooted under http://data. globalchange.gov/, allowing use of those identifiers for resource description framework (RDF) and linking with semantic Web and other linked data systems. Our representation of those provenance elements with the PROV ontology is built off of those URIs. A few example URIs are shown in Table I.

All of the URIs will also be resolvable locators through Hypertext Transfer Protocol content negotiation [9] to either human-readable HTML Web pages or machine-readable encodings of the metadata describing the item and linking back to the repository for that item (such as a journal site for a paper or an agency data center for an observational dataset). Where items are derived from or associated with other items, the derived items will link back to the items on which they depend. The "activity" representations associated with the derivation will contain sufficient detail to understand and, ultimately, to reproduce the process that created the derived items.

PROV can be extended with domain-defined types for "agents" like our agency and project organizations and specialized agent roles for the NCA process like the "convening lead authors."

Identifiers for people such as scientific research authors are particularly troublesome, since names can not be relied on as a unique identifier. Several efforts are attempting to address the problem, including ResearcherID¹ and ORCID,² and we plan to take advantage of them as they become more widespread. Although we can harvest basic publication metadata from some publisher Web sites, our early efforts with the NCA rely on a somewhat manual (and, we acknowledge, error-prone) process.

¹http://researcherid.com.

²http://orcid.org.

TABLE I Some Example URIS For GCIS

URI	Resource
http://data.globalchange.gov/report/nca2013	NCA 2013 Report
http://data.globalchange.gov/report/nca2013/chapter/13/figure/4	Figure 4 from Chapter 13 of the report
http://data.globalchange.gov/organization/Santa_Clara_University	Santa Clara University
http://data.globalchange.gov/person/Nancy_GMaynard	Convening Lead Author Nancy G. Maynard
http://data.globalchange.gov/publication/doi/10.1029/2005jc003136	Article Variability of ocean heat uptake: Reconciling observations and models

In the system, unique identifiers for authors are recorded where available and assigned where they are not, so we can distinguish multiple authors with the same name within our own database.

C. Granularity

Earth science data encompass a wide range of data types and forms. Some are as simple as a spreadsheet of *in situ* measurements gathered by hand. Others include millions of measurements from remote sensing earth observation satellite instruments. The organization of such data into meaningful useful portions is often referred to as partitioning or modularizing the data. The NASA Earth Observing System Data Model defines collections of data that are organized into archivable chunks or "granules." For example, the Moderate Resolution Imaging Spectrometer has a granule size of 5 min, with a unique identifier and "granule-level" metadata recorded for each 5-min granule.

When referring to such data, the GCIS will record and link information only at the collection or dataset level, with individual granule level data, metadata, provenance, etc., remaining solely the responsibility of the data center holding that data. In some cases, provenance or lineage information has only been recorded and presented by the data centers at the granule level. It must be summarized to the collection level to be usefully captured and linked into the GCIS. Depending on the processing scenarios, this summarization could be very simple, or it could be quite complicated. Good algorithms for succinctly and correctly determining and representing collection level provenance from granule level processing records are an area that needs further research.

Within the reports such as the NCA, our "granules" will be each identifiable portion of the content where knowledge of particular metadata, including provenance, is important. For the NCA, this will include chapters, which can be linked through attribution to their authors; key messages, which can be linked to their traceable accounts; individual figures; graphs; etc., which can be linked to other research papers or data sets from which they are derived.

Some of the decomposition of the report into those "granules" can be automated by parsing out the structured parts of the document. Some requires manual intervention and "cleanup" to ensure that the document is represented faithfully.

