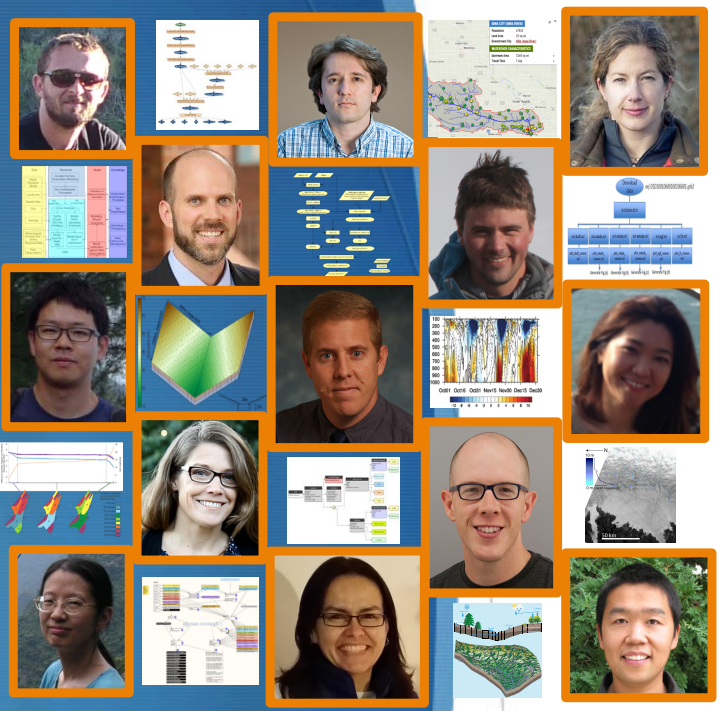
The Scientific Paper of the Future



http://www.scientificpaperofthefuture.org

OntoSoft Training

January 2017

ontosoft@gmail.com

http://dx.doi.org/10.5281/zenodo.159206

[CER-1440323
[CER-1343800

EarthCube

Instructors Today

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Gail Clement

Information Sciences Institute
University of Southern California

Research Library
California Institute of Technology

Acknowledgments

ICER-1440323
ICER-1343800

- The Scientific Paper of the Future training materials were developed and edited by Yolanda Gil (USC), based on the OntoSoft Geoscience Paper of the Future (GPF) training materials with contributions from the OntoSoft team including Chris Duffy (PSU), Chris Mattmann (JPL), Scott Peckham (CU), Ji-Hyun Oh (USC), Varun Ratnakar (USC), Erin Robinson (ESIP)
- The OntoSoft training materials were significantly improved through input from GPF pioneers Cedric David (JPL), Ibrahim Demir (UI), Bakinam Essawy (UV), Robinson W. Fulweiler (BU), Jon Goodall (UV), Leif Karlstrom (UO), Kyo Lee (JPL), Heath Mills (UH), Suzanne Pierce (UT), Allen Pope (CU), Mimi Tzeng (DISL), Karan Venayagamoorthy (CSU), Sandra Villamizar (UC), and Xuan Yu (UD)
- Thank you to Ruth Duerr (NSIDC), James Howison (UT), Matt Jones (UCSB), Lisa Kempler (Matworks), Kerstin Lehnert (LDEO), Matt Meyernick (NCAR), and Greg Wilson (Software Carpentry) for feedback on best practices
- Thank you also to the many scientists and colleagues that have taken the training and asked hard questions
- We are grateful for the support of the National Science Foundation and the EarthCube program

ICER-1440323
ICER-1343800

EarthCube

OntoSoft: Software Stewardship for the Geosciences

OntoSoft

Community

- Recommender system
- Interoperability

OntoSoft

Publication

- Structured metadata
- Interactive advice

GEOSCIENCE PAPERS OF THE FUTURE

Learning

- Best practices
- Multimedia lessons

The Geoscience Papers of the Future (GPF) Initiative

http://www.scientificpaperofthefuture.org/gpf

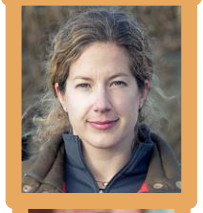
1. A Special Issue of a journal in all geoscience areas that includes only geoscience papers of the future

2. Training sessions for geoscientists to learn best practices in software and data sharing, provenance documentation, and scholarly publication

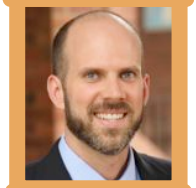
GPF Pioneer Authors

Cedric David, NASA/JPL
Hydrology modeling

Ibrahim Demir, U. of Iowa
Hydrology sensor networks

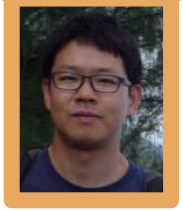


R. W. Fulweiler, Boston U.
Biogeochemistry in marine ecology



J. Goodall/B. Essawy, U. Virginia, Hydrology/visualization

Leif Karlstrom, U. Oregon
Volcanic vent clustering



Kyo Lee, NASA/JPL
Regional climate modeling

Heith Mills, U. Houston
Geochemistry, marine biology

Ji-Hyun Oh, USC
Tropical meteorology

Suzanne Pierce, UT Austin
Hydrogeology for decision support

Allen Pope, U. Colorado
Glaciology

Mimi Tzeng, Dauphin Island Sea Lab, Ocean fisheries

Sandra Villamizar, UC Merced
River ecohydrology

Xuan Yu, U. Delaware
Hydrologic modeling

Why Learn to Write a Scientific Paper of the Future

1. **Get credit** for all your research products
   - ★ Citations for software, data, samples, …
2. **Increase citations** of your papers
3. Write impressive **Data Management Plans**
4. **Extend your CV** with data and software sections
5. **Reproduce** your work from years ago
6. Comply with new **funder and journal requirements**

Training Goals

What Training Covers

- **Best practices**
  - Many are still being developed by the community
- **Major concepts and goals**, regardless of the platform, research area, or target journal
- **Mindful of effort**
  - How to implement best practices with simplest approach

What is Not Covered

- Metadata standards specific to particular research areas
- Improving software development skills
- Details of using code sharing sites

Scientific Paper of the Future Training

Part I

1. Motivation and overview: open science, reproducible publications, and digital scholarship
2. Making data accessible
3. Making software accessible
4. Documenting software with metadata

Part II

5. Documenting provenance and methods
6. Improving author citation profile and researcher impact
7. Summary of author checklist

CODATA

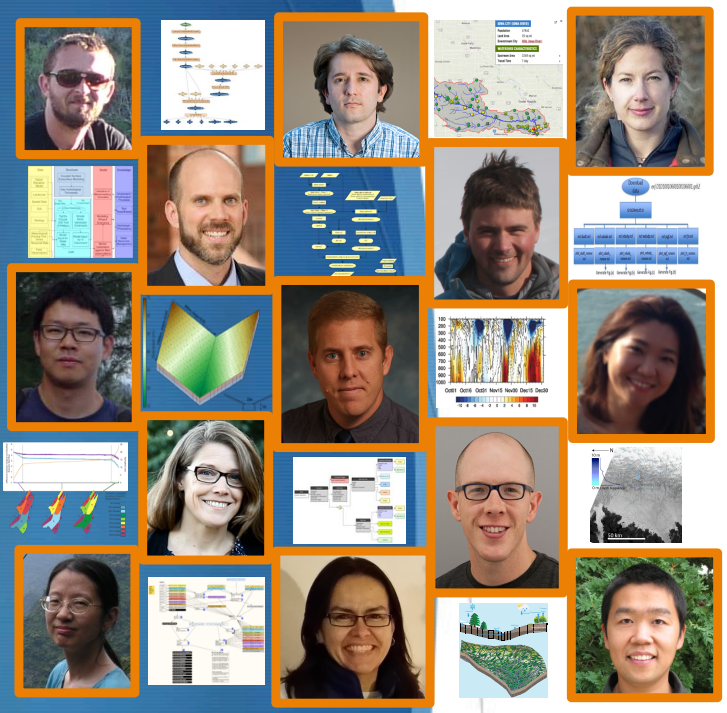
RDA
RESEARCH DATA ALLIANCE

DataCite

FORCE11
The Future of Research Communications and e-Scholarship

SIP

The Scientific Paper of the Future: Motivation and Overview



OntoSoft Training

Part 1

http://dx.doi.org/10.5281/zenodo.15920

http://www.scientificpaperofthefuture.org

NSF ICER-1440323
ICER-1343800

Modern Scientific Articles

Traditional Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Modern Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

Scientists Are Changing

Open data

figshare

DRYAD

The Dataverse Network™ Project

Open access

creative commons

open source initiative

Open publications

PLOS

Open source

github SOCIAL CODE HOSTING

Apache

sourceforge

wikigenes collaborative publishing

Scientists Are Changing

NATURE|METRICS SURVEY 2010

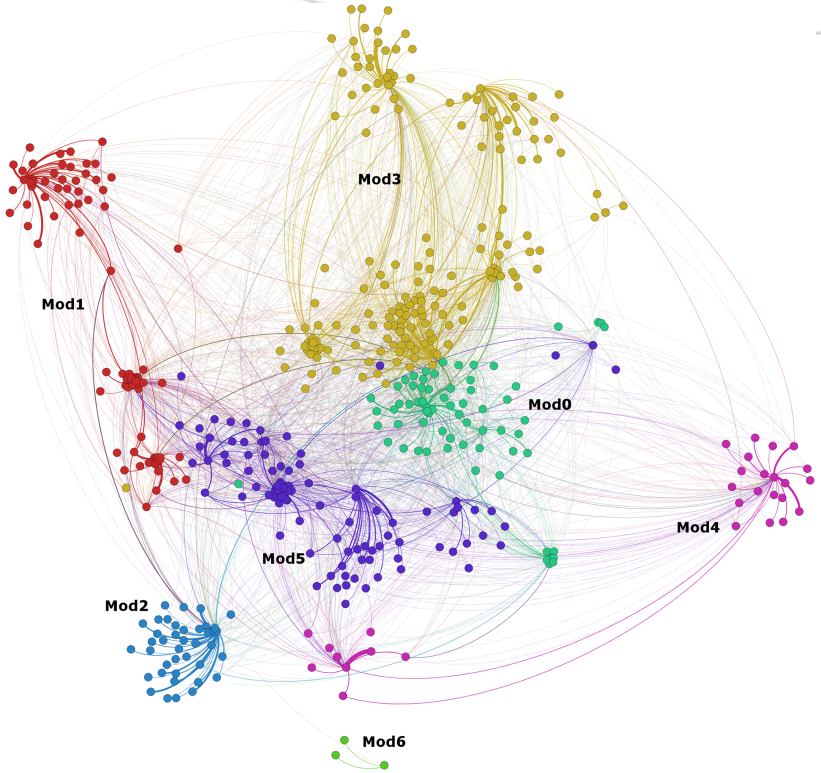
METRICS SURVEY RESULTS

Thinking about all of the possible measures of scientific contribution that are possible, please select your top 5 priorities.

	No. of times chosen	Relative ranking
Publication in high-impact journals	92	2.61
Grants earned	65	1.73
Training and mentoring students and postdocs	63	1.71
No. of citations on published research	58	1.62
No. of publications	53	1.38
Teaching courses	41	1.18
Collaborative work outside of your department/institution	37	0.97
Development of research resources for the scientific community (e.g. reagents, software, database development)	31	0.89
Departmental/institutional administration	5	0.16
Development of start-up business	5	0.14
Blogging, writing for lay press	4	0.10
Meeting abstracts	3	0.08
Data deposited in public repositories	3	0.08
Participation in departmental meetings	2	0.05

http://www.nature.com/nature/newspdf/metrics_survey.pdf

Scientists Are Changing



[Holmberg et al 2014]

altmetrics

Impact

usage	peer-review	citations	alt-metrics
downloads views	expert opinion		storage links bookmarks conversations

Crossref

depsy

Altmetric

Impactstory

http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0106086

Publishers Are Changing

Illuminating the black box

Note to biologists: submissions to *Nature* should contain complete descriptions of materials and reagents used.

nature

Reporting Checklist For Life Sciences Articles

This checklist is used to ensure good reporting standards and to improve the reproducibility of published results. For more information, please read Reporting Life Sciences Research.

Availability of Software

PLOS | ONE

PLOS supports the development of open source software and believes that, for submissions appropriate open source standards will ensure that the submission conforms to (1) our requi another researcher can reproduce the experiments described, (2) our aim to promote openn PLOS journals can be built upon by future researchers. Therefore, if new software or a new a that the software conforms to the Open Source Definition, have deposited the following three submission as Supporting Information:

- **The associated source code of the software described by the paper.** This should be licensed under a suitable license such as BSD, LGPL, or MIT (see http://www.ope commercial software such as Mathematica and MATLAB does not preclude a paper f preferred.
- **Documentation for running and installing the software.** For end-user applications prerequisite; for software libraries, instructions for using the application program inter
- **A test dataset with associated control parameter settings.** Where feasible, result test data should not have any dependencies — for example, a database dump.

eptable archives should provide a public repository of the described software. The code s reating user accounts, logging in or otherwise registering personal details. The repositor e than 1,000 projects. Examples of such archives are: SourceForge, Bioinformatics.Org, annah, GitHub and the Codehaus. Authors should provide a direct link to the deposited s

The Public is Changing

ZOONIVERSE
REAL SCIENCE ONLINE

foldit
Solve Puzzles for Science

oldWeather

eBird

PLOS ONE

Discovery of Western European R1b1a2 Y Chromosome Variants in 1000 Genomes Project Data: An Online Community Approach

Richard A. Rocca, Gregory Magoon, David F. Reynolds, Thomas Krahn, Vincent O. Tilroe, Peter M. Op den Velde Boots, Andrew J. Grierson

Published: July 24, 2012 • DOI: 10.1371/journal.pone.0041634

Funders Are Changing

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

February 22, 2013

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: John P. Holdren
Director

SUBJECT: Increasing Access to the Results of Federally Funded Scientific Research

1. Policy Principles

The Administration is committed to ensuring that, to the greatest extent and with the fewest constraints possible and consistent with law and the objectives set out below, the direct results of federally funded scientific research are made available to and useful for the public, industry, and the scientific community. Such results include peer-reviewed publications and digital data.

an approach for optimizing search, archival, and dissemination features that encourages innovation in accessibility and interoperability, while ensuring long-term stewardship of the results of federally funded research;

Funders Are Changing

NSF'S PUBLIC ACCESS PLAN:

Today's Data, Tomorrow's Discoveries

Increasing Access to the Results of Research Funded by the National Science Foundation

National Science Foundation

March 18, 2015

Modern Scientific Articles

Traditional Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Modern Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

Data Papers & Data Repositories

★ Data paper

Ecological Research
July 2013, Volume 28, Issue 4, p 541

Date: 10 May 2013

Monitoring records of plant species in the Hakone region of Fuji-Hakone-Izu National Park, Japan, 2001–2010

Takeshi Osawa

Abstract

The monitoring of species occurrences is a crucial aspect of biodiversity conservation, and regional volunteerism can serve as a powerful tool in such endeavors. The Fuji-Hakone-Izu National Park in the Hakone region of Kanagawa Prefecture, Japan, boasts a volunteer association of approximately 100 members. These volunteers have monitored plant species occurrences from 2001 to the present along several hiking trails in the region. In this paper, I present the annual observation records of plant occurrences in Hakone from 2001 to 2010. This data set includes 1,071 species of plants from 151 families. Scientific names follow the Y List, and this data set includes several threatened plant species. Data files are formatted based on the Darwin Core and Darwin Core Archives, which are defined by the Biodiversity Information Standards (BIS) or Biodiversity Information Standards Taxonomic Databases Working Group (TDWG). Data files filled on required and some additional item on Darwin Core. The data set can download from the author's personal Web site as of July 2012. These data will soon be published for the Global Biodiversity Information Facility (GBIF) through GBIF Japan. All users can then access the data from the GBIF portal site.

- *The complete data set for this abstract published in the Data Paper section of the journal is available in electronic format in Ecological Research Data Paper Archives at http://db.cger.nies.go.jp/JaLTER/ER_DataPapers/archives/2013/ERDP-2013-01.*

★ Data published in a repository

LTER — The US Long Term Ecological Research Network

+/- NTL LTER *"WDNR Yahara Lakes Fisheries: Fish Lengths and Weights 1987-1998" - Lathrop*

LTER Identifier:

knb-lter-ntl.279.1

Abstract:

These data were collected by the Wisconsin Department of Natural Resources (WDNR) from 1987-1998. Most of these data (1987-1993) precede 1995, the year that the University of Wisconsin Â NTL-LTER program Â took over sampling of the Yahara Lakes. However, WDNR data collected from 1997-1998 Â (unrelated to LTER sampling) is also included. In 1987 a joint project by the WDNR and the University of Wisconsin-Madison, Center for Limnology (CFL) was initiated on Lake Mendota. The project involved biomanipulation o...

Owners/Creators:

Lathrop

Metadata:

Select here for full metadata

Data File(s):

- wdnr_fyke_minifyke_seine_lengths_weights.csv
- wdnr_boomshock_lengths_weights.csv
- wdnr_gillnet_lengths_weights_93.csv
- wdnr_walleye_age_lengths_weights_87.csv
- wdnr_creel_survey_lengths_weights.csv
- wdnr_creel_survey_angler_counts.csv

"Dark Data"

Shedding Light on the Dark Data in the Long Tail of Science

P. Bryan Heidorn

From: Library Trends
Volume 57, Number 2, Fall 2008
pp. 280-299 | 10.1353/lib.0.0036

Abstract:

One of the primary outputs of the scientific enterprise is data, but many institutions such as libraries that are charged with preserving and disseminating scholarly output have largely ignored this form of documentation of scholarly activity. This paper focuses on a particularly troublesome class of data, termed *dark data*. "Dark data" is not carefully indexed and stored so it becomes nearly invisible to scientists and other potential users and therefore is more likely to remain underutilized and eventually lost. The article discusses how the concepts from long-tail economics can be used to understand potential solutions for better curation of this data. The paper describes why this data is critical to scientific progress, some of the properties of this data, as well as some social and technical barriers to proper management of this class of data. Many potentially useful institutional, social, and technical solutions are under development and are introduced in the last sections of the paper, but these solutions are largely unproven and require additional research and development.

Modern Scientific Articles

Traditional Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Modern Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

NOT published,
loosely recorded:

Software:
scripted codes + manual steps +
documentation in notes/emails

Reproducibility

Illuminating the black box

Note to biologists: submissions to *Nature* should contain complete descriptions of materials and reagents used.

nature

Reporting Checklist For Life Sciences Articles

This checklist is used to ensure good reporting standards and to improve the reproducibility of published results. For more information, please read Reporting Life Sciences Research

Methodology

A Biostatistic Paper Alleges Potential Harm To Patients In Two Duke Clinical Studies

By Paul Goldberg

Biostatistics journals aren't usually the pl

most recent issue of the Annals of Applied Statistics is an

Human lives

COMPUTER SCIENCE

Accessible Reproduc

Science

putation in research grows, needed to expand recording,

Friday, December 2, 2011 As of 12:00 AM New York 43° | 34°

THE WALL STREET JOURNAL. | HEALTH

HEALTH INDUSTRY | DECEMBER 2, 2011

Scientists' Elusive Goal: Reproducing Study Results

ping how it had halted nearly two-thirds of

experiments failed to match claims made

The New York Times

Science

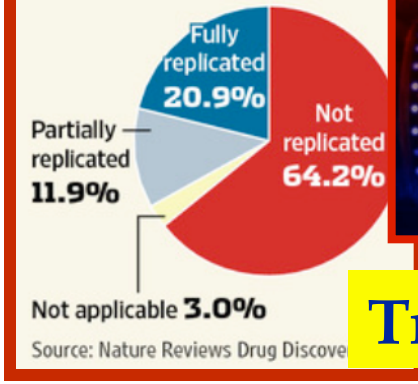
NYTimes: Home - Site Index - Archive - Help

Reliability

Nobel Laureate Retracts Two Paper

No Cure

When Bayer tried to replicate results of 67 studies published in academic journals, nearly two-thirds failed.



Source: Nature Reviews Drug Discove

Financial

The New York Times

Retracted Scientific Studies: A Growing List

Scientific integrity

Trust

Reproducible Publications and Executable Papers

Sweave = R · LaTeX

IP[y]: Notebook

Reproducible Articles

Modern Published Articles

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

NOT published,
loosely recorded:

Software:
scripted codes + manual steps +
documentation in notes/emails

Reproducible Publications

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

Software:
Data preparation,
data analysis, and visualization

Provenance and Workflow:
Workflow/scripts describing
dataflow, codes, and parameters

Beyond Reproducible Publications

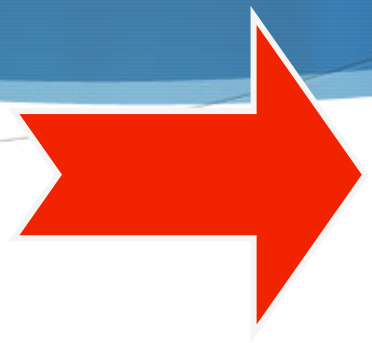
Reproducible Publications

Text:
Narrative of method,
the data is in tables, figures/plots,
the software used is mentioned

Data:
Supplementary materials,
pointers to data repositories

Software:
Data preparation,
data analysis, and visualization

Provenance and methods:
Workflow/scripts describing
dataflow, codes, and parameters



Is this sufficient?

The Scientific Paper of the Future has further requirements

Citations: Getting Credit

Citations: Getting Credit

OPEN ACCESS Freely available online

PLoS one

Sharing Detailed Research Data Is Associated with Increased Citation Rate

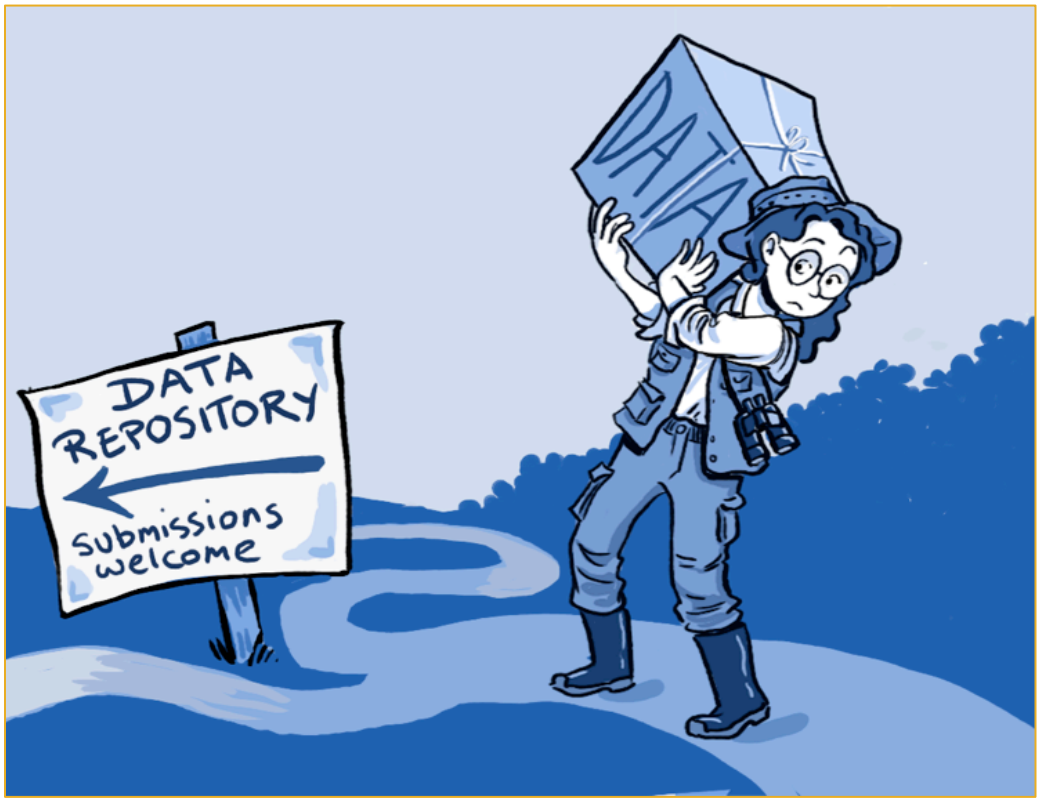
Heather A. Piwowar*, Roger S. Day, Douglas B. Fridsma

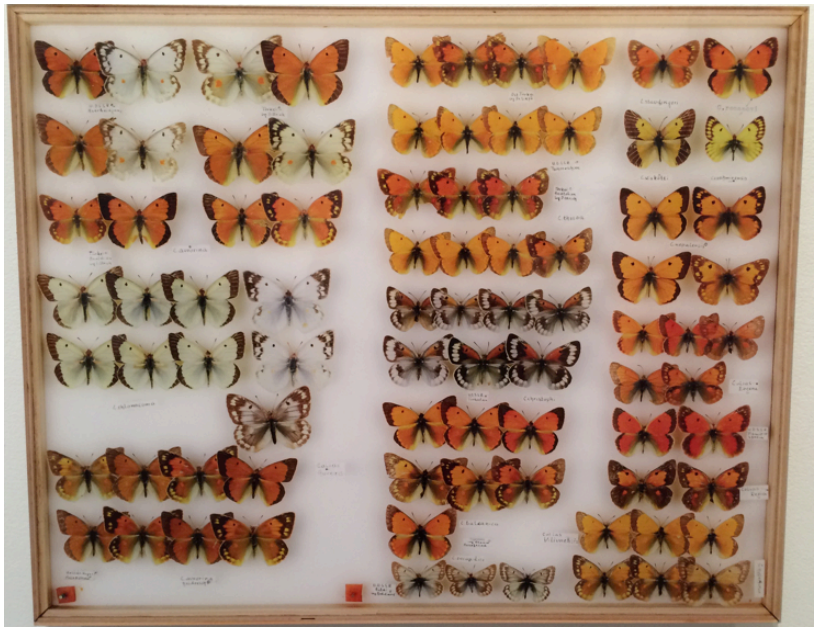
Department of Biomedical Informatics, University of Pittsburgh School of Medicine, Pittsburgh, Pennsylvania, United States of America

Background. Sharing research data provides benefit to the general scientific community, but the benefit is less obvious for the investigator who makes his or her data available. *Principal Findings*. We examined the citation history of 85 cancer microarray clinical trial publications with respect to the availability of their data. The 48% of trials with publicly available microarray data received 85% of the aggregate citations. Publicly available data was significantly ($p = 0.006$) associated with a 69% increase in citations, independently of journal impact factor, date of publication, and author country of origin using linear regression. *Significance*. This correlation between publicly available data and increased literature impact may further motivate investigators to share their detailed research data.

Licenses for Data and Software: Encouraging Safe Reuse

Discoverability through Shared Repositories and Metadata for Data and Software





Scientific Paper of the Future

Modern Paper

Text:
Narrative of the method, some data is in tables, figures/plots, and the software used is mentioned

Data:
Include data as supplementary materials and pointers to data repositories

Open Science

Sharing:
Deposit data and software (and provenance/workflow) in publicly shared repositories

Open licenses:
Open source licenses for data and software (and provenance/workflow)

Metadata:
Structured descriptions of the characteristics of data and software (and provenance/workflow)

Reproducible Publication

Software:
For data preparation, data analysis, and visualization

Provenance and methods:
Workflow/scripts specifying dataflow, codes, configuration files, parameter settings, and runtime dependencies

Digital Scholarship

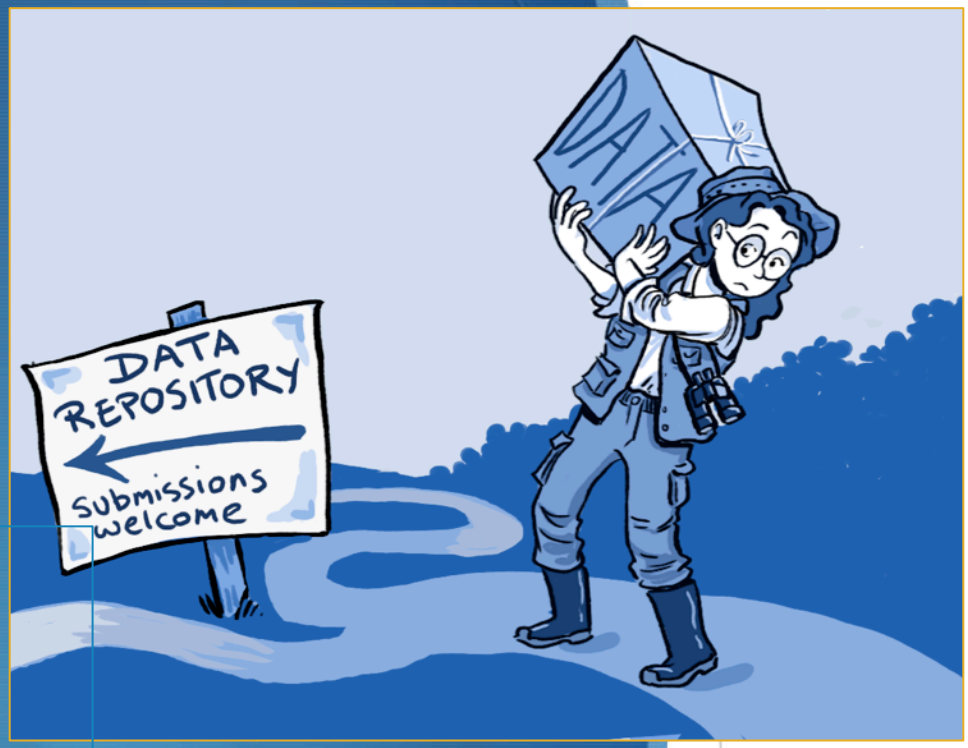
Persistent identifiers:
For data, software, and authors (and provenance/workflow)

Citations:
Citations for data and software (and provenance/workflow)

What is a Scientific Paper of the Future

- **Data**: Available in a public repository, including documentation (metadata), a clear license specifying conditions of use, and citable using a unique and persistent identifier.
- **Software**: Available in a public repository, with documentation (metadata), a license for reuse, and citable using a unique persistent identifier.
  - Not only major software used, but also other ancillary software for data reformatting, data conversions, data filtering, and data visualization.
- **Provenance**: Documented for all results by explicitly describing the series of computations and their outcome with a provenance record of the execution traces and a workflow sketch (or formal workflow)
  - Possibly in a shared repository and with a unique and persistent identifier.

Making Data Accessible



OntoSoft Training

Part 2

http://dx.doi.org/10.5281/zenodo.15920

SCIENTIFIC Onto Soft PAPER OF THE FUTURE

Onto Soft

NSF ICER-1440323 ICER-1343800

http://www.scientificpaperofthefuture.org

Problems with Current Practice

- Data is often not made available in publications
  - Limited reproducibility

Nature Genetics **41**, 149 - 155 (2009)
Published online: 28 January 2008 | doi:10.1038/ng.295

Repeatability of published microarray gene expression analyses

scientists. Here we evaluated the replication of data analyses in 18 articles on microarray-based gene expression profiling published in *Nature Genetics* in 2005–2006. One table or figure from each article was independently evaluated by two teams of analysts. We reproduced two analyses in principle and six partially or with some discrepancies; ten could not be reproduced. The main reason for failure to reproduce was data unavailability, and discrepancies were mostly due to incomplete data annotation or specification of data processing and analysis.

- Data made available through investigator's URL
  - URL does not resolve (i.e., ''rotten'')

PLOS ONE | DOI:10.1371/journal.pone.0115253 December 26, 2014

RESEARCH ARTICLE

Scholarly Context Not Found: One in Five Articles Suffers from Reference Rot

Martin Klein[1]*, Herbert Van de Sompel[1], Robert Sanderson[1], Harihar Shankar[1], Lyudmila Balakireva[1], Ke Zhou[2], Richard Tobin[2]

We analyze a vast collection of articles from three corpora that span publication years 1997 to 2012. For over one million references to web resources extracted from over 3.5 million articles, we observe that the fraction of articles containing references to web resources is growing steadily over time. We find one out of five STM articles suffering from reference rot, meaning it is impossible to revisit the web context that surrounds them some time after their publication. When only considering STM articles that contain references to web resources, this fraction increases to seven out of ten.

Better Approaches

★ Data paper

Ecological Research
July 2013, Volume 28, Issue 4, p 541

Date: 10 May 2013

Monitoring records of plant species in the Hakone region of Fuji-Hakone-Izu National Park, Japan, 2001–2010

Takeshi Osawa

Abstract

The monitoring of species occurrences is a crucial aspect of biodiversity conservation, and regional volunteerism can serve as a powerful tool in such endeavors. The Fuji-Hakone-Izu National Park in the Hakone region of Kanagawa Prefecture, Japan, boasts a volunteer association of approximately 100 members. These volunteers have monitored plant species occurrences from 2001 to the present along several hiking trails in the region. In this paper, I present the annual observation records of plant occurrences in Hakone from 2001 to 2010. This data set includes 1,071 species of plants from 151 families. Scientific names follow the Y List, and this data set includes several threatened plant species. Data files are formatted based on the Darwin Core and Darwin Core Archives, which are defined by the Biodiversity Information Standards (BIS) or Biodiversity Information Standards Taxonomic Databases Working Group (TDWG). Data files filled on required and some additional item on Darwin Core. The data set can download from the author's personal Web site as of July 2012. These data will soon be published for the Global Biodiversity Information Facility (GBIF) through GBIF Japan. All users can then access the data from the GBIF portal site.

- *The complete data set for this abstract published in the Data Paper section of the journal is available in electronic format in Ecological Research Data Paper Archives at http://db.cger.nies.go.jp/JaLTER/ER_DataPapers/archives/2013/ERDP-2013-01.*

★ Data published in a repository

The US Long Term Ecological Research Network

+/- NTL LTER *"WDNR Yahara Lakes Fisheries: Fish Lengths and Weights 1987-1998" - Lathrop*

LTER Identifier:

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Abstract:

These data were collected by the Wisconsin Department of Natural Resources (WDNR) from 1987-1998. Most of these data (1987-1993) precede 1995, the year that the University of Wisconsin Â NTL-LTER program Â took over sampling of the Yahara Lakes. However, WDNR data collected from 1997-1998 Â (unrelated to LTER sampling) is also included. In 1987 a joint project by the WDNR and the University of Wisconsin-Madison, Center for Limnology (CFL) was initiated on Lake Mendota. The project involved biomanipulation o...

Owners/Creators:

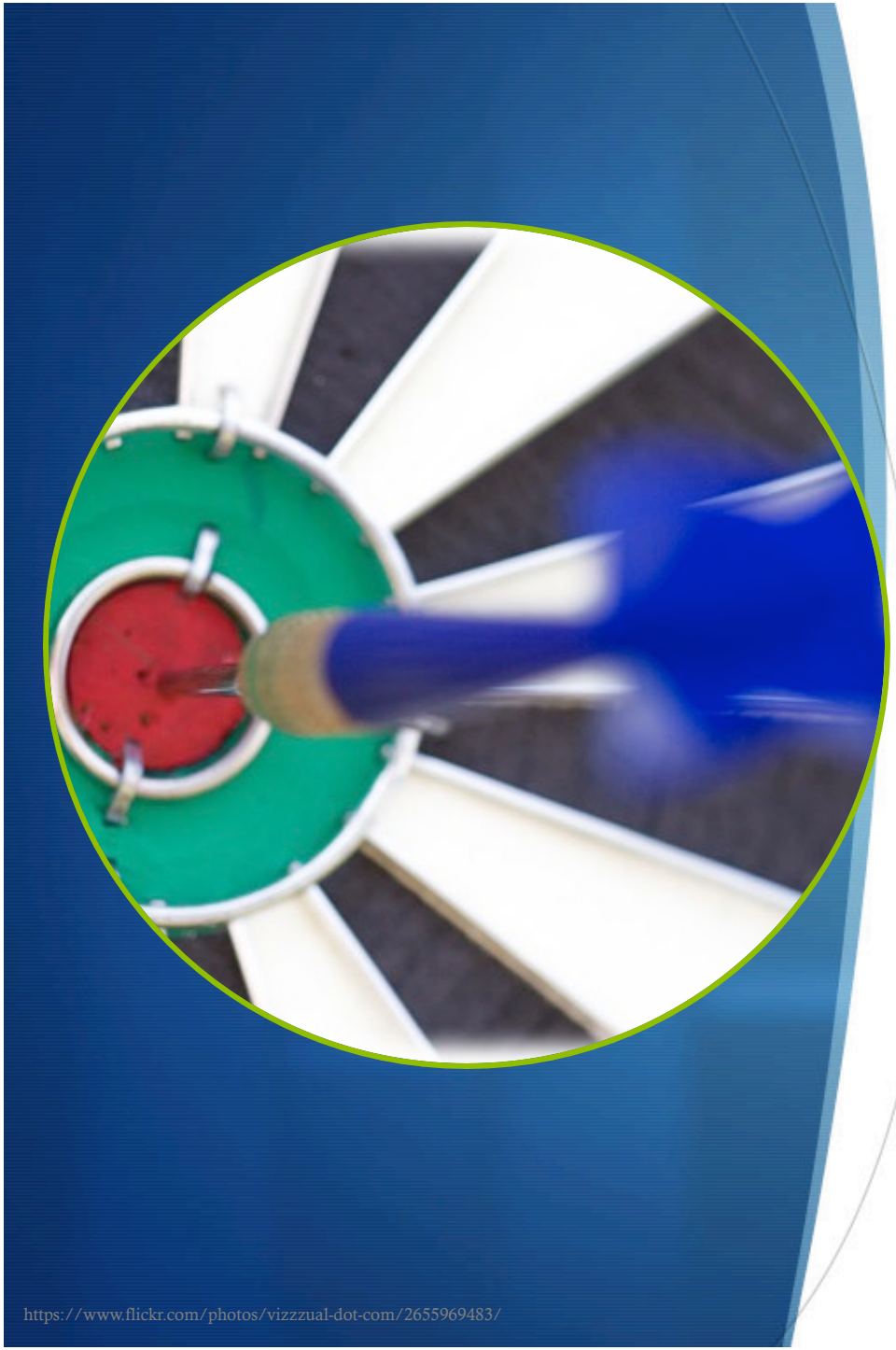
Lathrop

Metadata:

Select here for full metadata

Data File(s):

- wdnr_fyke_minifyke_seine_lengths_weights.csv
- wdnr_boomshock_lengths_weights.csv
- wdnr_gillnet_lengths_weights_93.csv
- wdnr_walleye_age_lengths_weights_87.csv
- wdnr_creel_survey_lengths_weights.csv
- wdnr_creel_survey_angler_counts.csv

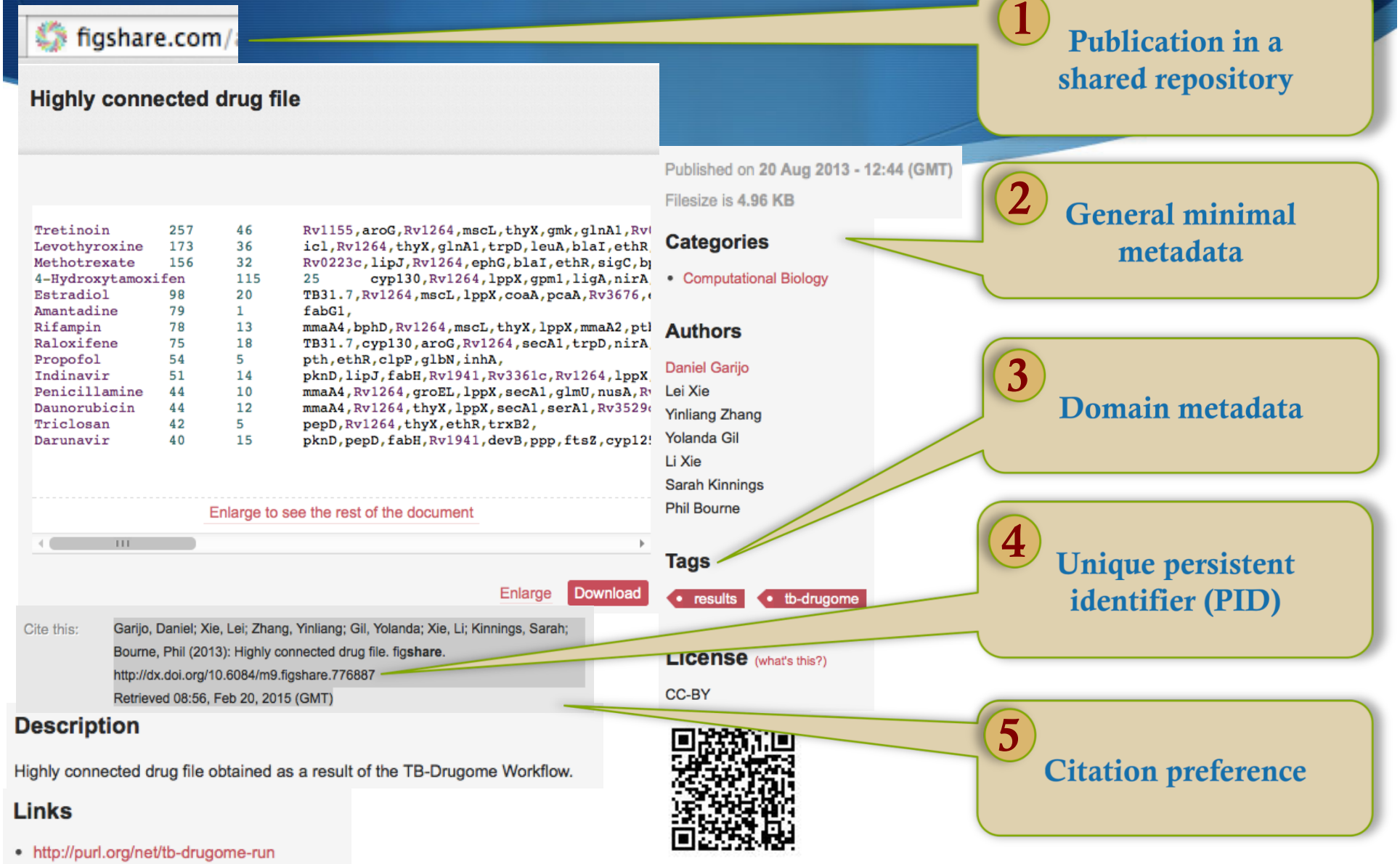


https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

1. Understand best practices
2. Understand how to implement those best practices

Making Data Accessible: Overview of Best Practices



Best Practices (1 of 5)

figshare.com/

Highly connected drug file

Tretinoin	257	46	Rv1155,aroG,Rv1264,mscL,thyX,gmk,glnA1,Rv
Levothyroxine	173	36	icl,Rv1264,thyX,glnA1,trpD,leuA,blaI,ethR
Methotrexate	156	32	Rv0223c,lipJ,Rv1264,ephG,blaI,ethR,sigC,b
4-Hydroxytamoxifen		115	25 cyp130,Rv1264,lppX,gpm1,ligA,nirA
Estradiol	98	20	TB31.7,Rv1264,mscL,lppX,coaA,pcaA,Rv3676,
Amantadine	79	1	fabG1,
Rifampin	78	13	mmaA4,bphD,Rv1264,mscL,thyX,lppX,mmaA2,ptl
Raloxifene	75	18	TB31.7,cyp130,aroG,Rv1264,secA1,trpD,nirA
Propofol	54	5	pth,ethR,clpP,glbN,inhA,
Indinavir	51	14	pknD,lipJ,fabH,Rv1941,Rv3361c,Rv1264,lppX
Penicillamine	44	10	mmaA4,Rv1264,groEL,lppX,secA1,glmU,nusA,R
Daunorubicin	44	12	mmaA4,Rv1264,thyX,lppX,secA1,serA1,Rv3529
Triclosan	42	5	pepD,Rv1264,thyX,ethR,trxB2,
Darunavir	40	15	pknD,pepD,fabH,Rv1941,devB,ppp,ftsZ,cyp12

Enlarge to see the rest of the document

Enlarge Download

Cite this: Garijo, Daniel; Xie, Lei; Zhang, Yinliang; Gil, Yolanda; Xie, Li; Kinnings, Sarah; Bourne, Phil (2013): Highly connected drug file. figshare. http://dx.doi.org/10.6084/m9.figshare.776887 Retrieved 08:56, Feb 20, 2015 (GMT)

Description

Highly connected drug file obtained as a result of the TB-Drugome Workflow.

Links

- http://purl.org/net/tb-drugome-run

Published on 20 Aug 2013 - 12:44 (GMT)

Filesize is 4.96 KB

Categories

- Computational Biology

Authors

Daniel Garijo
Lei Xie
Yinliang Zhang
Yolanda Gil
Li Xie
Sarah Kinnings
Phil Bourn

Tags

- results
- tb-drugome

License (what's this?)

CC-BY

1. Publication in a shared repository
2. General minimal metadata
3. Domain metadata
4. Unique persistent identifier (PID)
5. Citation preference

Popular Data Repositories

Not Curated

Curated

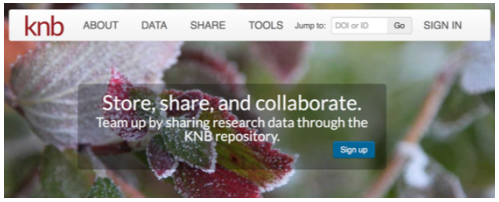
zenodo

figshare

zenodo

DRYAD

The Dataverse Project



PANGAEA®

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http://www.arqhys.com/articulos/ingeniero-inspector.html

Directories of Research Data Repositories

- http://www.re3data.org
- http://databib.org/index_subjects.php
- http://oad.simmons.edu/oadwiki/Data_repositories
- http://www.force11.org
- http://www.nature.com/sdata/data-policies/repositories

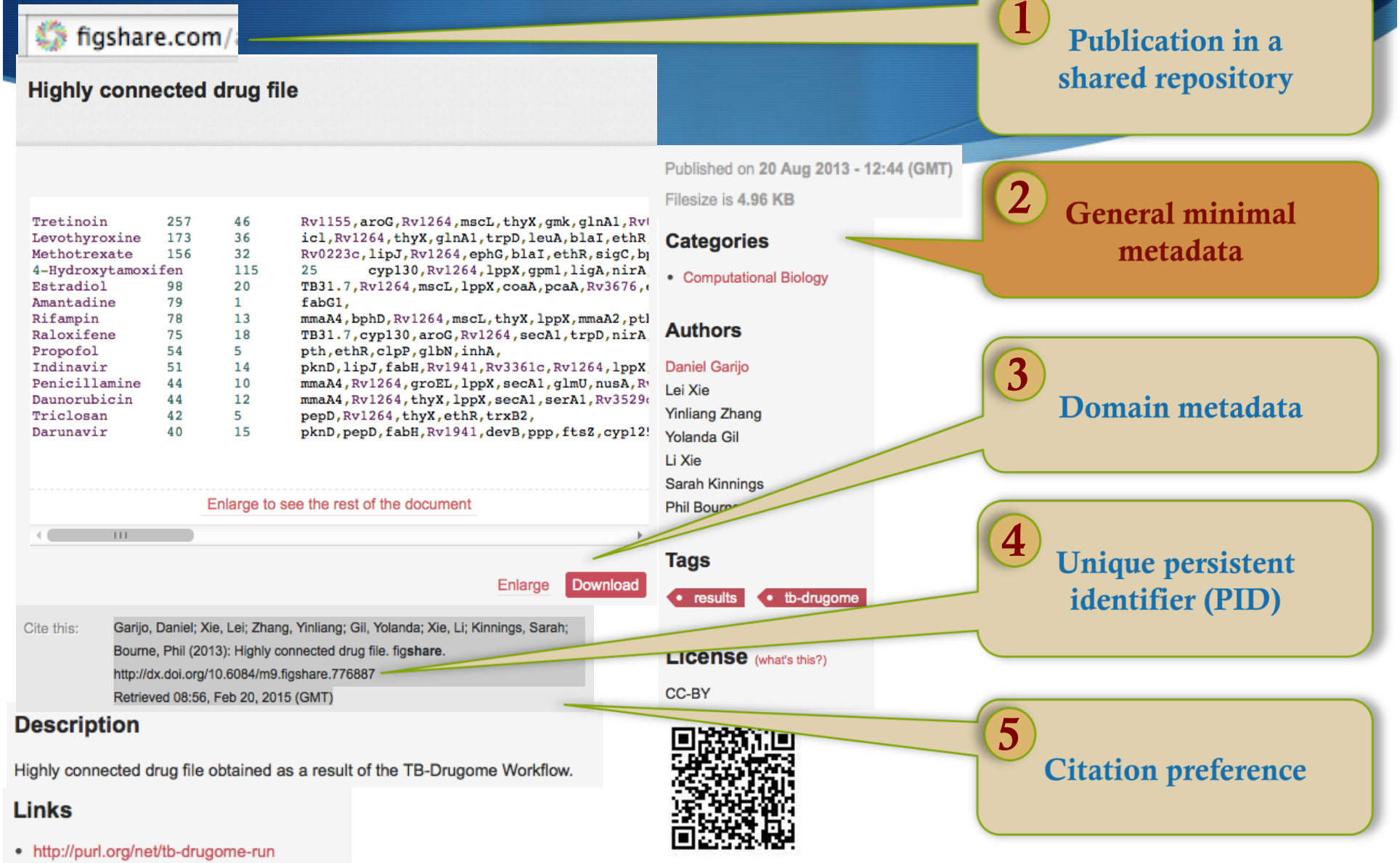
http://www.thestaffingstream.com/2012/08/06/the-buzz-about-talent-communities/

International Geo Sample Number: IGSN

- ★ Globally unique and persistent identifier for physical samples in the Earth Sciences
- ★ Obtain IGSNs for your samples
  - ★ Best upon collection or as soon as you are back online!
- ★ Go to http://www.geosamples.org/ or contact info@geosamples.org
- ★ Record and register quality metadata for your samples
  - ★ At a minimum: Location, Lithology, Contact, access restrictions
- ★ Use IGSNs in your publications: text, data tables,…

Credit: Kerstin Lehnert, LDEO, Columbia U.

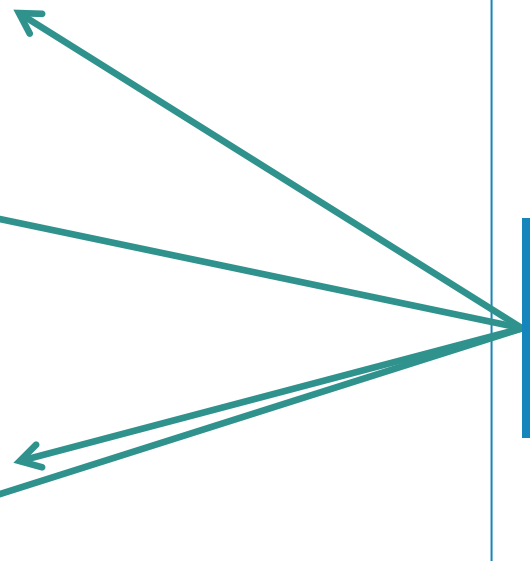
Best Practices (2 of 5)



Minimal Metadata

General

- ★ Dataset name/title
- ★ Description
- ★ Creator(s)
- ★ Publication date
- ★ License
- ★ Publisher/contact
- ★ Version
- ★ Resource type
- ★ Location of the data



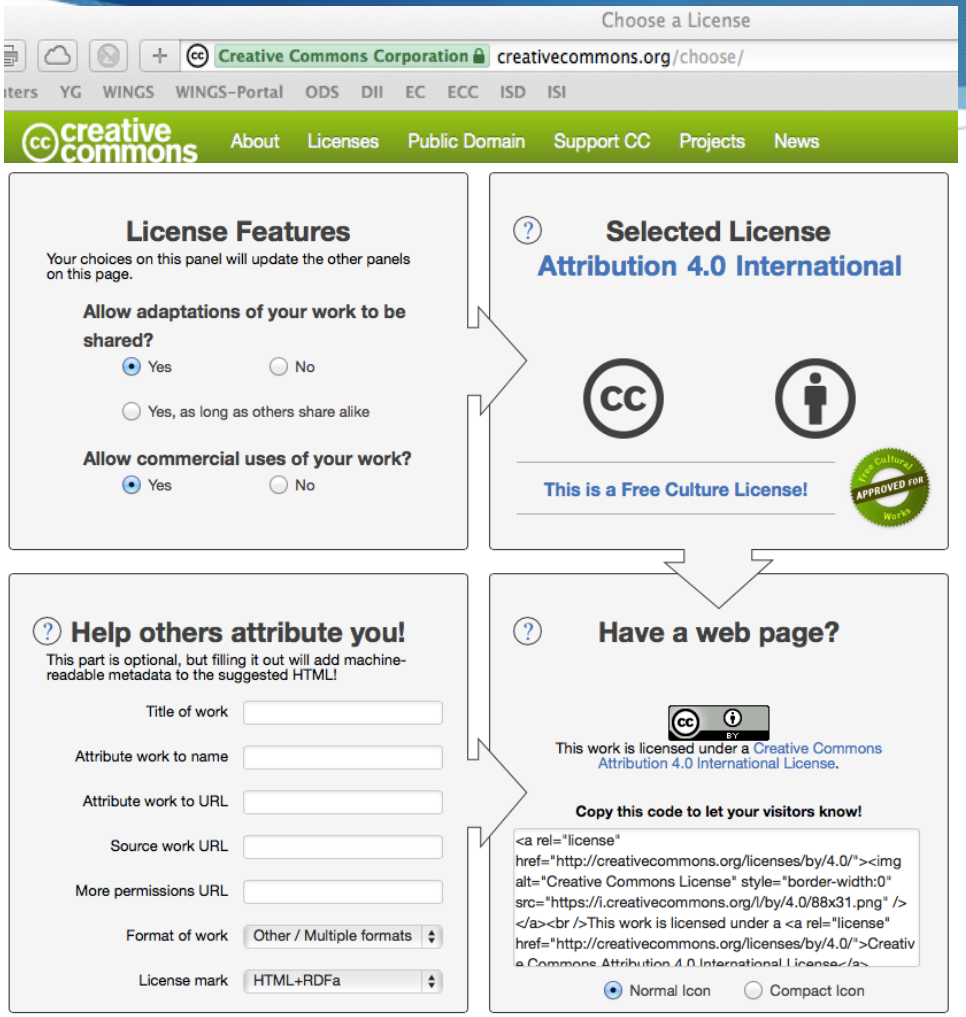
Typical of digital libraries,
eg the Dublin Core standard
(http://dublincore.org/documents/dcmi-terms/)

Minimal Metadata

General

- ★ Dataset name/title
- ★ Description
- ★ Creator(s)
- ★ Publication date
- ★ License
- ★ Publisher/contact
- ★ Version
- ★ Resource type
- ★ Location of the data

Choose a License



Recommended: CC-BY and CC0

Attribution
CC BY

This license lets others distribute, remix, tweak, and build upon your work, even commercially, as long as they credit you for the original creation. This is the most accommodating of licenses offered. Recommended for maximum dissemination and use of licensed materials.

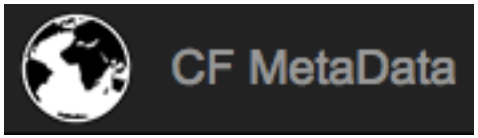
CC0 (datasets) "No rights reserved"

CC0 can be particularly important for the sharing of data and databases, since it otherwise may be unclear whether highly factual data and databases are restricted by copyright or other rights. Databases may contain facts that, in and of themselves, are not protected by copyright law.