III. PROVENANCE REPRESENTATION

Many models for provenance representation have been developed in various communities. For the general geoscience provenance and our particular focus for the needs of the GCIS, we have converged on two: the lineage elements for

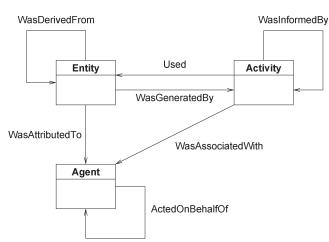


Fig. 2. PROV core structures.

the International Standards Organization (ISO) Geographic information–Metadata standards for specific data production provenance and the W3C PROV standard for representation and interoperability of the overall provenance. These standards overlap in some areas but, in general, are complementary, and each has its uses. In general, we encourage data producers and archives to adopt ISO metadata for complete documentation of their data products and, specifically, to populate the lineage elements with their sources and process for creating those products so that we (and any other users of their products) can discover and use provenance facts about those products. We will use the W3C PROV model for our linking of that data product provenance with all of the other provenance that we are presenting.

A. ISO Lineage Elements

Earth science data centers are gradually converging on ISO metadata for representation of basic provenance for their data products. ISO 19115:2003, *Geographic information—Metadata* includes a section LI_Lineage with elements LI_Source and LI_ProcessStep that can represent basic provenance information. ISO 19115-2:2009 extends the data lineage model, allowing more detail (LE_Source, LE_Processing, LE_Algorithm, etc.). Where data producers or archives are describing their data with ISO Extensible Markup Language metadata, we can obtain information about provenance directly from those descriptions and link it into our overall provenance chain.

The description of the provenance of the data products themselves is primarily the responsibility of the data producers and archivers. Unfortunately, few data producers or archives are

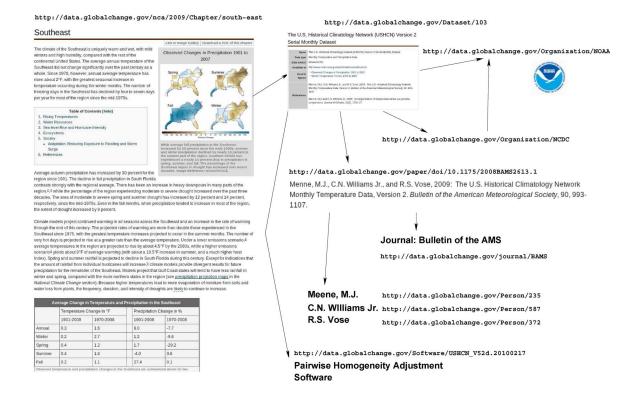


Fig. 3. NCA 2009 figure example provenance.

publishing ISO metadata, and of those even fewer populate the lineage elements with consistent descriptions and identifiers. In this early phase of the GCIS, where our focus is on the primary provenance of the NCA report itself, we are unable to determine and produce complete provenance for data products where the producers have failed to do so. We will be working with producers and archives to encourage good provenance capture and representation using standards like those of the ISO. As they do so, we plan to link their provenance with ours.

B. W3C PROV

The W3C Provenance Working Group is finalizing definition of the PROV data model (PROV-DM) [10]. PROV-DM is a "generic data model for provenance that allows domain and application specific representations of provenance to be translated into such a data model and *interchanged* between systems." The PROV specification family also includes PROV-O, an OWL2 ontology [11].

The PROV-DM allows some quite complex provenance relationships to be represented. The GCIS, starting with the NCA, will focus on using PROV for some very basic relationships in the short term. These could be extended in the future.

The core types defined by PROV include Entity, Activity, and Agent. Those types and the most basic relationships between them are depicted in Fig. 2. Early representations of the NCA provenance will use the most important and useful PROV concepts: Attribution ("WasAttributedTo") and Derivation ("Was-DerivedFrom"). Those simple concepts alone are sufficient to build a graph of contributing entities and agents and construct a Web site for a user to browse the collection.

Where appropriate and useful, we will extend those by further describing the activities involved and attaching additional attributes to the relationships between entities, activities, and agents.

IV. NCA 2009 W3C PROV-O EXAMPLE

In order to express the functionality of the GCIS in terms of how the user will interact with it for provenance information, we applied a number of use cases. In this use case, we will describe an application of provenance in the GCIS, with a focus on the NCA report, shown with a simple example from the NCA 2009 report depicted in Fig. 3.