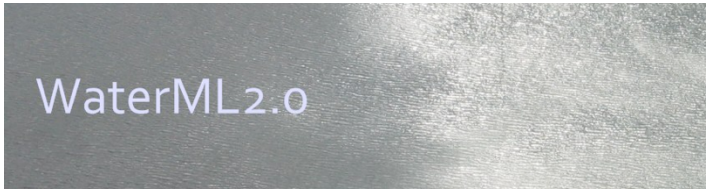
CC0 is recommended for data and databases and is used by hundreds of organizations. It is especially recommended for scientific data. Although CC0 doesn't legally require users of the data to cite the source, it does not take away the moral responsibility to give attribution, as is common in scientific research.

http://creativecommons.org/licenses/

Domain-Specific Metadata Standards

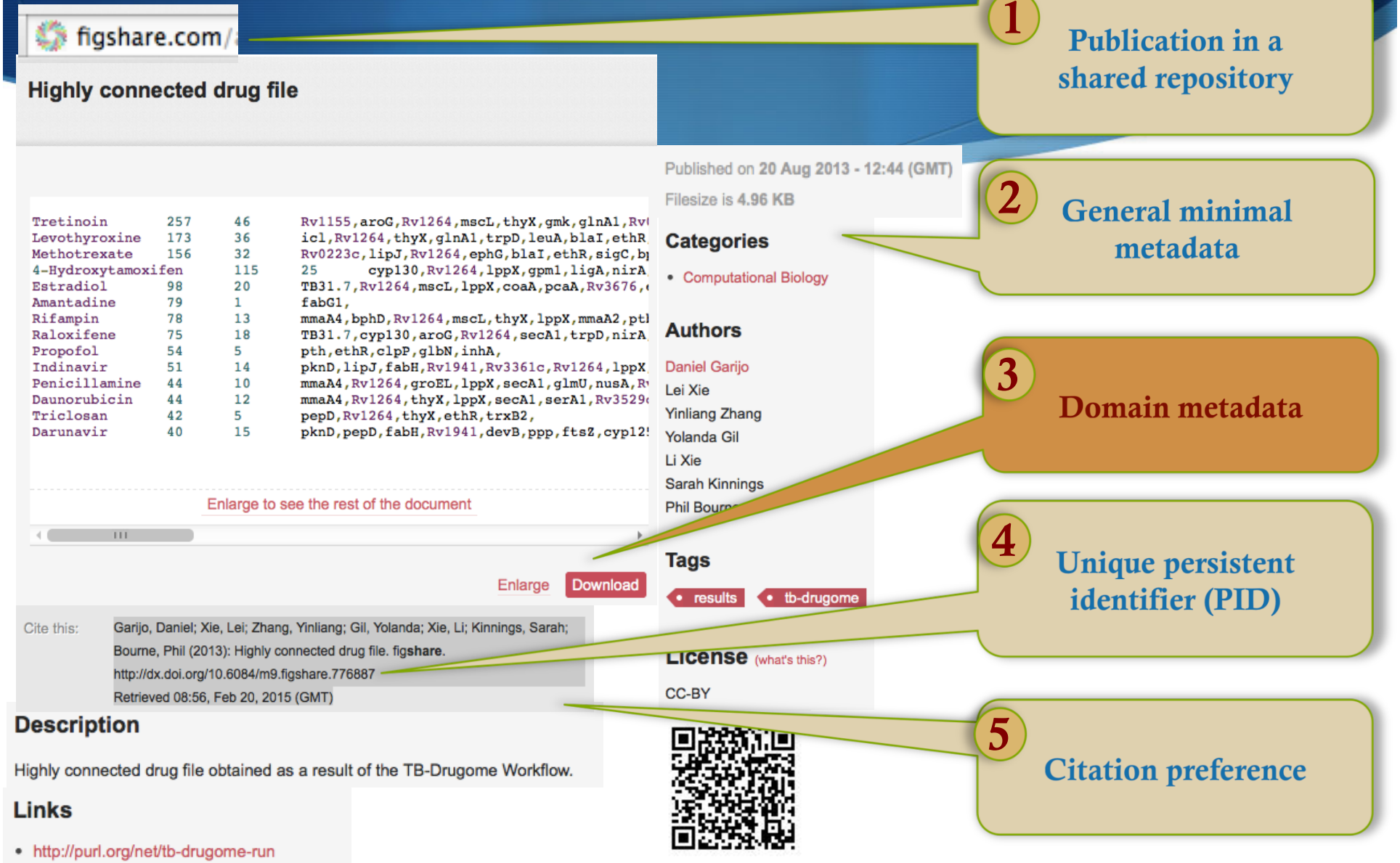


ISO 19115



- A data repository in a given discipline may request metadata using accepted standards

Best Practices (3 of 5)



Domain-Specific Metadata

General

- Dataset name/title
- Description
- Creator(s)
- Publication date
- License
- Publisher/contact
- Version
- Resource type
- Location of the data

Domain Specific

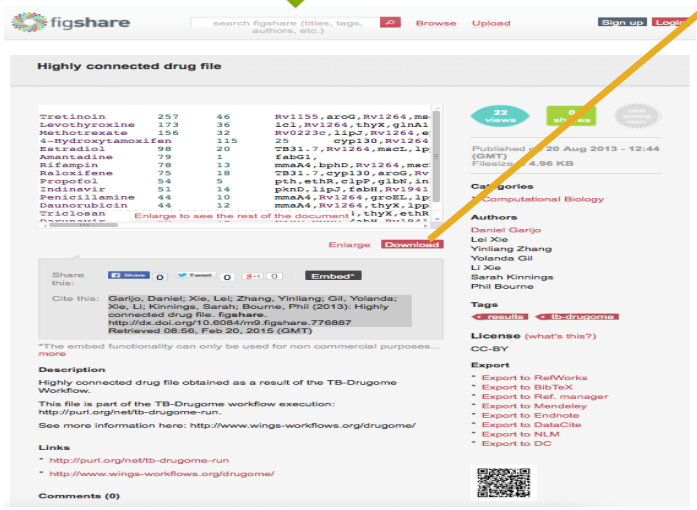
- Collection information
- Pre-processing
- Dataset characteristics

Domain data repositories use metadata standards for that domain and guide you to provide the information needed

Manual Accessibility

SEARCHING AND BROWSING METADATA

- http://figshare.com/articles/Highly_connected_drug_file/776887



DATA

- http://files.figshare.com/1175525/highlConnectedDrugs.txt

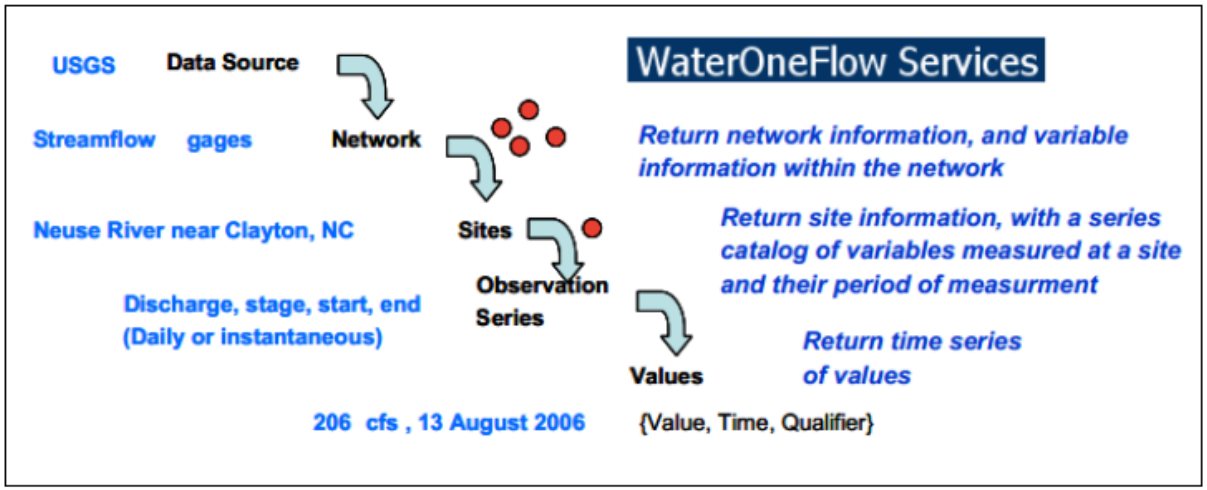
```
Tretinoin          257     46      Rv1155,aroG,Rv1264,mscL,thyX,gmk,glnA1,Rv
Levothyroxine      173     36      icl,Rv1264,thyX,glnA1,trpD,leuA,blaI,ethR
Methotrexate       156     32      Rv0223c,lipJ,Rv1264,ephG,blaI,ethR,sigC,b
4-Hydroxytamoxifen         115     25      cyp130,Rv1264,lppX,gpm1,ligA,nirA
Estradiol          98      20      TB31.7,Rv1264,mscL,lppX,coaA,pcaA,Rv3676,
Amantadine         79      1       fabG1,
Rifampin           78      13      mmaA4,bphD,Rv1264,mscL,thyX,lppX,mmaA2,pt
Raloxifene         75      18      TB31.7,cyp130,aroG,Rv1264,secA1,trpD,nirA
Propofol           54      5       pth,ethR,clpP,glbN,inhA,
Indinavir          51      14      pknD,lipJ,fabH,Rv1941,Rv3361c,Rv1264,lppX
Penicillamine      44      10      mmaA4,Rv1264,groEL,lppX,secA1,glmU,nusA,R
Daunorubicin       44      12      mmaA4,Rv1264,thyX,lppX,secA1,serA1,Rv3529
Triclosan          42      5       pepD,Rv1264,thyX,ethR,trxB2,
Darunavir          40      15      pknD,pepD,fabH,Rv1941,devB,ppp,ftsZ,cyp12
```

Machine Accessibility: Metadata is a Necessity!

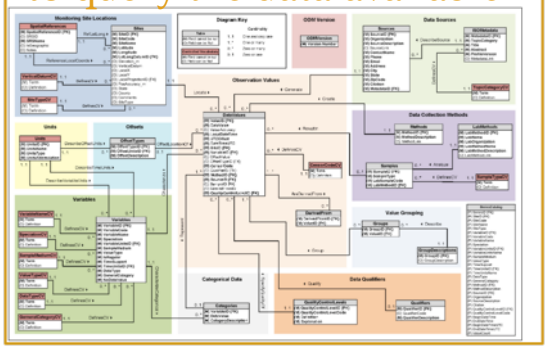
CUAHSI
UNIVERSITIES ALLIED FOR WATER RESEARCH

WaterOneFlow Web Services

Web services are computer applications that interact with and exchange information with other applications over the internet. The CUAHSI HIS uses a family of web services, called WaterOneFlow (WOF), that have been developed as a standard mechanism for the transfer of hydrologic data between hydrologic data servers (databases) and users' computers. Web services streamline the often time consuming tasks of extracting data from a data source, transforming it into a usable format, and loading it in to an analysis environment. The WaterOneFlow Web Services format the data as the type of XML described above, WaterML 1.1.

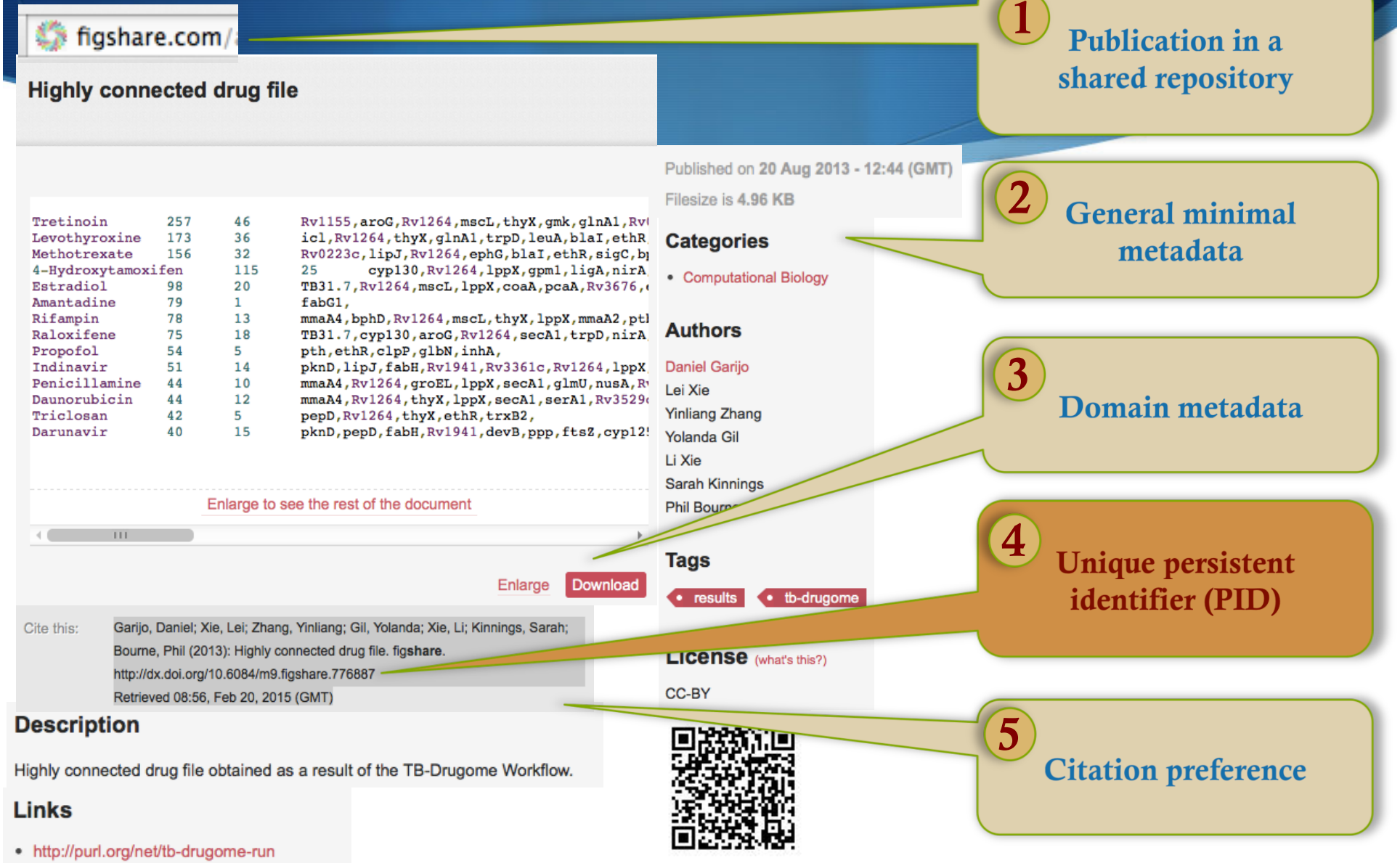


Data model specifies how to query the data available



https://www.cuahsi.org/Standards

Best Practices (4 of 5)



Main Types of Unique Identifiers

1. Uniform Resource Locator (URL)
2. Persistent URL (PURL)
3. Digital Object Identifier

"Internet1" by Rock1997 - Own work. Licensed under GFDL via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Internet1.jpg#mediaviewer/File:Internet1.jpg

URL/URI

- Minimal effort to create
- No guarantee of persistence
  - i.e., almost guaranteed it will not have persistence
  - e.g., http://www.greatuniversity.edu/gradstudents/joesmith/awesomedata/

Do not use in papers!!

Persistent URL (PURL)

- The same PURL can be resolved to different Web address over time
  - Go to https://w3id.org (run by W3C), or other PURL services
    - Create a PURL, and direct it to where you actually have the data today eg: http://www.wisc.edu/myadvisorsgroup/awesomedata.html
  - Always refer to your data with the same PURL: http://w3id.org/mydataandme/awesomedata.html
    - Tomorrow you have graduated and tell w3id.org to resolve your PURL to: http://www.stanford.edu/myowngroup/awesomedata.html
- It is easy to create your own PURLs, just remember to update whenever you move the data

Digital Object Identifier (DOI)

PLoS Biol. 2003 Nov; 1(2): e57.
Published online 2003 Nov 17. doi: 10.1371/journal.pbio.0000057

DOIs can only be issued by a DOI authority (eg a journal publisher) that guarantees to always resolve it

The What and Whys of DOIs

Susanne DeRisi, Rebecca Kennison, and Nick Twyman

Data repositories can issue DOIs for data

DOIs are **free**

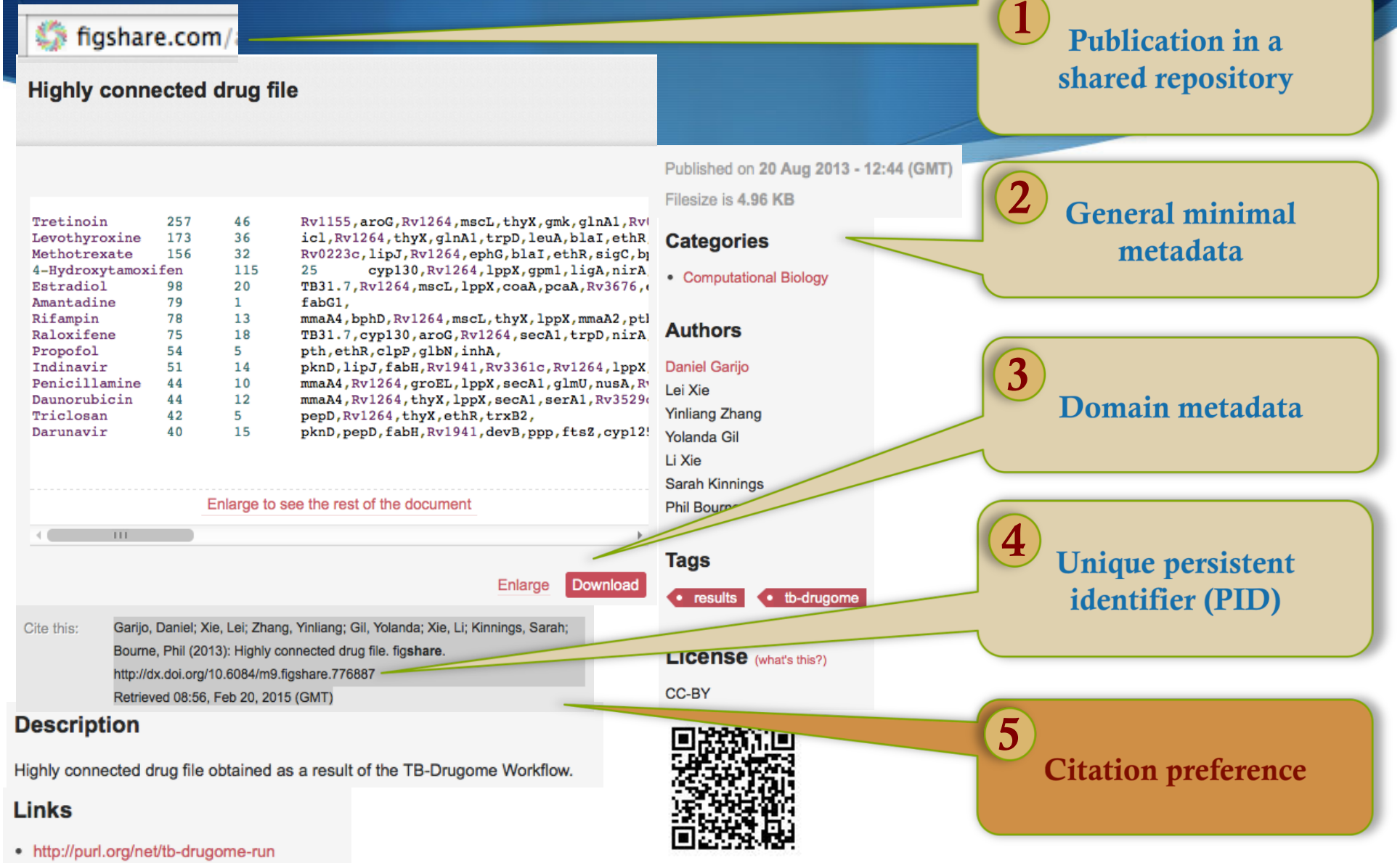
As you may have noticed in the first issue of *PLoS Biology* and again in this issue, there are many places where an alphanumeric string appears after the letters "DOI," such as 10.1371/journal.pbio.0000005 or 10.1371/journal.pbio.0000005.g005. Although some of you may already be acquainted with DOIs, others of you may wonder what they are, how they are used, and why we are using them.

What Are DOIs?

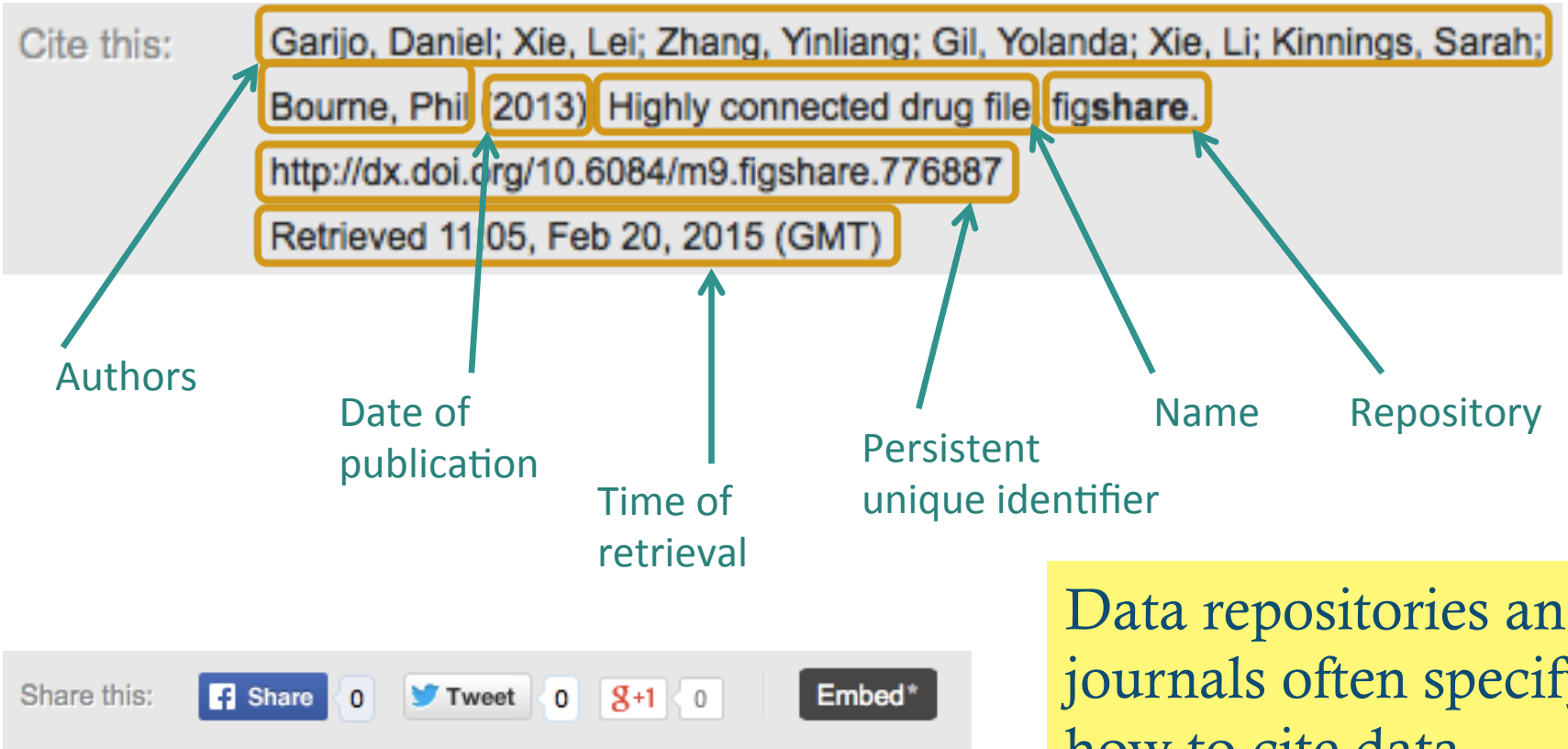
Go to:

A Digital Object Identifier (DOI) is an URN (Uniform Resource Name), a compact string that provides a unique, persistent, and actionable identifier for the digital object with which it is associated. DOIs are commonly assigned to scientific articles in their electronic form, but DOIs may also be used as identifiers for any object in any location, although this usage is not yet common outside the online world. The International DOI Foundation (IDF), which governs the DOI system, has several hundred registrant organizations and in August 2003 reported that over 10 million DOIs have been issued since the foundation was created in 1998 (http://www.doi.org/news/03augnews.html).

Best Practices (5 of 5)

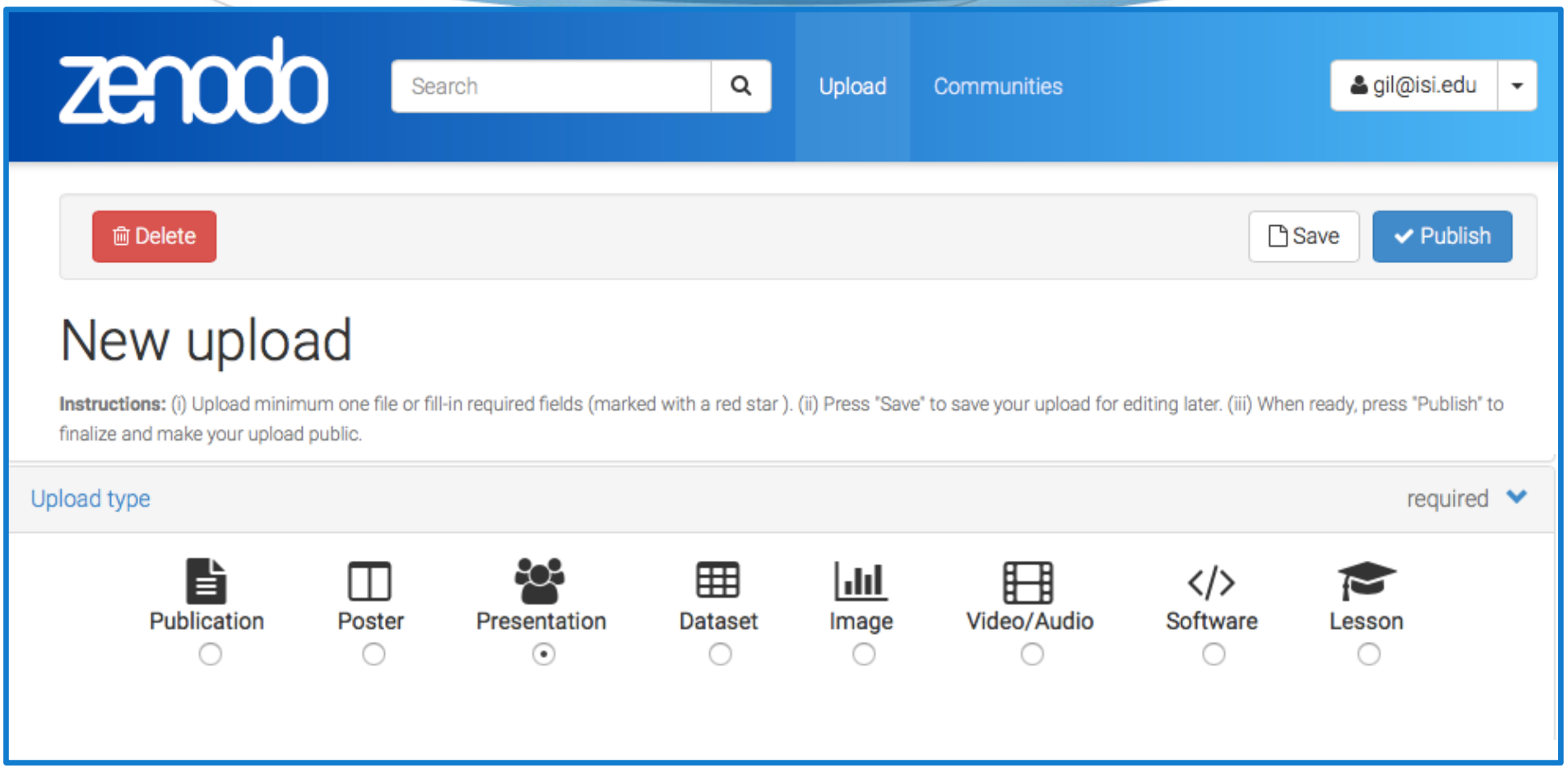


Data Citation Format



Data repositories and journals often specify how to cite data

Versatility of Data Repositories



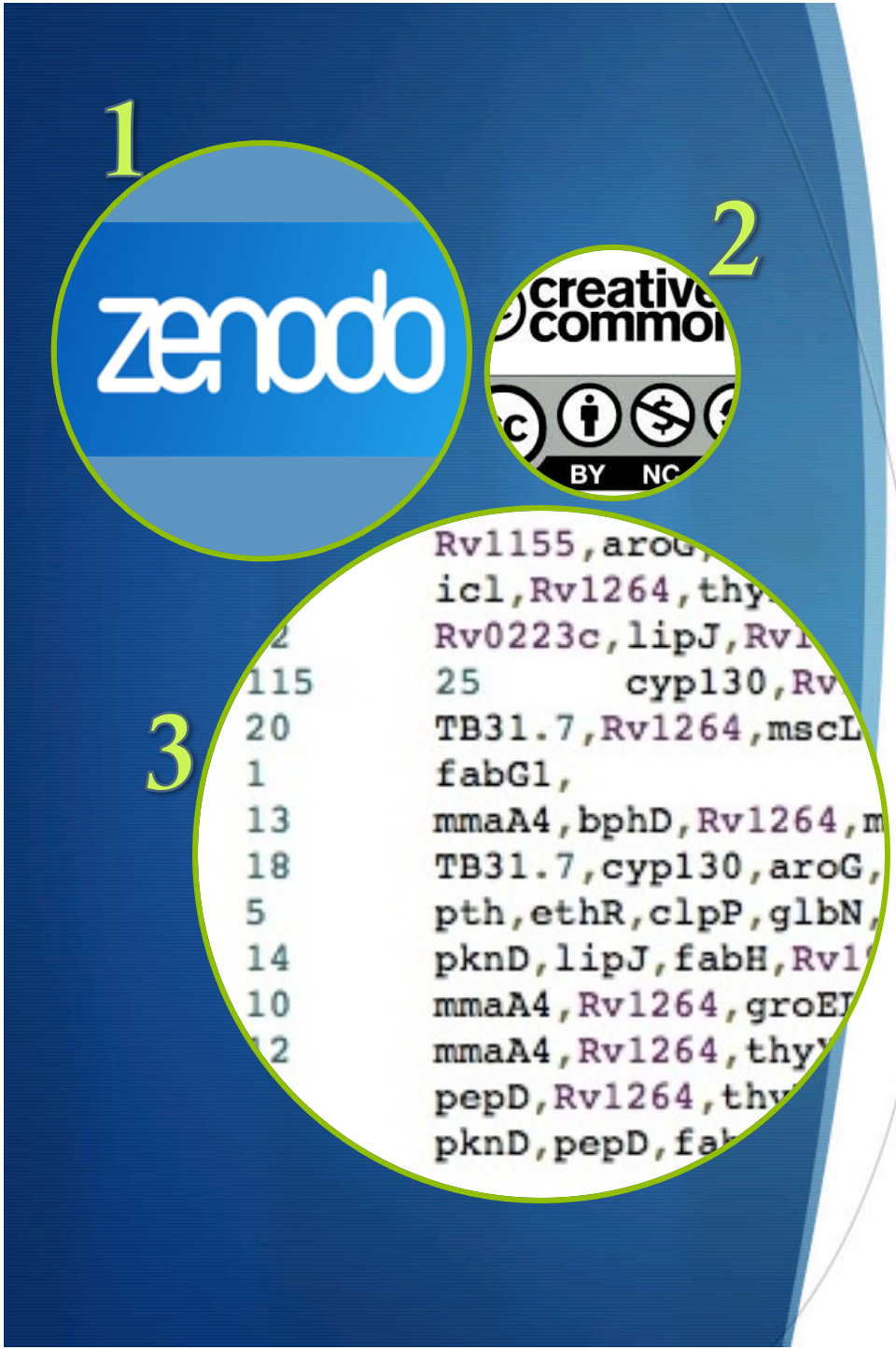
What if…

- **… there are several datasets in several files?**
  - Create a DOI for each file and a DOI for the whole set
- **… the data is from a public repository?**
  - Publish the query, create a DOI + metadata for it, mention the original source in the metadata, point to the original data source
- **… the data is from a colleague?**
  - Get permission in advance and make an agreement, then do as with the data from a public repository
- **… the data comes from many sources?**
  - Credit each source, create URIs as needed
  - Can create a table with "microattributions" that summarize each data source
- **… the data comes from a database?**
  - Create a file (or files) from it
- **… the data has many versions?**
  - Create a DOI either for each slice or for each snapshot

https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

1. Understand what those best practices mean
2. Understand how to implement those best practices



Making Data Accessible:
Simplest Approach

1. **Create a public entry for your dataset with a persistent unique identifier**
   - Go to a domain repository (use a general repository, e.g.., zenodo.org, if you cannot find one), create an account
   - Create an entry for your dataset
2. **Specify the metadata**
   - Including license -- choose from http://www.creativecommons.org/licenses
3. **Upload/point to the data**

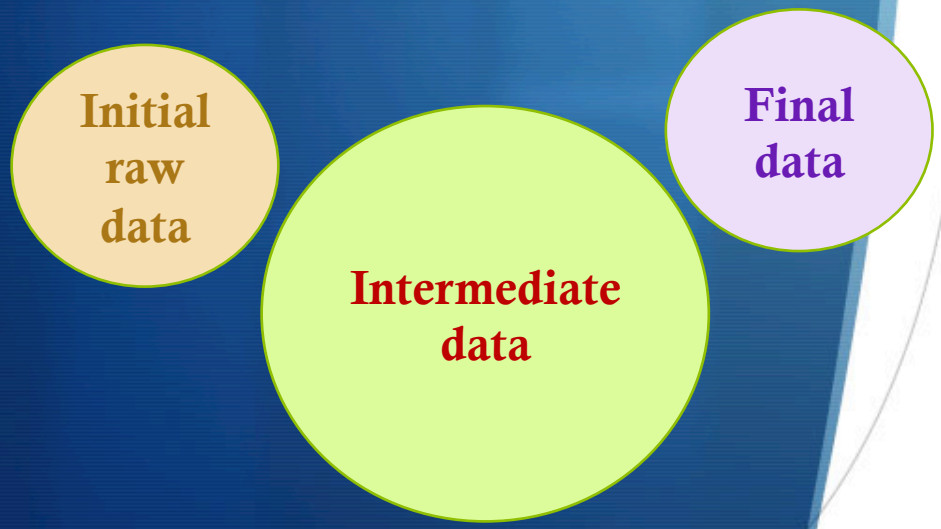
Voilà! The repository will give you a data citation

Making Data Accessible: Ideal Approach

1. Find a repository that your community uses, if there is not one then organize one!
2. **Create a public entry for your dataset with a persistent unique identifier**
   - Create an entry for your dataset
3. **Specify the metadata**
   - Including license -- choose from http://www.creativecommons.org/licenses
4. **Upload/point to the data**
5. **Get a data citation from the repository**

Making Data Accessible:

Cite the data in your paper



- **Citation goes in the References section**
- **How to cite the data? You choose:**
  - With an in-text pointer as you would cite any other paper (recommended)
  - With an in-text pointer in a special "Data Resources" section
  - With an in-text pointer in the "Acknowledgments" section

Making Software Accessible

OntoSoft Training

Part 3

http://dx.doi.org/10.5281/zenodo.15920

NSF ICER-1440323
ICER-1343800

http://www.scientificpaperofthefuture.org

http://www.flickr.com/photos/gemmerich/6365692623/in/photostream/

The Value of Software

Availability of Software

PLOS | ONE

PLOS supports the development of open source software and believes that, for submissions
appropriate open source standards will ensure that the submission conforms to (1) our requi
another researcher can reproduce the experiments described, (2) our aim to promote openn
PLOS journals can be built upon by future researchers. Therefore, if new software or a new a
that the software conforms to the Open Source Definition, have deposited the following three
submission as Supporting Information:

- **The associated source code of the software described by the paper.** This should be licensed under a suitable license such as BSD, LGPL, or MIT (see http://www.ope commercial software such as Mathematica and MATLAB does not preclude a paper f preferred.
- **Documentation for running and installing the software.** For end-user applications prerequisite; for software libraries, instructions for using the application program inter
- **A test dataset with associated control parameter settings.** Where feasible, result test data should not have any dependencies — for example, a database dump.

Acceptable archives should provide a public repository of the described software. The code s for creating user accounts, logging in or otherwise registering personal details. The repositor more than 1,000 projects. Examples of such archives are: SourceForge, Bioinformatics.Org, Savannah, GitHub and the Codehaus. Authors should provide a direct link to the deposited s

Software Papers and Software Repositories

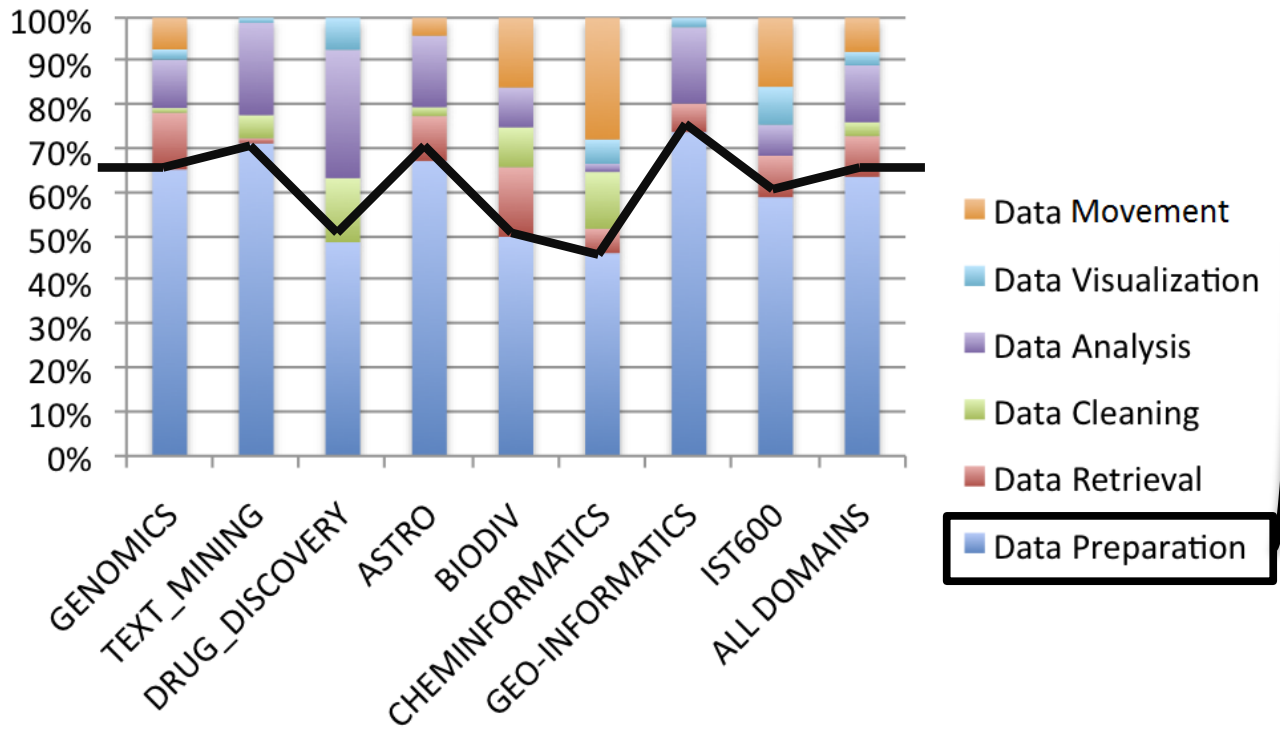
- ★ Some journal articles describe a piece of software
- ★ Some publications have "software papers" or "software metapapers"

Why Is Scientific Software Not Shared?

- "No one would use my code if I shared it"
- "My code is really bad"
- "My code is not ready to be shared"
- "Sharing my software will take a lot of time"
- "I won't get anything out of sharing my software"
- "I've shared software before, bad things happened"
- "I work for the government"
- "I want to commercialize my software"
- "I don't want anyone to commercialize my software"
- "I don't know where to start!"

Data Preparation Software Dominates but is Least Shared

- "Scientists and engineers spend more than 60% of their time just preparing the data for model input or data-model comparison" (NASA A40)

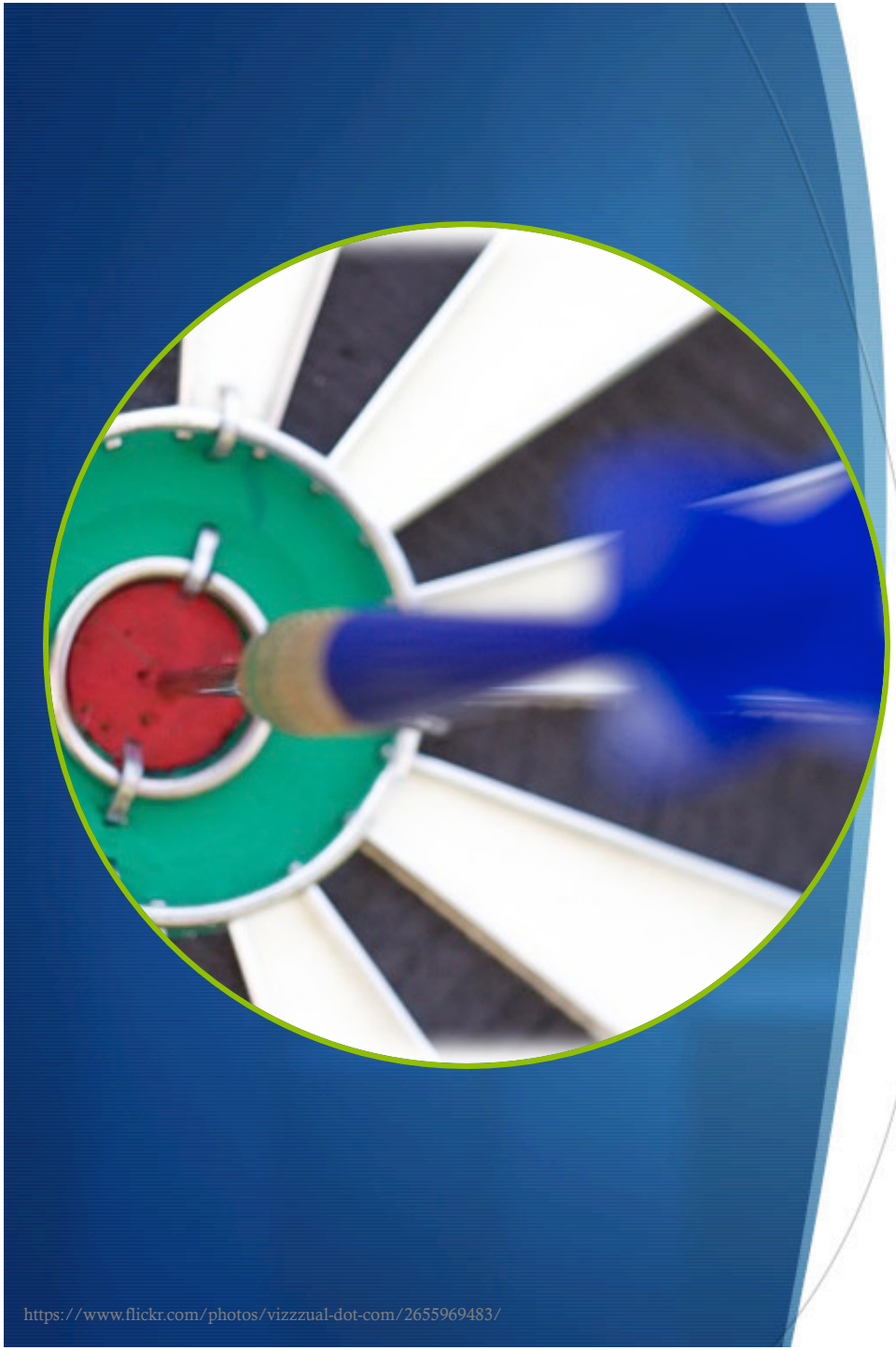


"Common Motifs in Scientific Workflows: An Empirical Analysis." Garijo, D.; Alper, P.; Belhajjame, K.; Corcho, O.; Gil, Y.; and Goble, C. Future Generation Computer Systems, 2013.

“Dark Software”

- Models that are not published
  - Eg from a PhD thesis
- Data preparation software
- Visualization software

“Dark Software” is the counterpart of “Dark Data” [Heidorn 2008]



https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

1. Making software ready for publication
2. Understand best practices in software publication
3. Understand how to implement those best practices

Some Notes on Making Software Ready for Publication

① Source code vs executable

② Making software run elsewhere

③ Making software modular

④ Making software configurable

⑤ Making software report errors

⑥ Providing test data

⑦ Code analysis

1 Publishing Source Code vs Executable

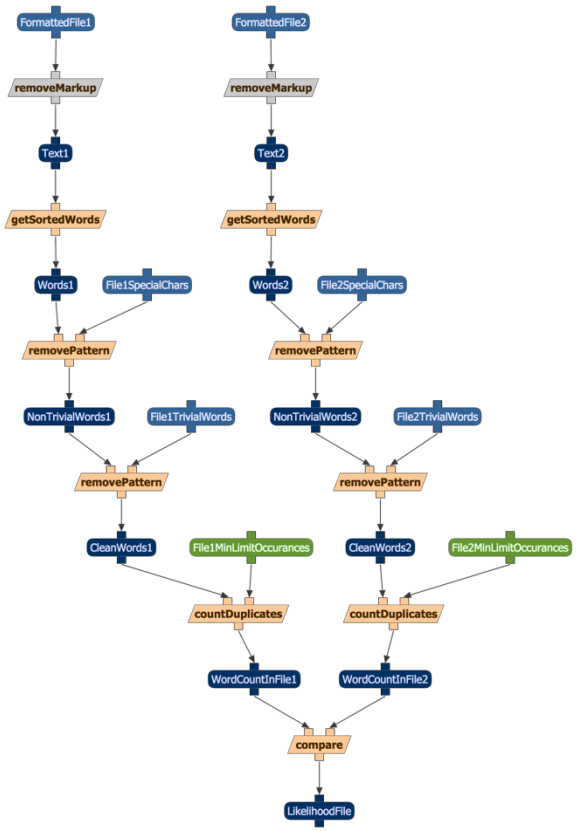
- **Source code**
  - Improve transparency
  - Opportunity for others to extend the code
  - Software repositories (e.g., GitHub, BitBucket) provide:
    - Version control
    - Community contributions: bugs, extensions, documentation…
- **Executable**
  - **Harder to maintain** as you have to build for various systems
  - **Faster** for people to use
- **Important: document run-time dependencies**
  - libraries and other third-party software required both for building the software from source and for running the software

2 Making Software Run Elsewhere

- **Portability:** If your software runs on machine A, will it run on machine B too?
  - List **required dependencies** (software and libraries that are needed to be installed on a machine to get your software to run)
  - **No Hard-Coded** machine specific details in the source code
    - Machine specific details such as file location, server name, etc.. should either go in a configuration file, or be provided as a parameter to the software

3 Making Software Modular

- Split code into multiple parts, where each part can be invoked separately if so desired
  - Provides finer grained functionality that someone might want to re-use




```
All Constraints:
 File2TrivialWords  rdf:type  dcdom:CommonTermsFile
 FormattedFile1  wflow:hasDifferentDataFrom  FormattedFile2
 File1TrivialWords  rdf:type  dcdom:CommonTermsFile
 File1SpecialChars  rdf:type  dcdom:SpecialCharsFile
 File2SpecialChars  rdf:type  dcdom:SpecialCharsFile
```

4 Making Software Configurable

- Expose important parameters in the software in the form of configuration files or parameter values
  - Helps to make your software more useful to people working in slightly different areas but with similar problem scenarios

5 Making Software Report Errors

- Instead of having the code fail silently if something goes wrong:
  - Show an expressive error for users.
  - Return a failure exit code for catching failures from software

6 Providing Test Data

- Provide test input data, and test results, and instructions on how to run the tests
- Share real input data if possible, and explain data formats
- Provide information about how to create (or where to get) new input data, and what to do with the result data

7

Code Analysis

- Automated tools are available for many languages
  - Code profilers
  - Code analyzers
- "Code review" sessions among colleagues to critique each other's code

Best Practices

1. Accessible from a public location
2. License
3. Citation

Making Software Accessible from a Public Location

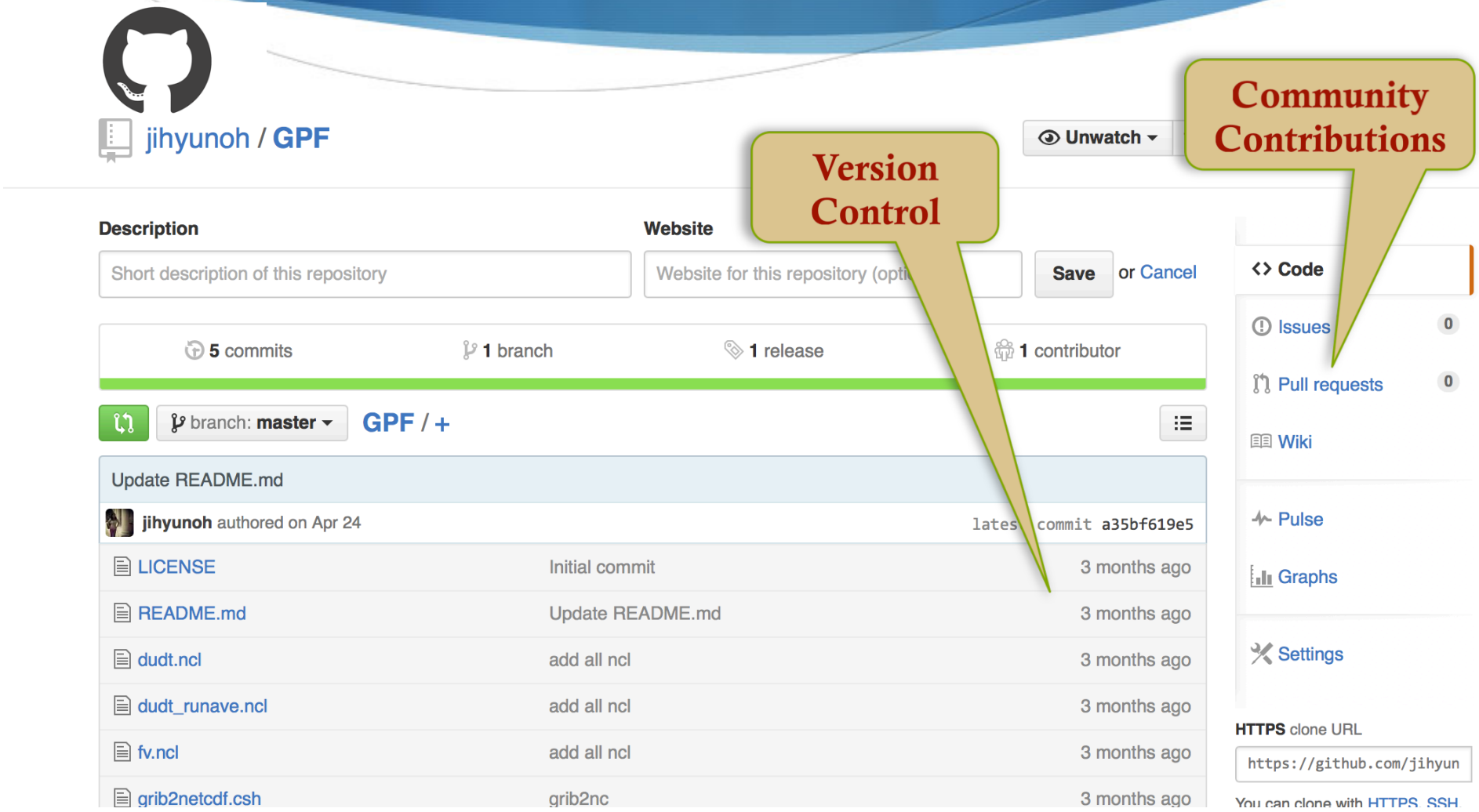
PURL

zenodo

Options:

- **Publish in your web site**
  - Very easy and simple
  - Get a PURL for the version you use in the paper
- **Use a data repository** (eg zenodo), treating code like data
  - Very easy and simple
  - It allows you to get a DOI
- **Use a code repository** (eg GitHub, BitBucket)
  - Beneficial if you have other users or want to track new versions
  - Some will give you a DOI (eg GitHub)
- **Create a formal community project** (eg in Apache)
  - Very involved, but very beneficial if you have many users

Publishing Software in a Code Repository



Publishing Software through a Software Foundation

- Oversight of software projects
- Characterized by a collaborative, consensus-based development process and an open and pragmatic software license.