The reader of the NCA report wishes to identify the dataset used to generate a particular figure in the report. S/he is directed first to the figure caption. Selecting the caption displays a page of information about the figure, and if the figure was originally published in another paper, it includes a link via the paper's DOI to the publisher's site describing that paper, offering it for download. The page of information also includes references to the datasets used in the paper on which the figure was based. Following each of the dataset links presents a page of information about the dataset, including links back to the agency/data center Web page which provides more details on the dataset (metadata) and from which the actual data may be available for order or download.

More formally, the primary *actor* in this use case is a reader of the NCA report. The *precondition* is that the reader is browsing the NCA report online, and after consulting the basic flow of information described previously, the *postcondition* is that the reader has visited the dataset Web page on the data center Web site. The components in the use case include a report, a chapter, a figure, a paper, and a dataset.

We captured provenance information required to support the aforementioned use case and modeled it using the PROV-O

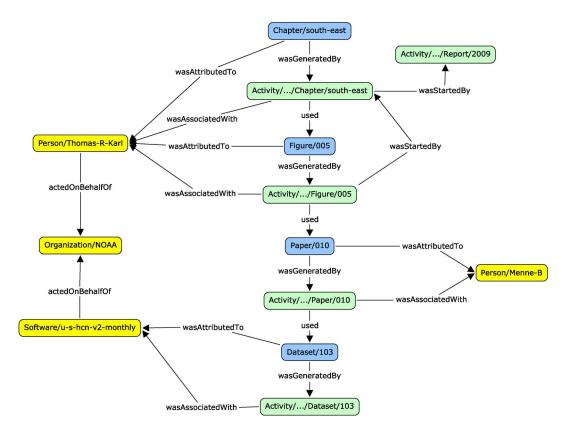


Fig. 4. PROV-O example graph representation.

ontology [11]. The example in Fig. 4 illustrates the provenance history of a figure in a chapter of the NCA report. This fulfills the requirements of the aforementioned use case. Aside from chapter, figure, paper, and dataset, we also captured provenance information such as persons involved in generating a chapter, paper, or figure, software used to collect the dataset, etc. Fig. 4 applies the three starting point classes (i.e., Entity, Activity, and Agent) in the PROV-O ontology to depict the provenance information. For example, the entity "Chapter south-east" (a chapter) was generated by the activity "Chapter south-east," which used another entity "Figure 005." Entities "Chapter south-east" and "Figure 005" were attributed to the agent "Person Thomas-R-Karl," and the activity "Chapter south-east" was associated to the same agent. Another PROV relationship "wasStartedBy" was used to indicate that the activity of producing "Figure 005" was started by the activity of creating the "Chapter southeast," which, in turn, was started by the activity of creating the whole report. Fig. 5 shows an RDF serialization of the resources depicted in Fig. 4. The components shown in the provenance history also reflect the aforementioned consideration on the granularity of data and information in GCIS. This example shows that data provenance and data transparency can be easily captured and supported by adopting the PROV-O ontology.

V. CONCLUSION AND FUTURE WORK

Using the semantic Web approach to organizing and presenting the provenance of the NCA through the GCIS has resulted in a more structured and interoperable representation, allowing other tools and services to interact with the data behind the Web site, increasing its usefulness for other purposes, including data mining and service integration beyond what is possible with a simple Web site. This is a significant feature of the semantic Web and/or linked data approach.

The current focus for the GCIS in support of the NCA is "simple" provenance. A reader of the report will be able to read the content of the report, including a prose description of the rationale for the key messages of the report. From that, the reader can explore the papers, datasets, etc., that contributed to those descriptions and conclusions.

This approach initially uses relatively lightweight annotations and associated reasoning. Some of the authors have created and used a conversion tool to take in data and create lightly annotated data automatically [12]. This can be done with little effort since it is an automated effort. Additional tools are in process that support enhancements with minimal human effort.