- Apache Software Foundation:
  - https://www.apache.org/foundation/how-it-works.html#structure

Choosing an Open Source License

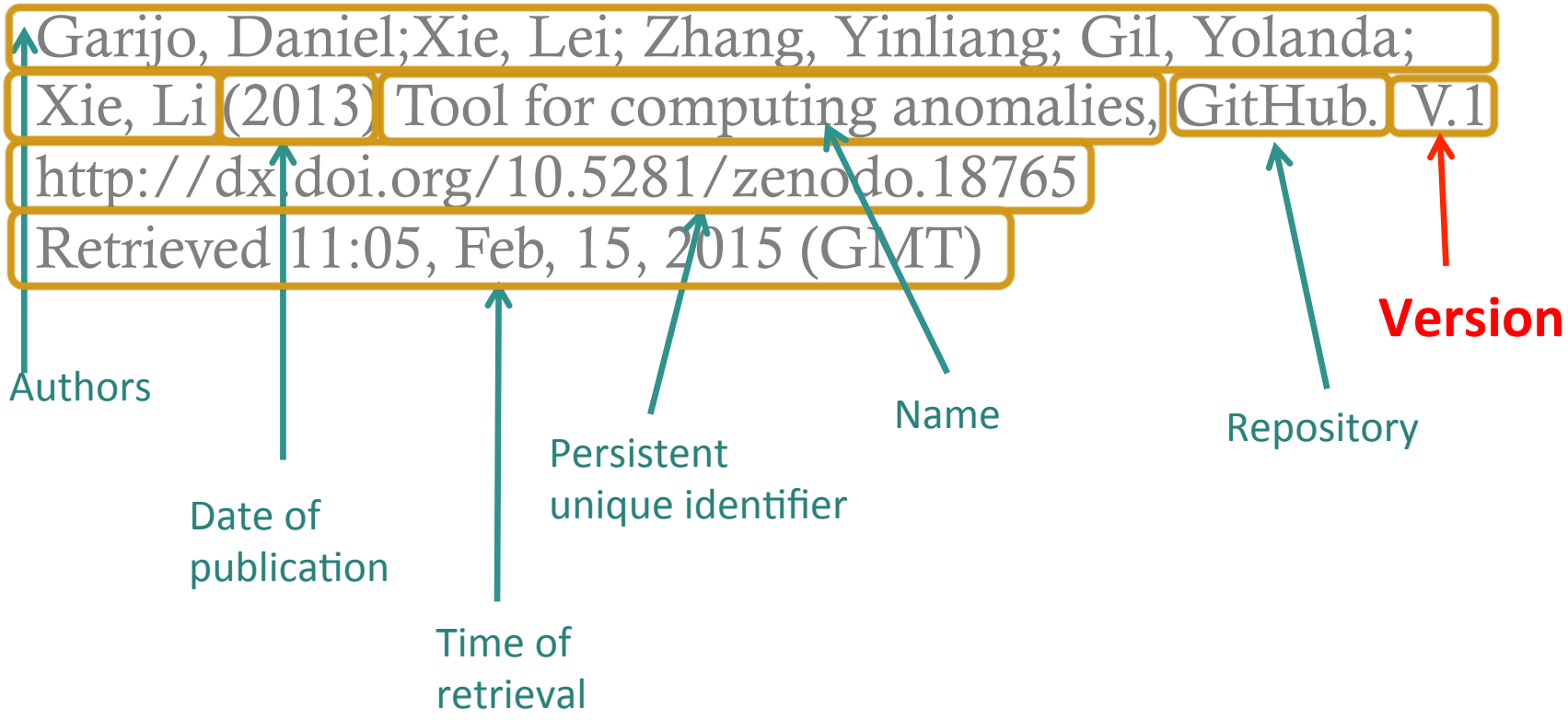
- Copyright: automatically applied to software when it is created to grant *the creator* exclusive rights as an intellectual property
- **Open source license**: reduce constraints and enable software developers to make their source code available to public
  1. "Copyleft" license (ex: GNU General Public License (GPL))
  2. "Permissive" license (ex: Apache 2 or MIT licenses)
- **Open Source Initiative**
  - Choose a license from: http://opensource.org/licenses
  - Recommend that you choose a permissive license
    - Apache v2

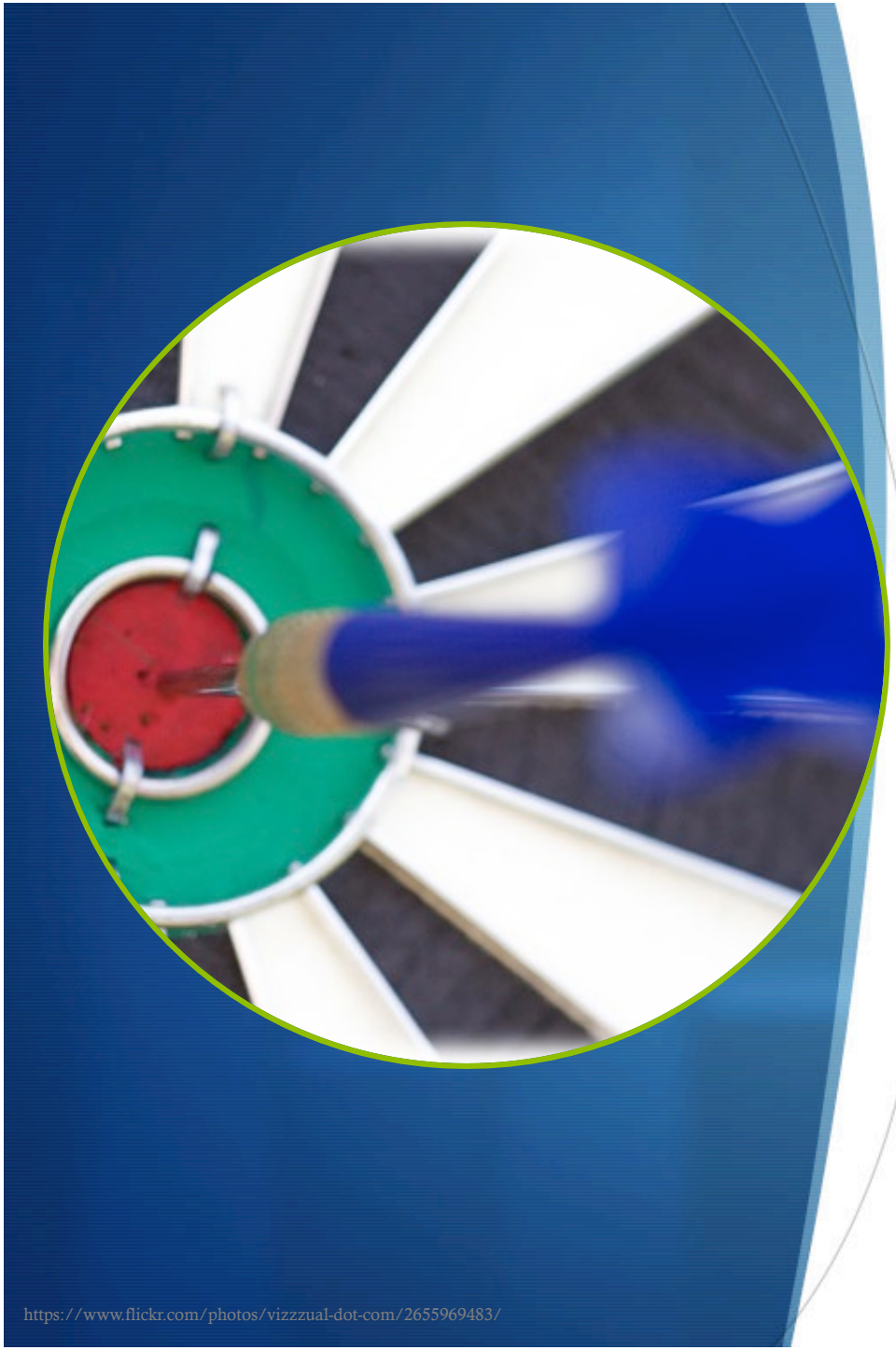
Software Citation

- Use a persistent unique identifier (PURL or DOI)
  - Analogous to identifiers for data
- Software sharing repositories are beginning to offer the ability to assign DOIs

Software Citation Format

★ Similar to data citation format, but includes software version





https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

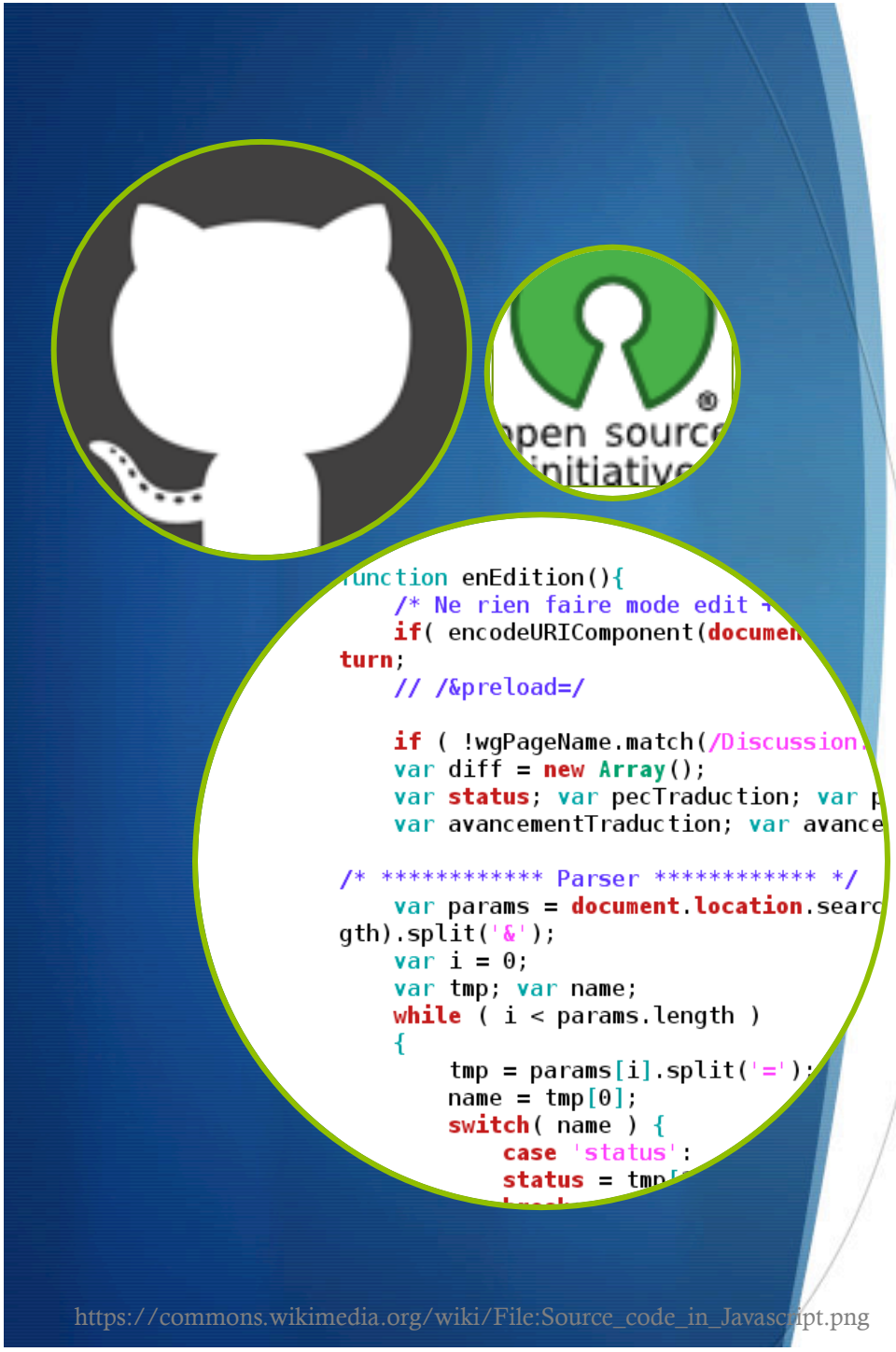
1. Making software ready for publication
2. Understand best practices in software publication
3. Understand how to implement those best practices

https://commons.wikimedia.org/wiki/File:Source_code_in_Javascript.png

Making Software Accessible:

Simplest Approach

1. Create a public entry for your software with a persistent unique identifier
   - Upload to a data repository (e.g., Zenodo) as you would data, and get a DOI
     - Or post on your web site and use a PURL
2. Specify basic metadata
   - Including license -- choose from http://opensource.org/licenses, preferably Apache v2.0
3. Specify desired citation



https://commons.wikimedia.org/wiki/File:Source_code_in_Javascript.png

Making Software Accessible:

Ideal Approach

1. Learn to use a code repository that allows version tracking and collaborative software development
   - GitHub, BitBucket, etc.
2. Create a public entry for your software with a persistent unique identifier
3. Specify the metadata
   - Including license -- choose from http://opensource.org/licenses, preferably Apache v2.0
4. Specify desired citation

Making Software Accessible:

Cite the software in your paper

Analogous to citing data:

- Citation goes in the References section
- How to cite the software? You choose:
  - With an in-text pointer as you would cite any other paper (recommended)
  - With an in-text pointer in a special "Data Resources" (or "Software Resources") section
  - With an in-text pointer in the "Acknowledgments" section

Scientific Paper of the Future Training

Part I

1. Motivation and overview: open science, reproducible publications, and digital scholarship
2. Making data accessible
3. Making software accessible
4. Documenting software with metadata

Part II

5. Documenting provenance and methods
6. Improving author citation profile and researcher impact
7. Summary of author checklist

Documenting Software through Metadata

OntoSoft Training

Part 4

http://dx.doi.org/10.5281/zenodo.15920

NSF ICER-1440323
ICER-1343800

http://www.scientificpaperofthefuture.org

http://www.flickr.com/photos/gemmerich/6365692623/in/photostream

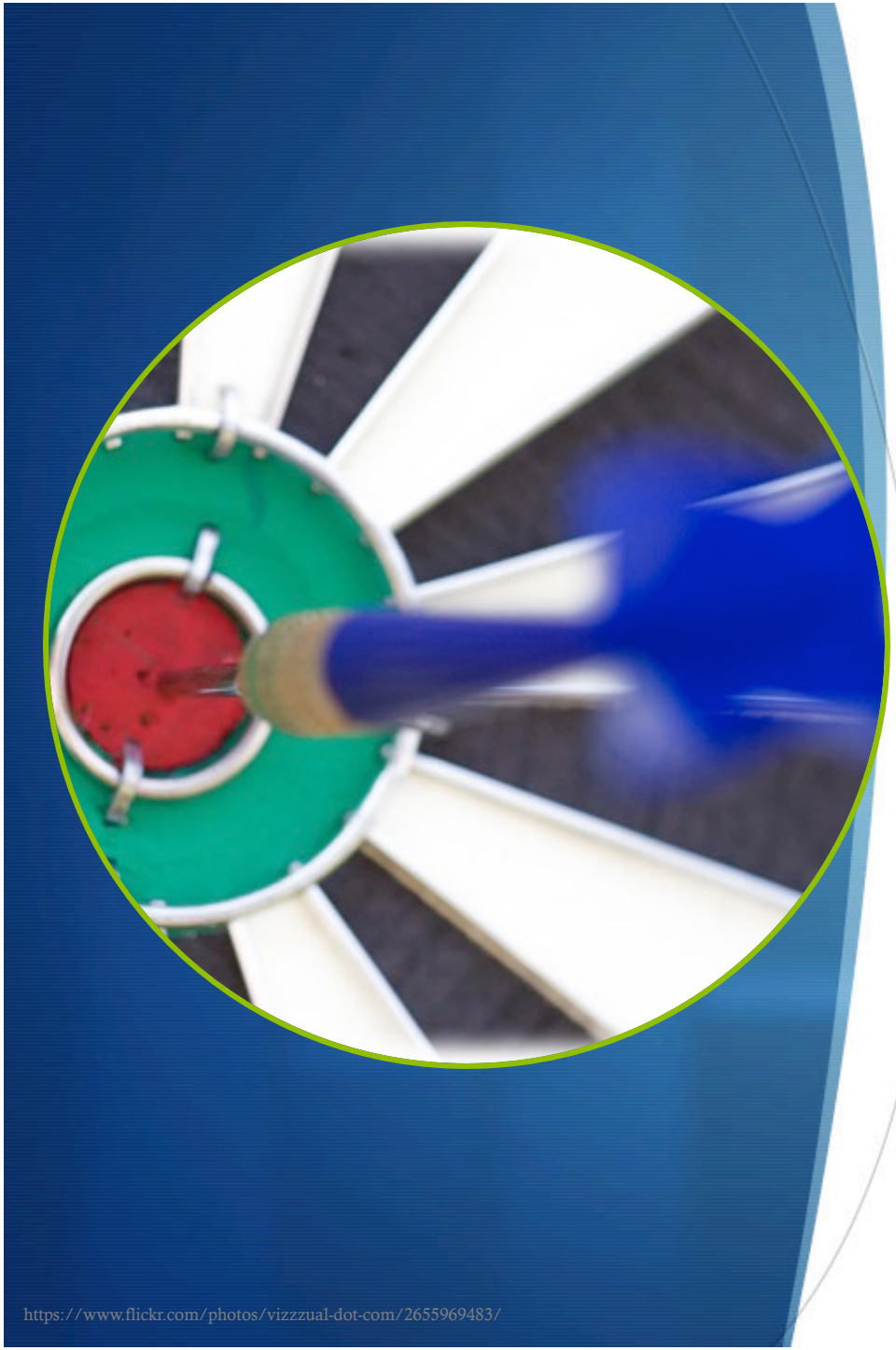
Software Repositories

So you have published your software in a repository…

Is that sufficient for others to reuse it?

Software Repository vs Software Registry

- **Software repository**
  - Code resides there
  - Support software evolution
  - Support groups of developers of open source software
- **Software registry**
  - Capture metadata
    - Useful structured information about the code



https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

1. Understand what metadata needs to be documented about software to promote reuse
2. Understand how to use a software registry to specify that metadata

Software Metadata

- Describe characteristics of the software that others can understand, discover (find), and compare software
- Six major categories of software metadata
  - Developed as part of the OntoSoft project
    - http://www.ontosoft.org/software

http://www.ontosoft.org/software

OntoSoft Metadata Categories

Locate
unique description

Contribute
evolution

Track
versions

Trust
quality and ratings

Relate
domain knowledge

Discuss
support and community

Access
download

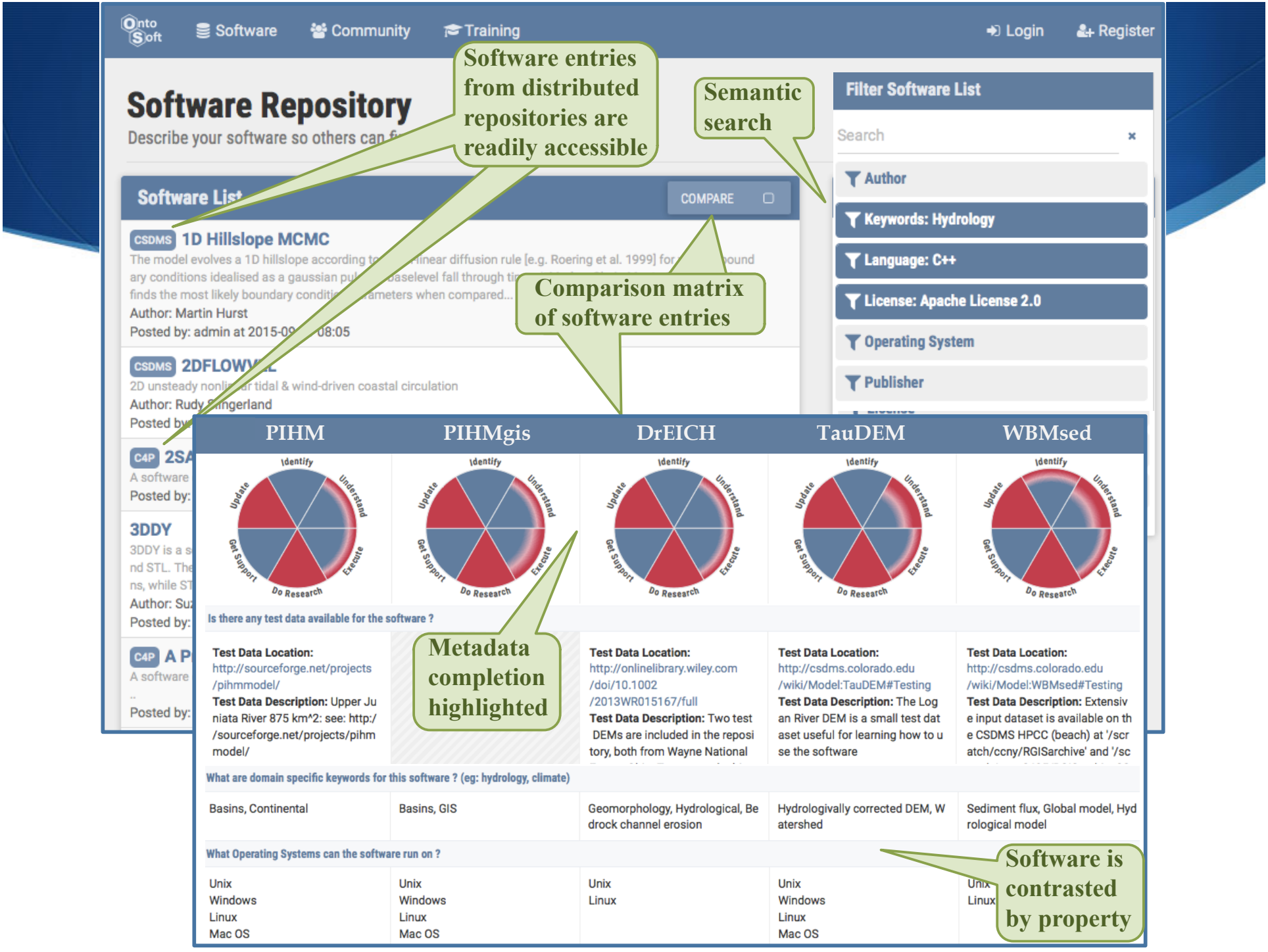
Install
execution requirements

Run
testing execution

Experiment
run with other data

Compose
run with other software

Cite
scientific publications

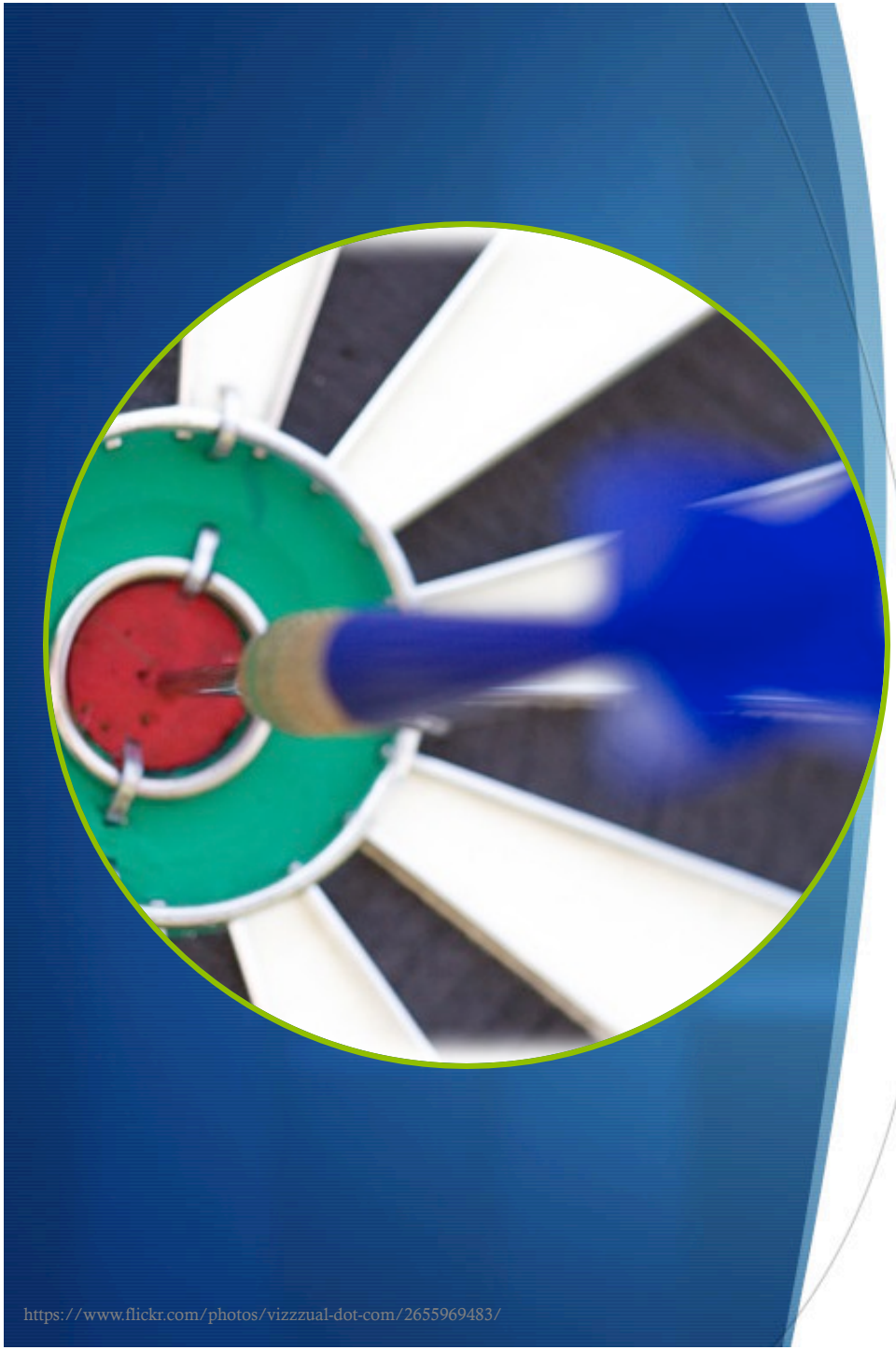

Onto Soft
Software
Community
Training
Login
Register
Software Repository
Describe your software so others can
Software entries from distributed repositories are readily accessible
Semantic search
Filter Software List
Search
Author
Keywords: Hydrology
Language: C++
License: Apache License 2.0
Operating System
Publisher
Software List
COMPARE
CSDMS 1D Hillslope MCMC
Author: Martin Hurst
Posted by: admin at 2015-09
08:05
CSDMS 2DFLOWVEL
2D unsteady nonlinear tidal & wind-driven coastal circulation
Author: Rudy Slingerland
C4P 2SA
A software
Posted by:
3DDY
Author: Suz
Posted by:
C4P A P
A software
Posted by:
Comparison matrix of software entries
PIHM
PIHMgis
DrEICH
TauDEM
WBMsed
Identify
Understand
Execute
Do Research
Get Support
Update
Is there any test data available for the software ?
Test Data Location: http://sourceforge.net/projects/pihmmodel/
Test Data Description: Upper Juniata River 875 km^2: see: http://sourceforge.net/projects/pihmmodel/
Test Data Location: http://onlinelibrary.wiley.com/doi/10.1002/2013WR015167/full
Test Data Description: Two test DEMs are included in the repository, both from Wayne National
Test Data Location: http://csdms.colorado.edu/wiki/Model:TauDEM#Testing
Test Data Description: The Logan River DEM is a small test dataset useful for learning how to use the software
Test Data Location: http://csdms.colorado.edu/wiki/Model:WBMsed#Testing
Test Data Description: Extensive input dataset is available on the CSDMS HPCC (beach) at '/scratch/ccny/RGISarchive' and '/sc
Metadata completion highlighted
What are domain specific keywords for this software ? (eg: hydrology, climate)
Basins, Continental
Basins, GIS
Geomorphology, Hydrological, Bedrock channel erosion
Hydrologically corrected DEM, Watershed
Sediment flux, Global model, Hydrological model
What Operating Systems can the software run on ?
Unix
Windows
Linux
Mac OS
Unix
Linux
Software is contrasted by property

Finding Software

- Any kind of software metadata can be useful to find software
  - "I want R code…"
  - "I want to see software by John Smith…"
  - "I want software that is well supported…"
  - "I want software that simulates water runoff…"
  - "I want software that uses elevation data…"

What if…

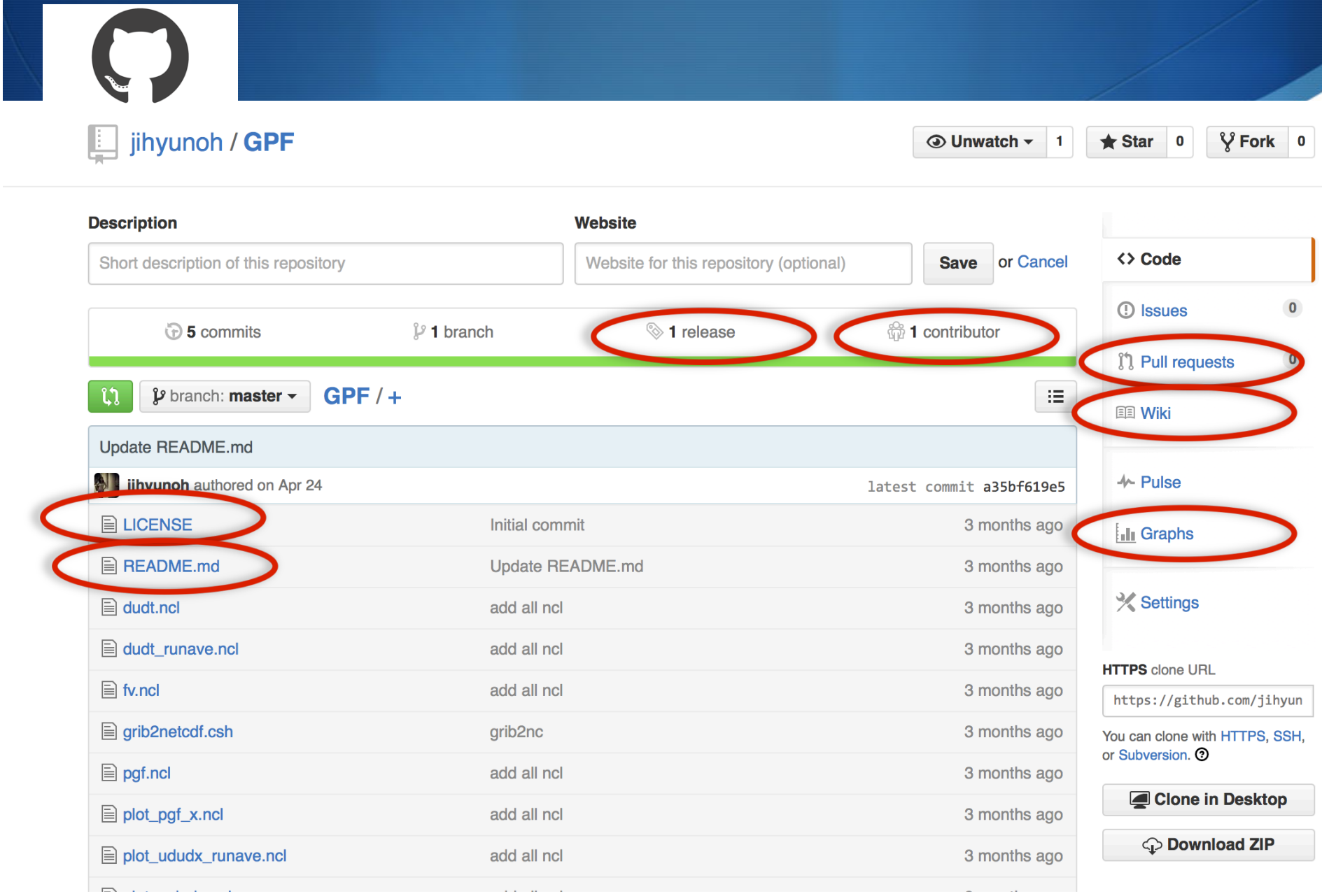
- **… there are many versions of the software?**
  - Give unique identifiers to the most significant versions that you want to release
  - Relate those versions to one another
- **… the software is already in a public repository?**
  - Create a proper documentation and description of the software
- **… the software is relatively small?**
  - If you think it may be useful to someone (think of people who do not program!), then release it
- **… the software is a large package with many functions?**
  - Consider releasing the large package as a whole for those who want all the functionality
  - Consider also releasing pieces of it with limited functionality that may have a broader audience



Goals of this Section

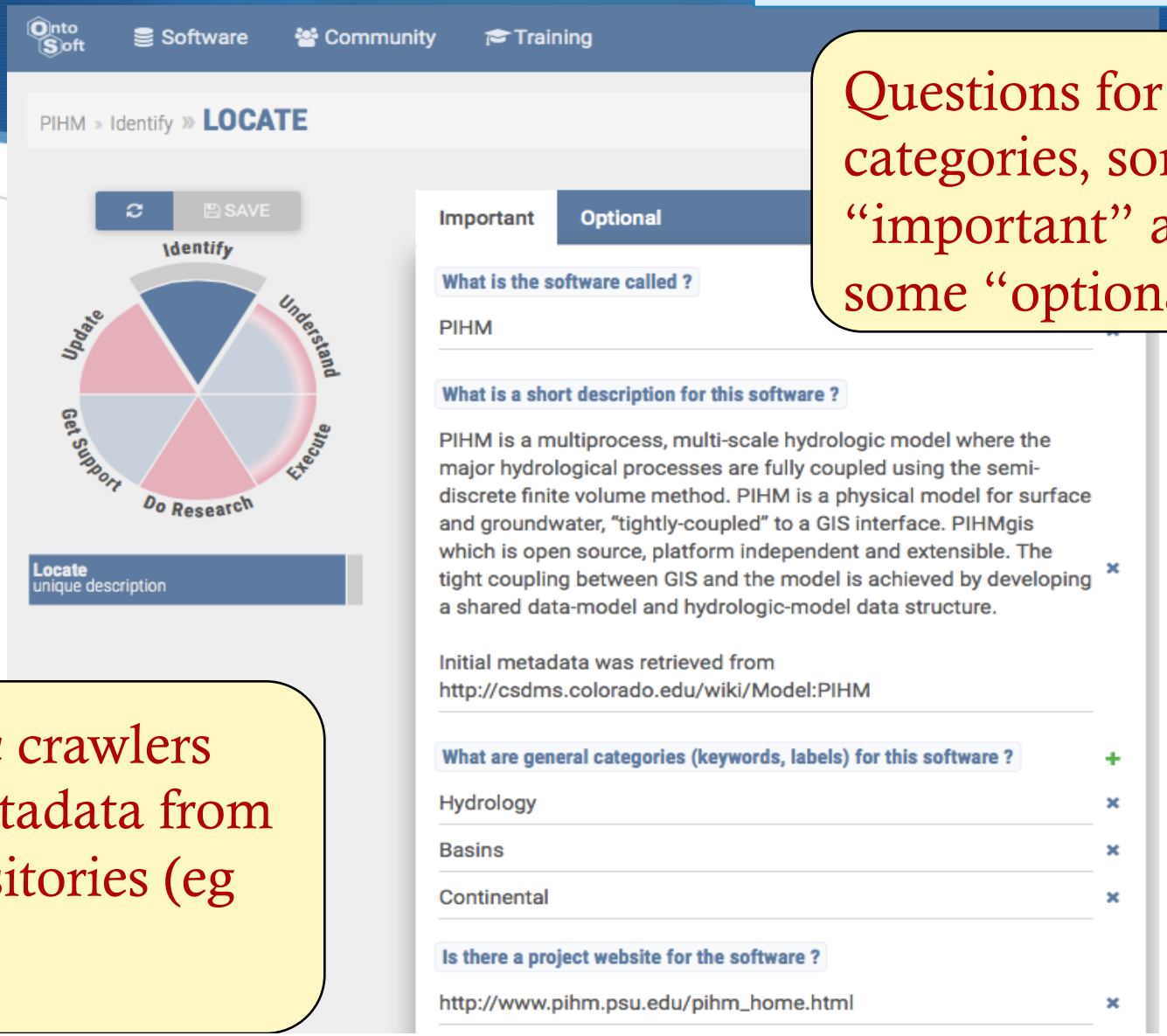
1. Understand what needs to be documented about software to promote reuse
2. Understand how to use a software registry to specify that metadata

Describing Software in a Repository



Describing Software with OntoSoft

http://www.ontosoft.org/portal

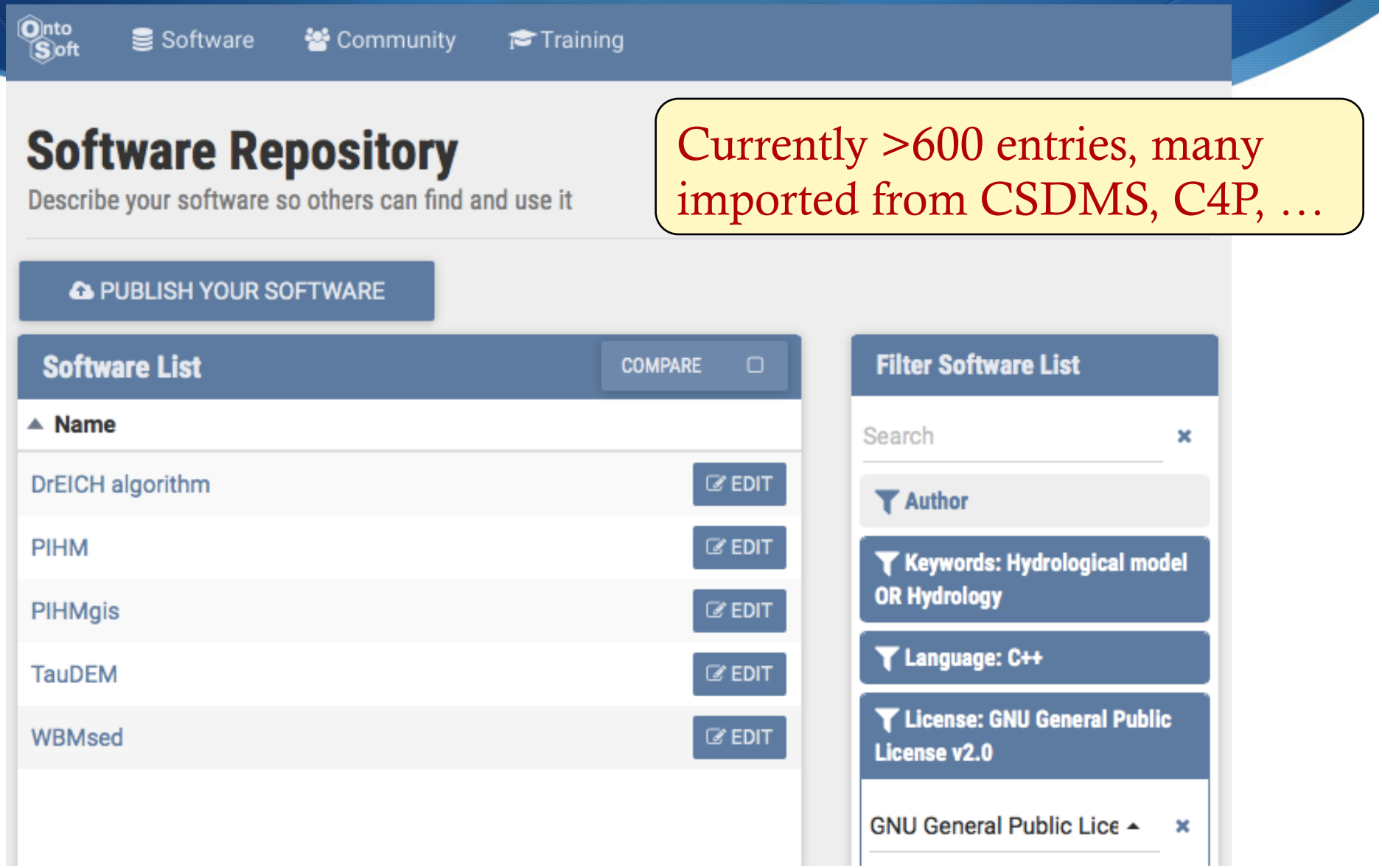


Questions for 6 top categories, some "important" and some "optional"

Automatic crawlers import metadata from code repositories (eg GitHub)

Finding Software with OntoSoft

http://www.ontosoft.org/portal



Currently >600 entries, many imported from CSDMS, C4P, …

Comparing Alternatives with OntoSoft

Select software and features, get a comparison table

Onto Soft | Software | Community | Training

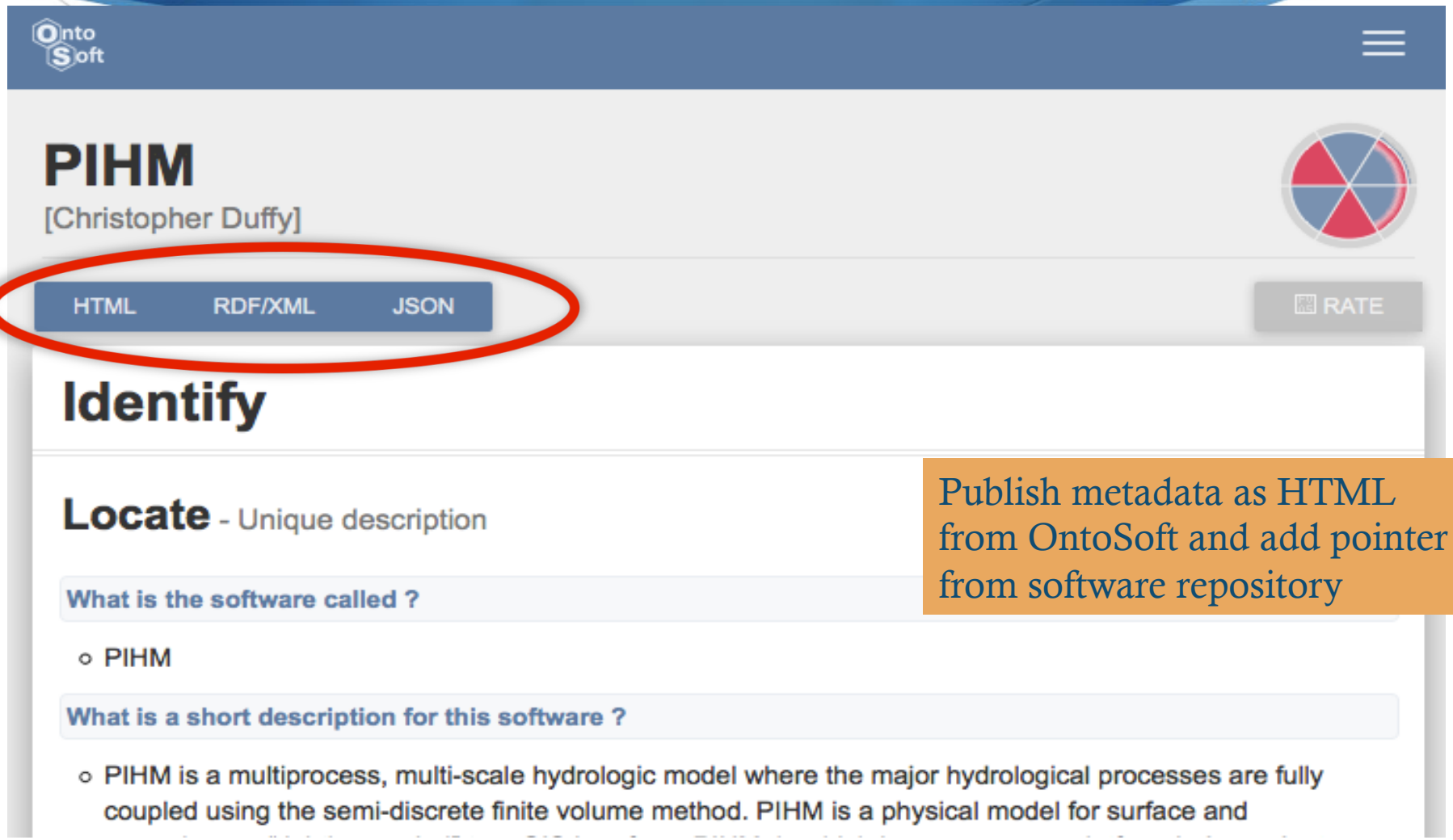
Compare Software

DrEICH algorithm, PIHM, PIHMgis, TauDEM, WBMsed

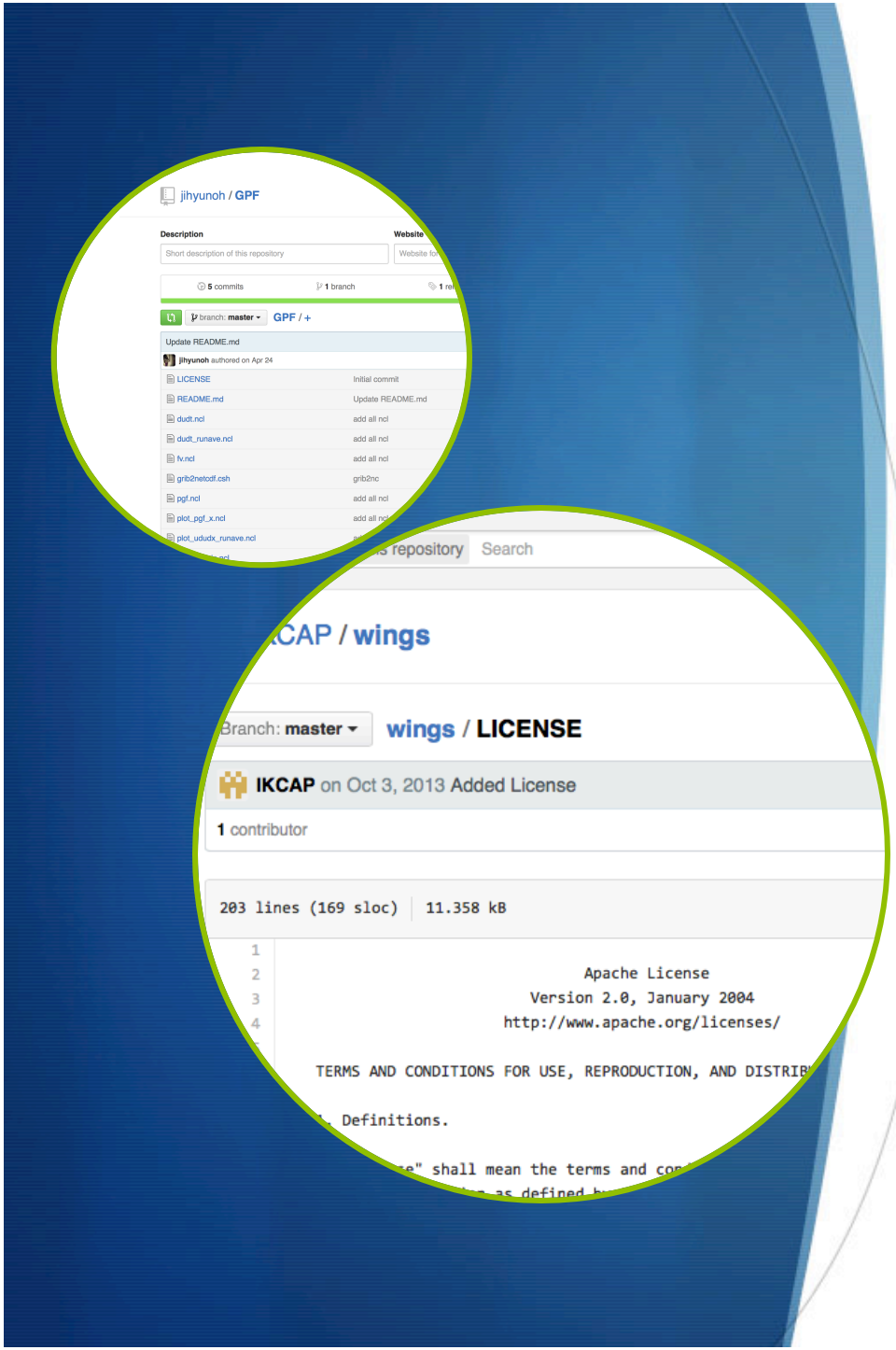
	PIHM	PIHMgis	DrEICH	TauDEM	WBMsed
					
What are domain specific keywords for this software ? (eg: hydrology, climate)					
	Geomorphology, Hydrological, Bedrock channel ero-	Basins, Continental	Basins, GIS	Hydrologically corrected DEM, Watershed	Sediment flux, Global model, Hydrological model
What Operating Systems can the software run on ?					
	Unix Linux	Unix Windows Linux Mac OS	Unix Windows Linux Mac OS	Unix Windows Linux Mac OS	Unix Linux
Is there any test data available for the software ?					
	Test Data Location: http://onlinelibrary.wiley.-com/doi/10.1002/2013WR015167/full **Test Data Description:** Two test DEMs are included in the repository,	**Test Data Location:** http://source-forge.net/projects/pih-mmodel/ **Test Data Description:** Upper Juniata River 875 km^2: see: http://source-		**Test Data Location:** http://csdms.colorado.e-du/wiki/Model:Tau-DEM#Testing **Test Data Description:** The Logan River DEM is a small test dataset useful	**Test Data Location:** http://csdms.colorado.e-du/wiki/Mod-el:WBMsed#Testing **Test Data Description:** Extensive input dataset is available on the CSDMS

Publishing Software Metadata with OntoSoft

http://www.ontosoft.org/portal



Publish metadata as HTML from OntoSoft and add pointer from software repository



Documenting Software through Metadata: Simplest Approach

1. Describe as much metadata as you can in your software site
    1. Document the basic metadata discussed earlier
    2. If you use a code repository, there is some basic structure you can follow

Ideal Approach

1. Use a software registry
   - http://www/ontosoft.org/portal, csdms.colorado.edu, etc.
   - Guides through questions to provide metadata
2. Save the metadata as HTML, XML,…
3. Post the metadata on your code site

Documenting Provenance and Methods

OntoSoft Training

Part 5

http://dx.doi.org/10.5281/zenodo.15920

http://www.scientificpaperofthefuture.org

NSF ICER-1440323
ICER-1343800

http://en.wikipedia.org/wiki/Certificate_of_origin#mediaviewer/File:Coal_from_the_Titanic.jpg

http://commons.wikimedia.org/wiki/File:The_seal_of_National_Taiwan_University.png

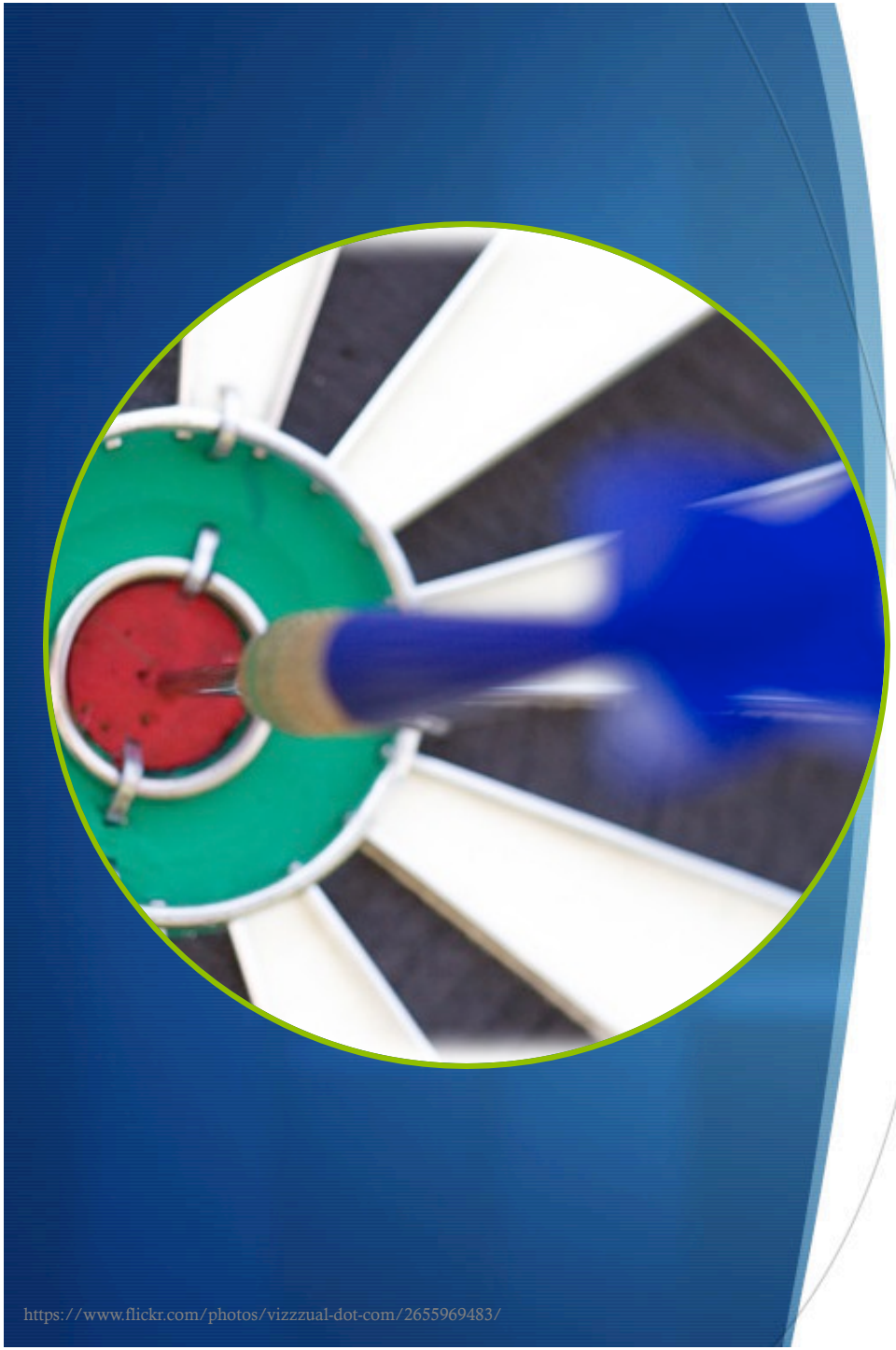
https://www.flickr.com/photos/alterschwede08/3203630740/ (CC BY-ND 2.0)

Methods Described in Text Are Incomplete

- Analysis of 18 quantitative papers published in Nature Genetics in the past two years found that reproducibility was not achievable even in principle in 10 cases, even when datasets are published [Ioannidis et al 09]
- "Data processing, however, is often not described well enough to allow for exact reproduction of the results, leading to exercises in '**forensic bioinformatics**' where aspects of raw data and reported results are used to infer what methods must have been employed." [Baggerly and Coombes 09]

Methods Described in Text Are Ambiguous

- "**Ambiguity** in program descriptions leads to the possibility, if not the certainty, that a given natural language description can be converted into computer code in various ways, each of which may lead to different numerical outcomes." [Ince et al 2012]
- "Ambiguity can occur at the **lexical, syntactic or semantic** level and is not necessarily the result of incompetence or bad practice. It is a natural consequence of using natural language and is unavoidable. " [Ince et al 2012]



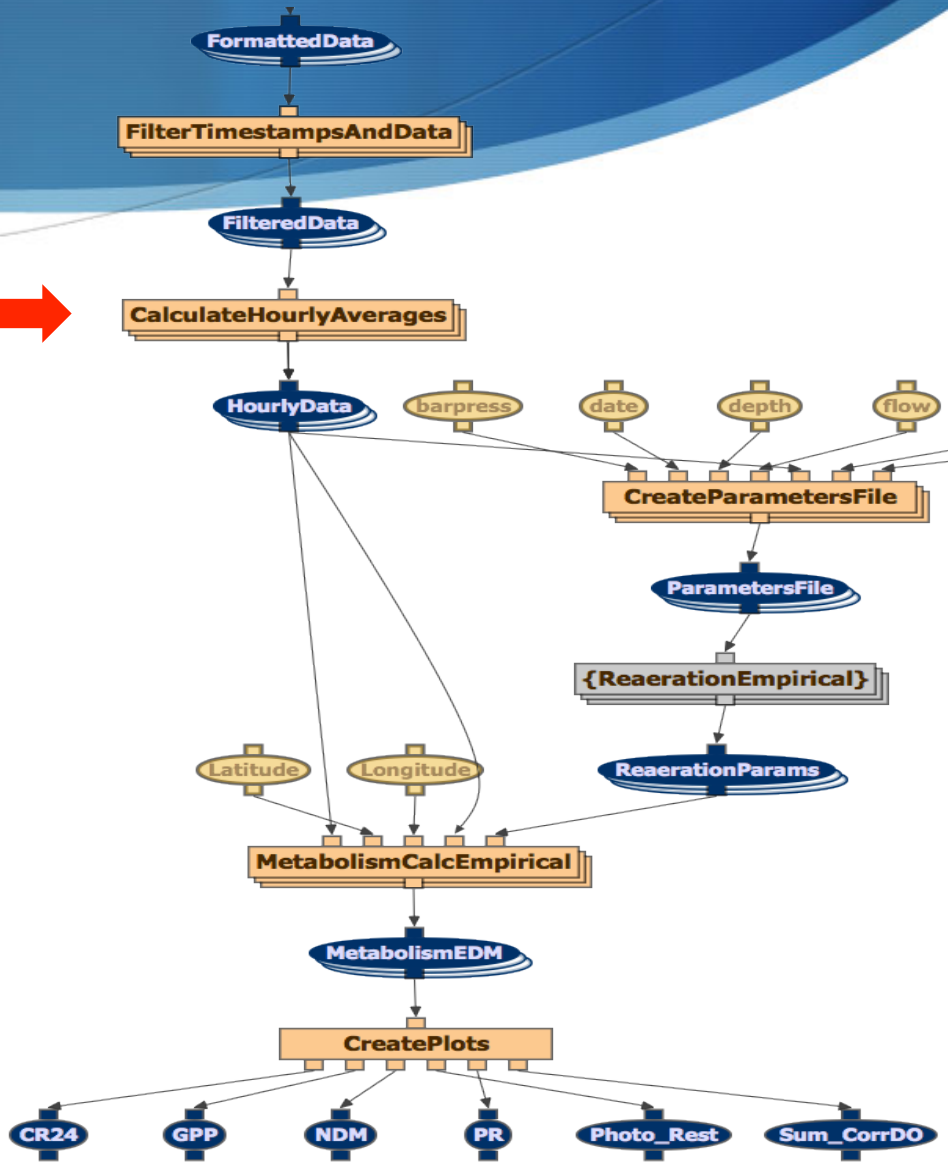
https://www.flickr.com/photos/vizzzual-dot-com/2655969483/