Starting with the core of entities represented in support of the NCA, the GCIS will build its database of papers, datasets, etc., eventually covering the entire scope of global change. By linking those items through provenance and other relationships, the resulting database could support more complicated data mining beyond the simple walking step by step through the graph on a Web site. It could, for example, produce metrics such as the number of papers that use data derived from each of the Earth observing satellites. It could provide the basis for discovery of interagency dependences such as an Environmental Protection Agency analysis that used data from a Department of Energy model that used data from a NASA satellite. It can be very difficult

<pre><http: 2009="" chapter="" data.globalchange.gov="" nca="" south-east=""> a prov:Entity; prov:wasGeneratedBy <http: 2009="" activity="" chapter="" data.globalchange.gov="" nca="" south-east="" writing="">; prov:wasAttributedTo <http: data.globalchange.gov="" person="" thomas-r-karl="">;</http:></http:></http:></pre>
<http: 2009="" activity="" chapter="" data.globalchange.gov="" nca="" south-east="" writing=""></http:>
<pre>a prov:Activity; prov:used <http: 005="" data.globalchange.gov="" figure="">; prov:wasAssociatedWith <http: data.globalchange.gov="" person="" thomas-r-karl="">; prov:wasStartedByActivity <http: 2009="" activity="" data.globalchange.gov="" nca="" report="" writing="">; .</http:></http:></http:></pre>
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<http: 005="" activity="" data.globalchange.gov="" figure="" writing=""> a prov:Activity; prov:used <http: 010="" data.globalchange.gov="" paper="">;</http:></http:>
<pre>prov:wasAssociatedWith <http: data.globalchange.gov="" person="" thomas-r-karl="">; prov:wasStartedByActivity <http: 2009="" activity="" chapter="" data.globalchange.gov="" nca="" south-east="" writing="">; .</http:></http:></pre>
<pre><http: 010="" data.globalchange.gov="" paper=""> a prov:Entity; prov:wasAttributedTo <http: data.globalchange.gov="" menne-b="" person="">; prov:wasGeneratedBy <http: 010="" activity="" data.globalchange.gov="" paper="" writing="">; .</http:></http:></http:></pre>
<pre><http: 010="" activity="" data.globalchange.gov="" paper="" writing=""> a prov:Activity; prov:used <http: 103="" data.globalchange.gov="" dataset="">; prov:wasAssociatedWith <http: data.globalchange.gov="" menne-b="" person="">;</http:></http:></http:></pre>
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<pre>prov:wasGeneratedBy <http: 103="" activity="" data.globalchange.gov="" dataset="" generating="">; rdfs:seeAlso <http: climate="" oa="" research="" ushcn="" www.ncdc.noaa.gov=""></http:>; prov:wasAttributedTo <http: data.globalchange.gov="" software="" u-s-hcn-v2-monthly="">; .</http:></http:></pre>
<pre><http: 103="" activity="" data.globalchange.gov="" dataset="" generating=""> a prov:Activity; prov:wasAssociatedWith <http: data.globalchange.gov="" software="" u-s-hcn-v2-monthly="">; .</http:></http:></pre>

Fig. 5. PROV-O example turtle representation.

and manpower intensive to manually trace such relationships in the absence of a standard representation of provenance crossing those interagency boundaries.

In future work in the GCIS and for the continuing sustained assessment activities, we plan to capture more details concerning rationales for decisions. We are moving toward more descriptive traceable accounts that capture not only the basic sources of data and analyzers but also more details of how the analysis progressed along with its assumptions and manipulations. We are exploring how this can be captured using the the Proof Markup Language (PML) [13]. PML was initially designed to provide a formal foundation for capturing information concerning basic provenance, information manipulations, and trust in a unified formal framework. It was one of the provenance languages that influenced today's W3C proposal for a provenance language recommendation. The next generation of PML provides compatibility with PROV and extends it to support encodings of more detailed information manipulation steps such as those used in coming to recommendations in a global change report. The next generation of traceable accounts would include formal encoding of the rationale and would not just be consumable by humans but they could also be analyzed mechanically for correctness and consistency.

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