Goals of this Section

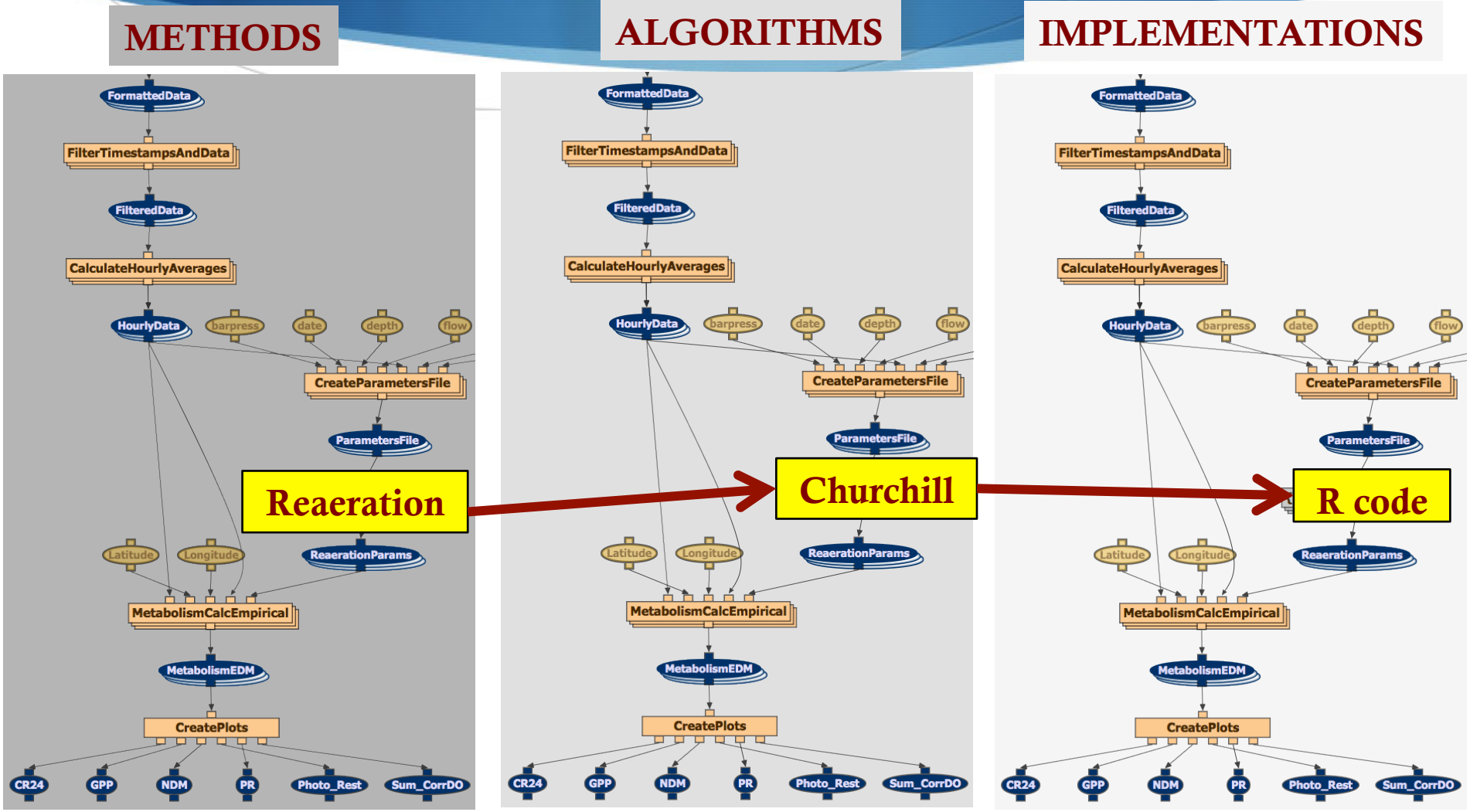
1. Understand what are methods and provenance is in a scientific article
2. Understand how to document methods and provenance properly in an article

Workflows as Representations of Computational Methods

- Computational workflow
  - Eg, water metabolism
- Workflows can include manual steps
  - Eg, creating a figure, cleaning data
- Workflows may access web services
  - Eg, access databases in biology

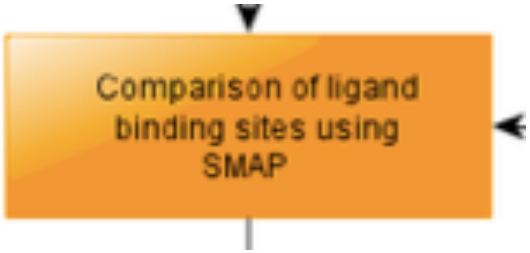


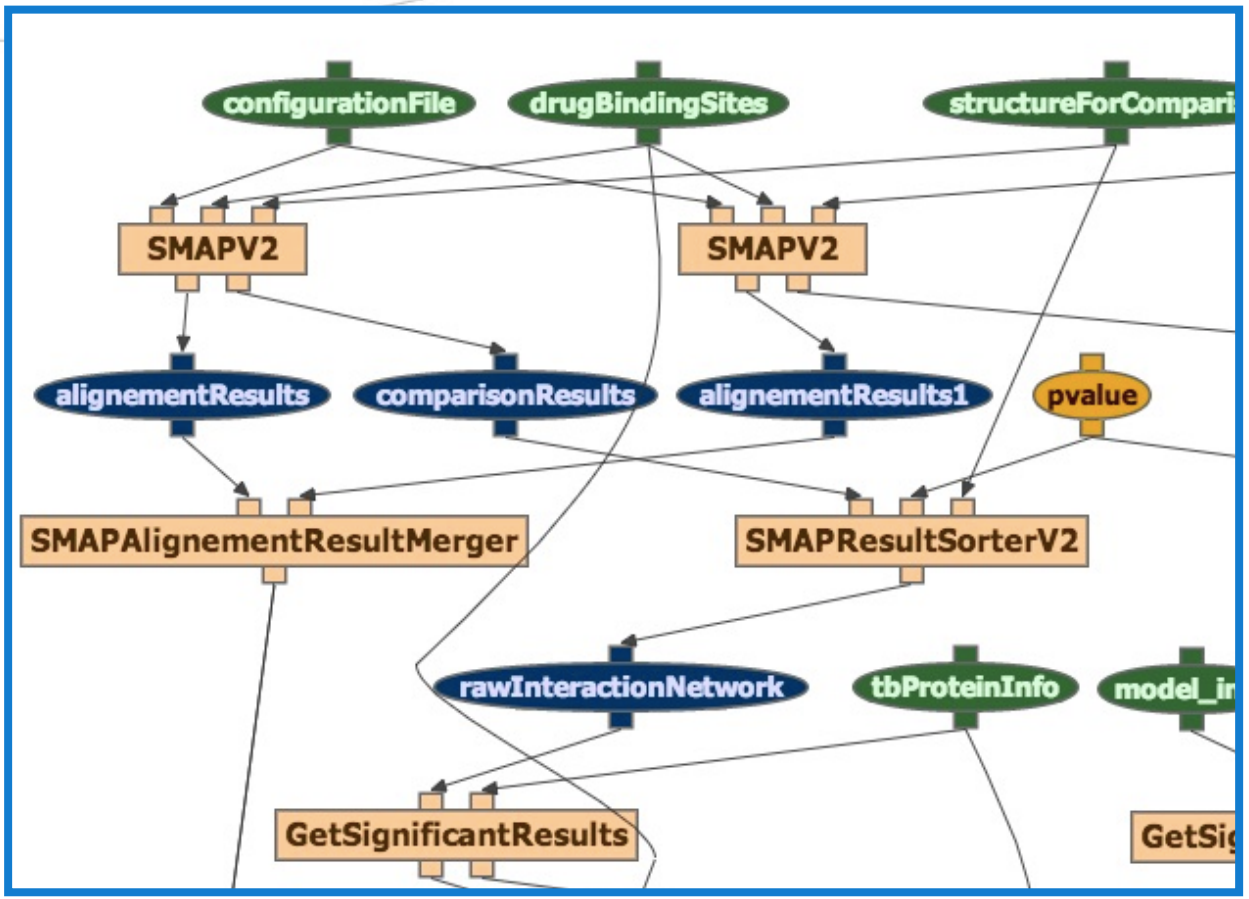
Describing a Method at Different Levels of Abstraction



What the Paper Says Versus What the Actual Software Does

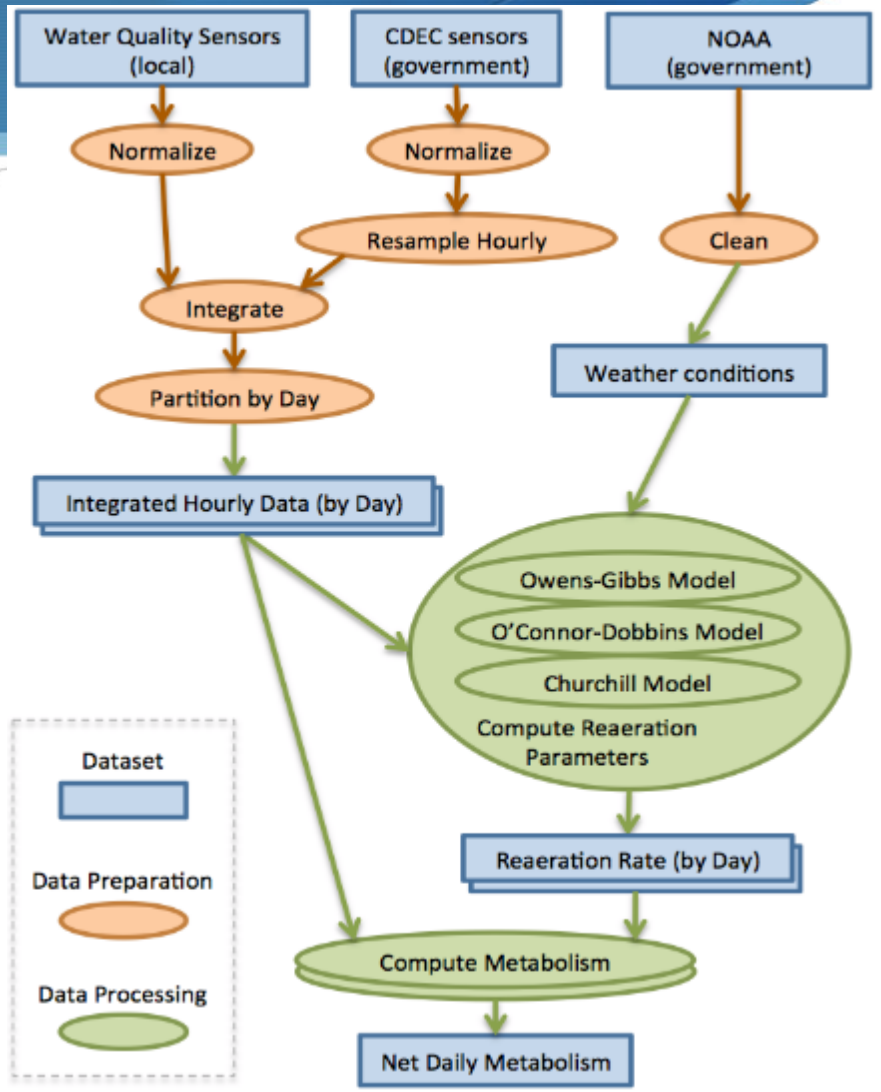
(from [Garijo et al 2013])



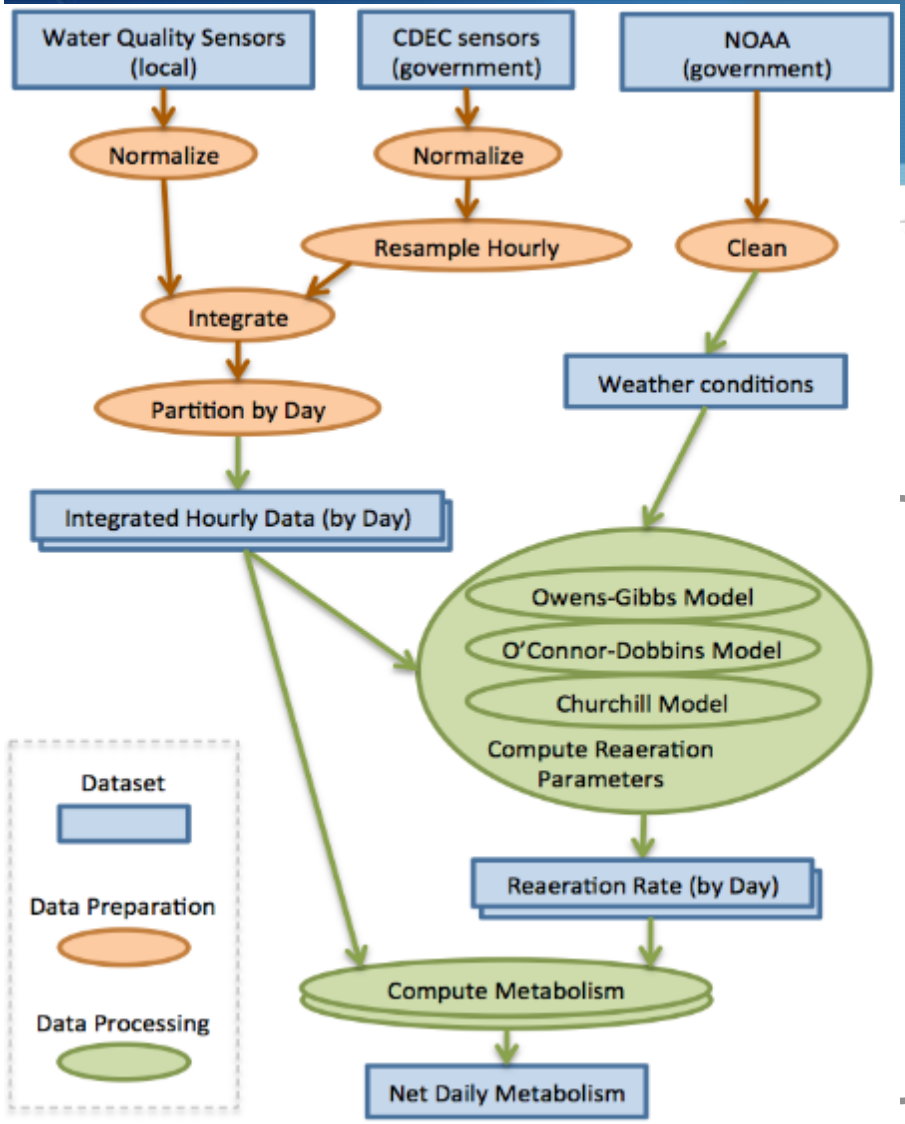


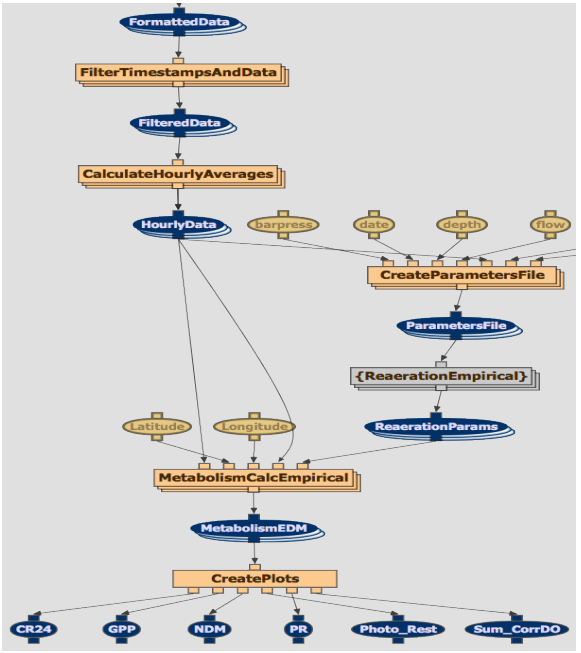
Developing Workflows: How to Sketch a Workflow

1. Compile the command line invocation to all your codes
   - ★ Input data, parameters, configuration files
   - ★ Include data preparation codes
2. Consider how the data flows from code to code
3. Starting with the input data, work your way to the results
4. If any steps were done with manual intervention, indicate that
5. Create subworkflows if it gets large



From a Workflow Sketch to a Formal Workflow





Workflow Systems

- Capture method as a workflow
- Workflow can be easily shared and reused
- Other benefits
  - Workflow validation
  - Scalable computations
  - Comprehensive software libraries
- Many workflow systems
  - Each has different capabilities

Electronic Notebooks

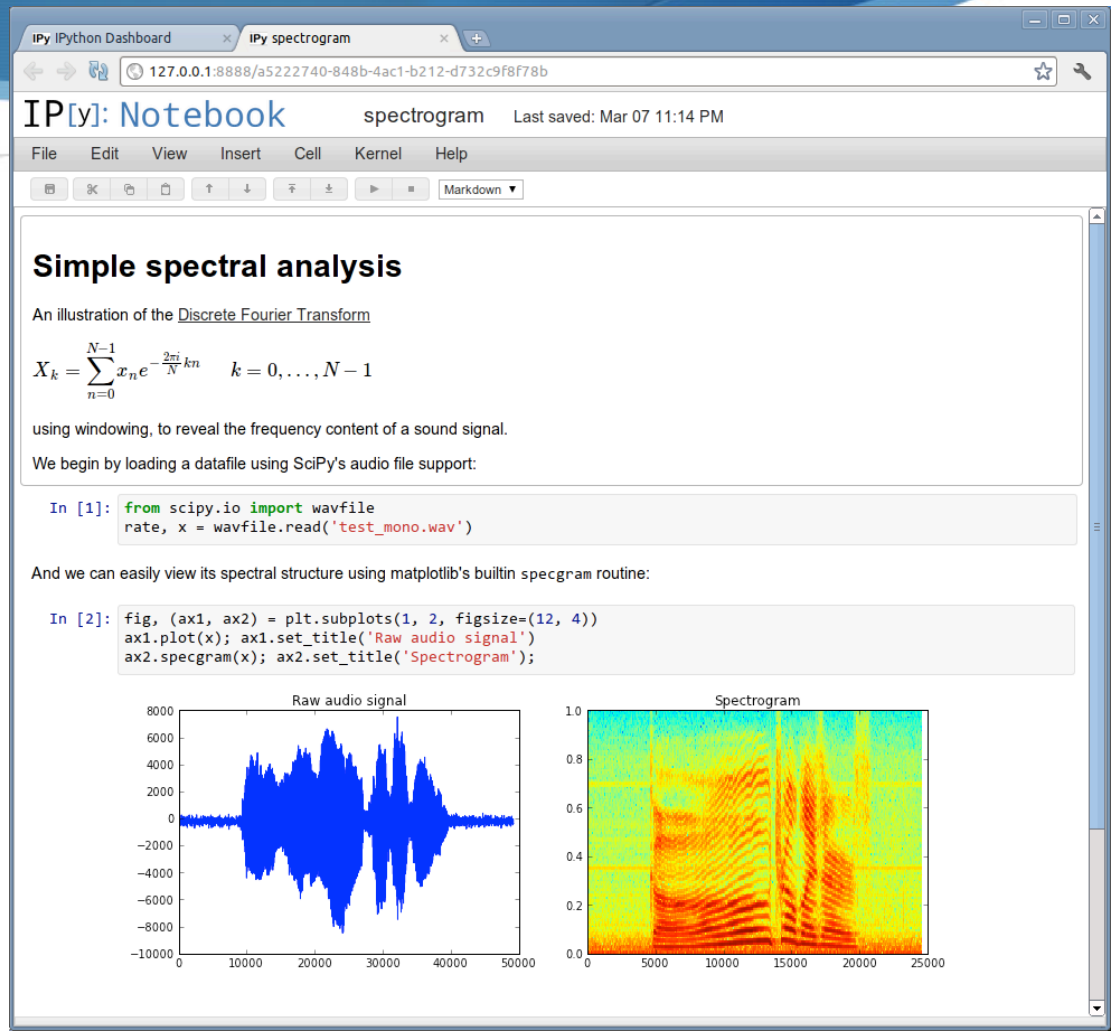
IP[y]: Notebook

Sweave = R · LaTeX

CDF **Computable Document Format**
Documents come alive with the power of computation

MADAGASCAR

http://ipython.org/notebook.html



http://en.wikipedia.org/wiki/Certificate_of_origin#mediaviewer/File:Coal_from_the_Titanic.jpg

http://commons.wikimedia.org/wiki/File:The_seal_of_National_Taiwan_University.png

https://www.flickr.com/photos/alterschwede08/3203630740/ (CC BY-ND 2.0)

What is Provenance

Provenance covers:

1. Processes
2. Documents ("resources")
3. Entities

http://www.w3.org/2005/Incubator/prov/wiki/What_Is_Provenance

A Working Definition of Provenance

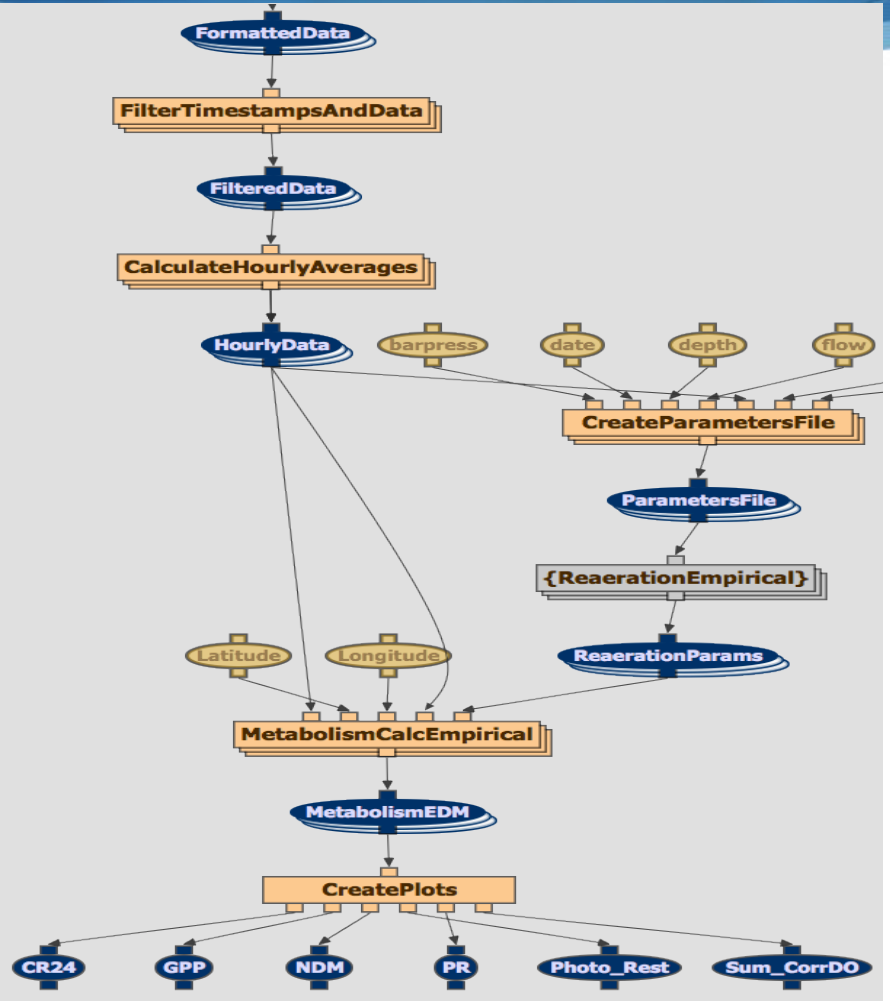
Provenance of a resource is a record that describes entities and processes involved in producing and delivering or otherwise influencing that resource.

Provenance provides a critical foundation for assessing authenticity, enabling trust, and allowing reproducibility.

- ★ Provenance results from past actions

- ★ Provenance can be seen as metadata, but not all metadata is provenance

1) Provenance as Process (Computing steps, actions, etc)



2) Provenance as Resources (Documents, Data, etc)

WIKIPEDIA
The Free Encyclopedia

Main page
Contents
Featured content
Current events
Random article
Donate to Wikipedia
Wikimedia Shop

Interaction
Help
About Wikipedia
Community portal
Recent changes
Contact page

Tools
What links here
Related changes
Upload file
Special pages

Article Talk

Stratovolcano

From Wikipedia, the free encyclopedia

A **stratovolcano**, also known as a **composite volcano**,[1] is a conical volcano built up by many layers (strata) of hardened lava, tephra, pumice, and volcanic ash. Unlike shield volcanoes, stratovolcanoes are characterized by a steep profile and periodic explosive eruptions and effusive eruptions, although some have collapsed craters called calderas. The lava flowing from stratovolcanoes typically cools and hardens before spreading far due to high viscosity. The magma forming this lava is often felsic, having high-to-intermediate levels of silica (as in rhyolite, dacite, or andesite), with lesser amounts of less-viscous mafic magma. Extensive felsic lava flows are uncommon, but have travelled as far as 15 km (9.3 mi).[2]

Stratovolcanoes are sometimes called "composite volcanoes" because of their composite layered structure built up from sequential outpourings of eruptive materials. They are among the most common types of volcanoes, in contrast to the less common shield volcanoes. Two famous stratovolcanoes are Krakatoa, best known for its catastrophic eruption in 1883 and Vesuvius, famous for its destruction of the towns Pompeii and Herculaneum in 79 AD. Both eruptions claimed thousands of lives.

Existence of stratovolcanoes has not been proved on other terrestrial bodies of solar system[3] with one exception. Their existence was suggested for some isolated massifs on Mars, e.g., Zephyria Tholus.[4]

Mount Vesuvius erupted in AD 79 and the last eruption of this stratovolcano near Naples, Italy occurred in March 1944. It has been essentially dormant since then.

References [edit]

1. ^ This article incorporates public domain material f
Retrieved 2009-01-19.
2. ^ "Garibaldi volcanic belt: Garibaldi Lake volcanic field"
2010-06-27.
3. ^ Barlow, Nadine (2008). *Mars : an introduction to its in*
ISBN 9780521852265.
4. ^ Stewart, Emily M.; Head, James W. (1 August 2001).
Geophysical Research **106** (E8): 17505. doi:10.1029/20
5. ^ *a b c d e f g h i j k l m* This article incorporates public
Jacquelyne; Tilling, Robert I. "Plate tectonics and people

3) Provenance as Entities (People, institutions, etc)

Ex: NY Times article from REUTERS reporting "At a press conference last Monday, Buckingham Palace was adamant that Prince Larry did not inhale."

Title	Prince Larry did not take drugs
Creator	CREUTERS journalist
Subject	
Description	
Publisher	FA Times
Contributor	Duckingham Palace
Date	
Type	
Format	
Identifier	
Source	original CREUTERS article
Language	
Relation	Tapes of the press conference
Coverage	
Rights	

e Larry took drugs

Prince Larry did not take drugs **is dismissable**

Prince Larry did not take drugs

[more]

according to source Duckingham Palace which is
completely reliable (A)
and improbable because They want to save the reputation of the Monarchy

Prince Larry took drugs **is elaborated in** Prince Larry took cannabis and The trou
Larry

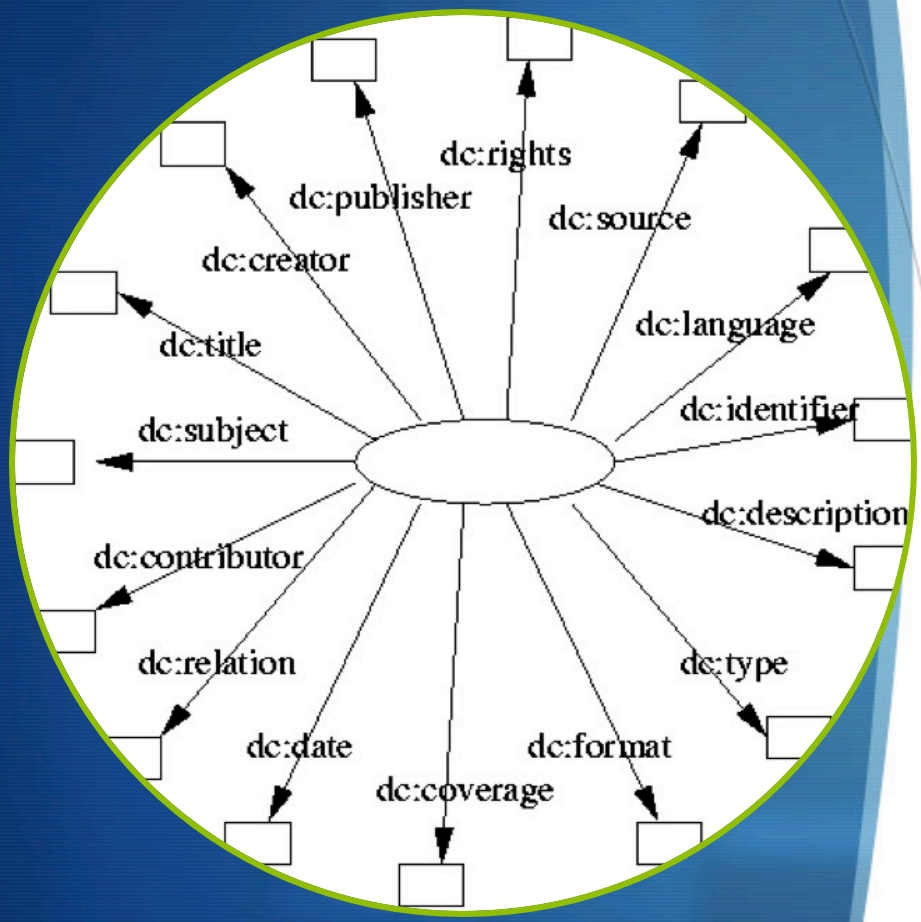
Prince Larry took cannabis

[more]

according to source BBC News which is
completely reliable (A)
and confirmed by other sources

The trouble with Prince Larry

more drug problems



http://dublincore.org/documents/dcq-rdf-xml/

A Well-Known Provenance Vocabulary:

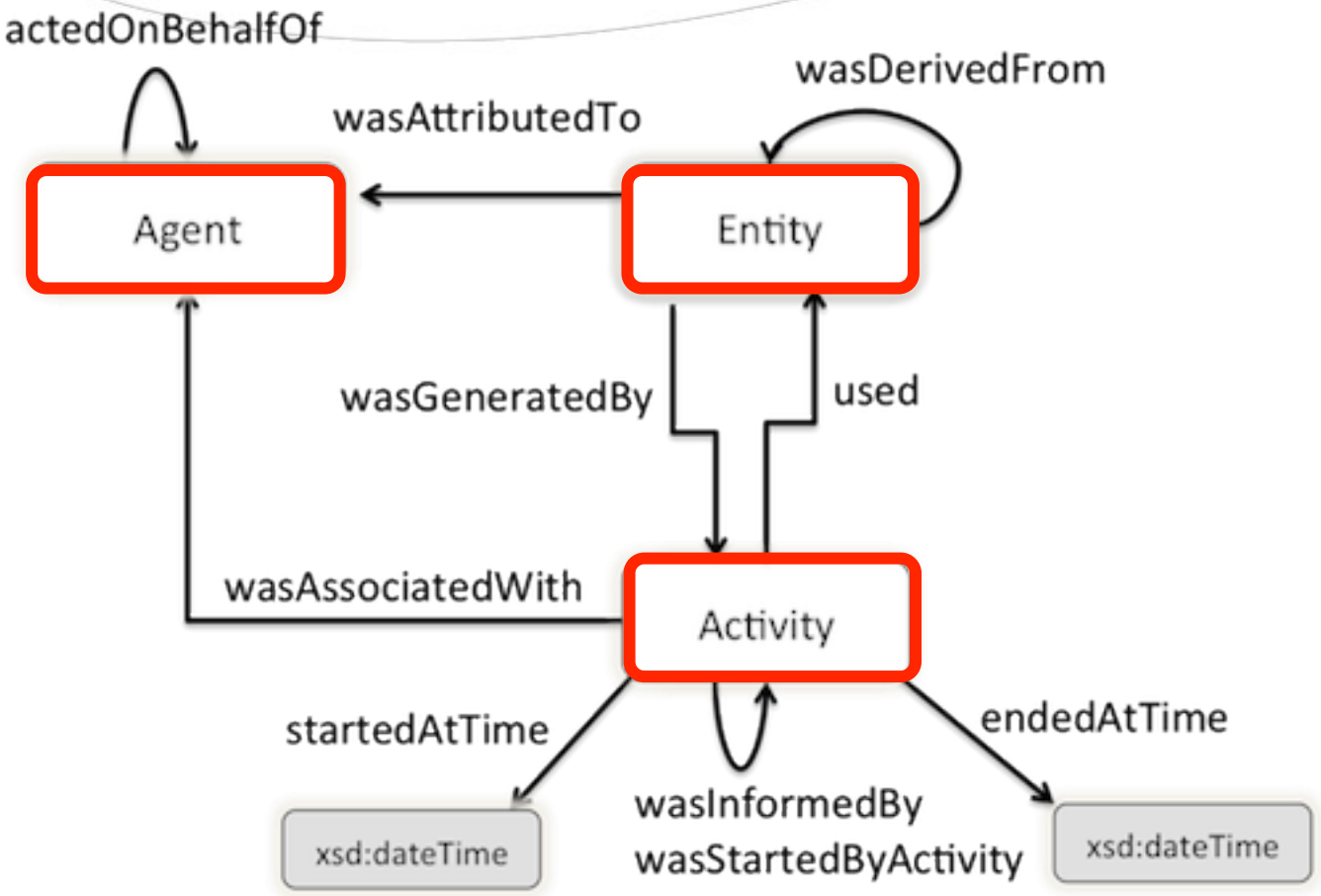
The Dublin Core

From library sciences

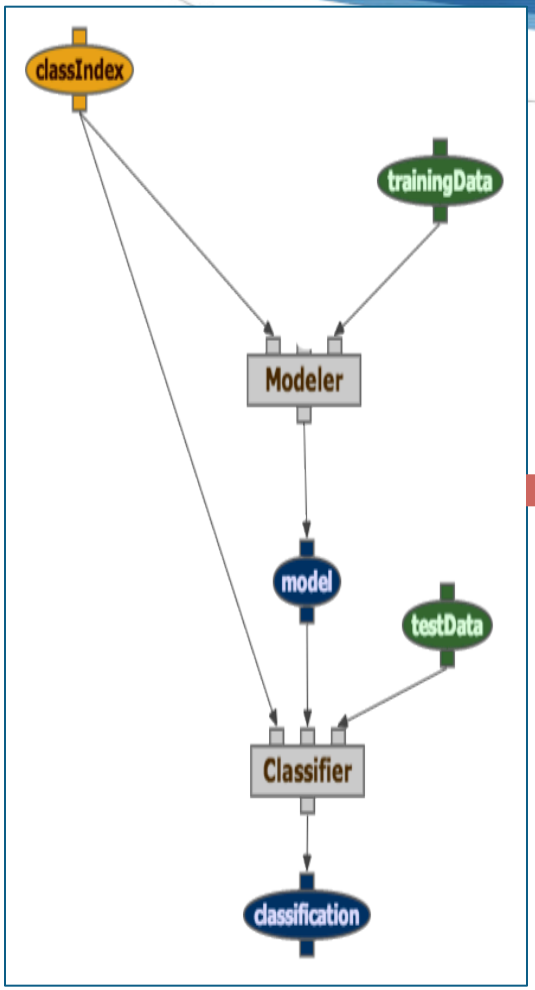
http://dublincore.org/documents/dcmi-terms/

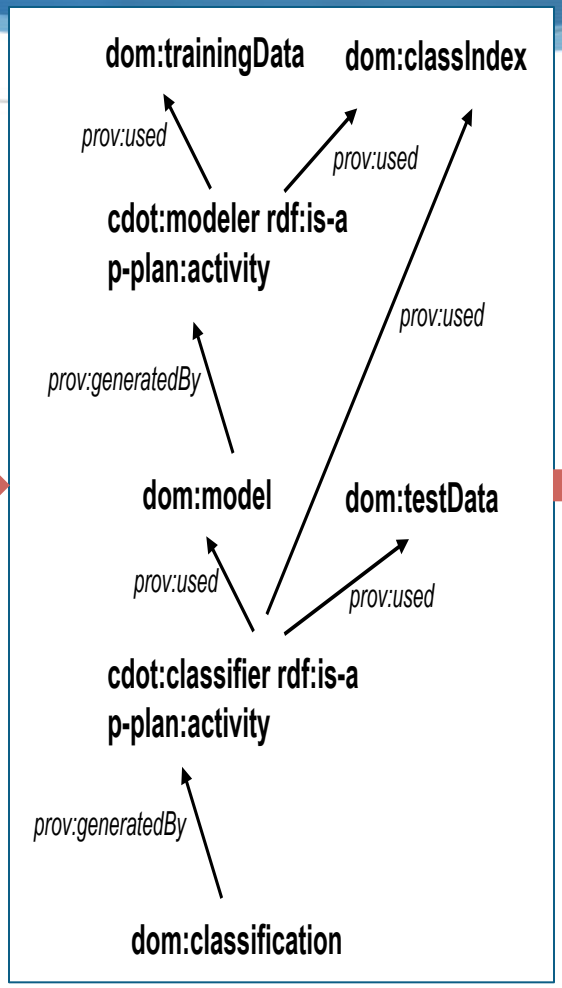
http://www.w3.org/TR/prov-primer/

A Provenance Standard for the Web: W3C PROV



Representing Provenance with the W3C PROV Standard





 # Entities

ex:testData1 a prov:Entity .

ex:model1 a prov:Entity .

ex:classification1 a prov:Entity .

 # Activities

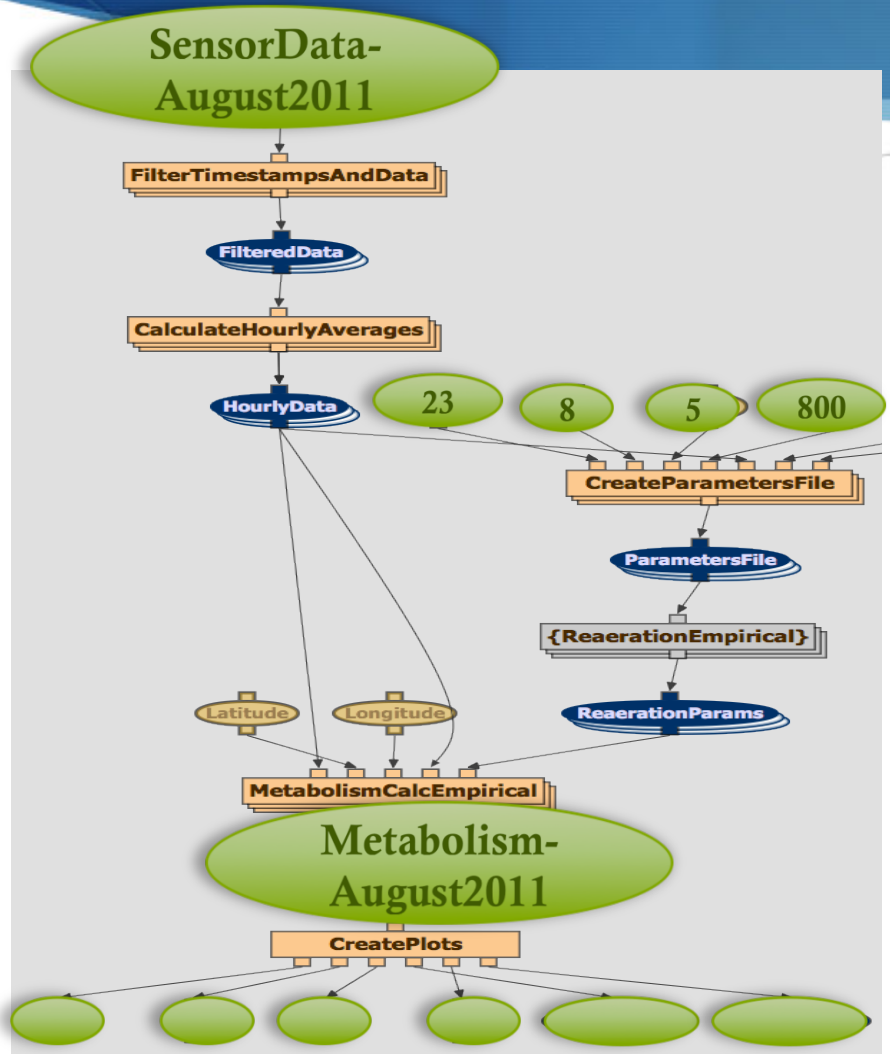
ex:Classifier1 a prov:Activity .

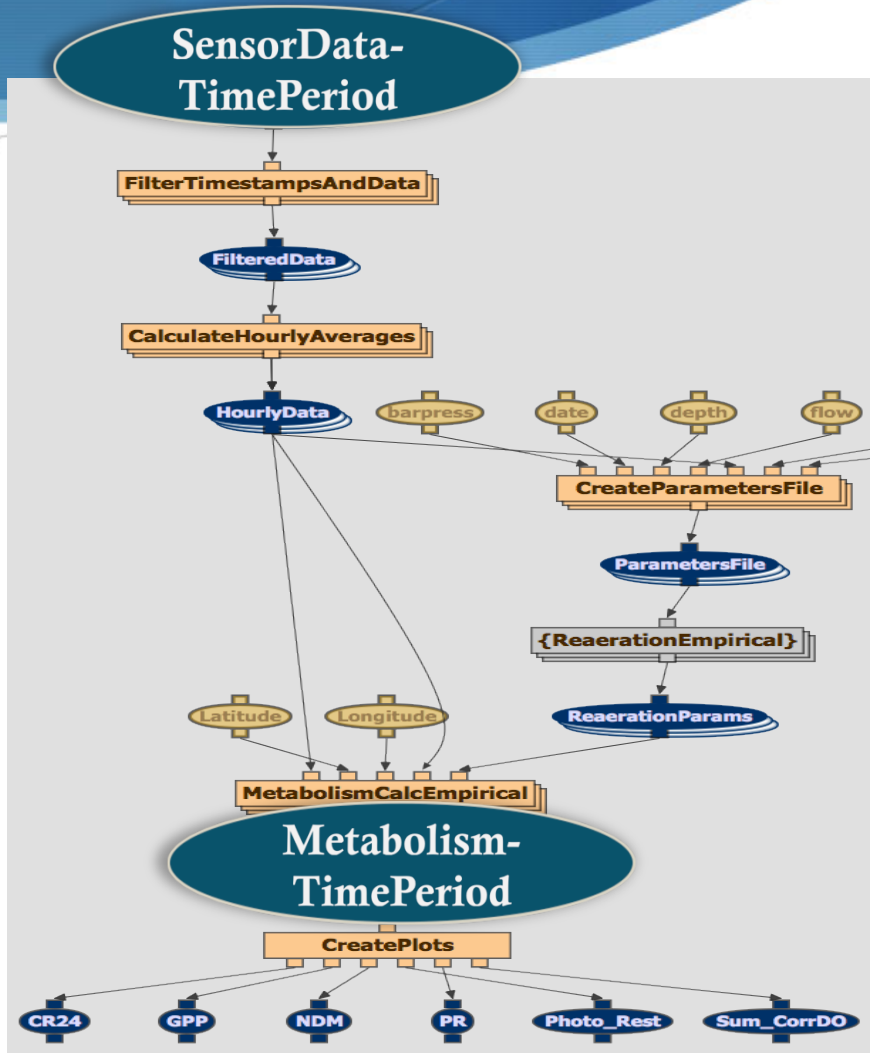
 # Usage and Generation relations between entities and activities

```
ex:Classifier1
    prov:used ex:testData1 ;
    prov:used ex:model1 .

ex:classification1
    prov:wasGeneratedBy
        ex:Classifier1 .
```

Describing Execution (Provenance) vs General Method (Workflow)





Publishing Provenance and Workflows

- Hard to deposit workflows or provenance in a repository
  - Not many repositories available
  - Not many communities sharing repositories
  - This will change in the near future
- Publish workflow and/or provenance in a data repository, get a persistent identifier, and cite

myexperiment

crowdLabs

SHIWA Workflow Repository
Click to visit

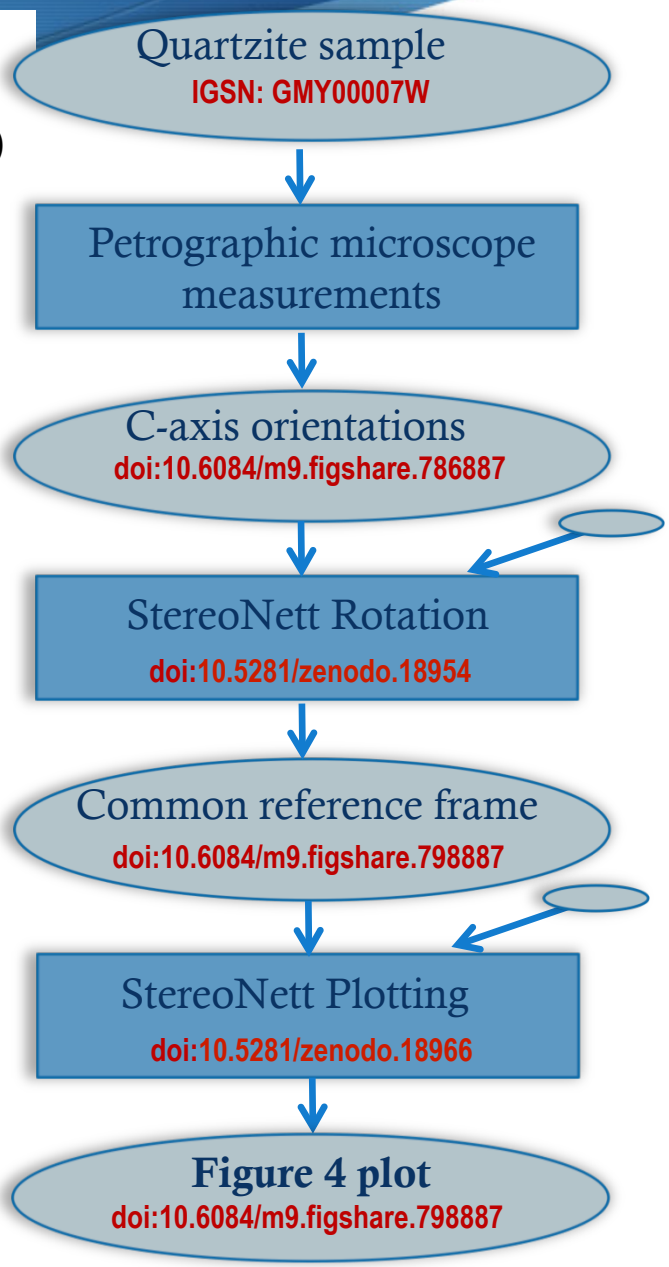
OPMW Workflow repository

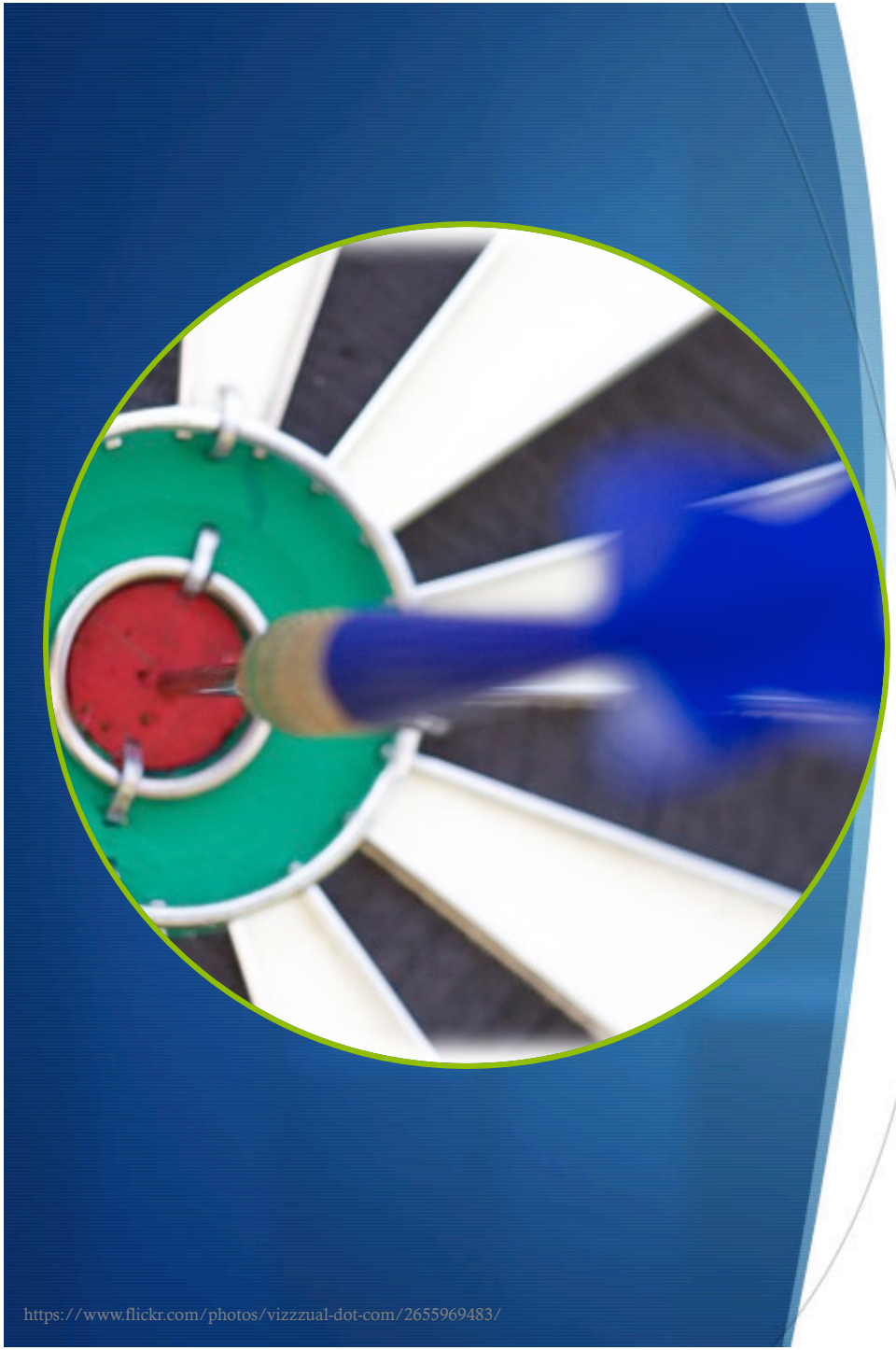
Example: Text and Provenance

Understanding kinematic data from the Moine thrust zone (doi:10.1016/j.ess.2009.08.012)

Jade Silverstein (orcid.org/0000-0001-8455-8431)

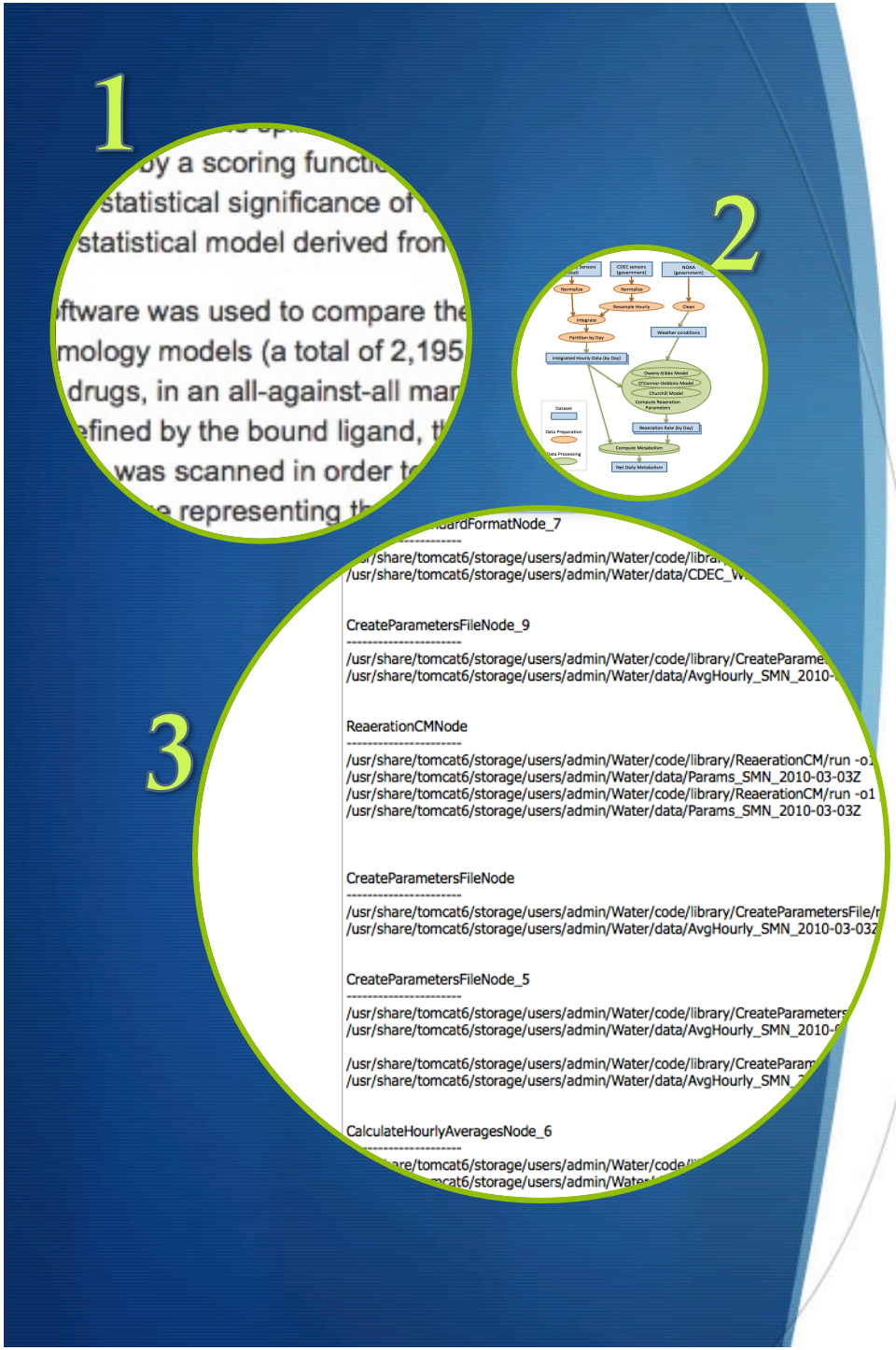
[…] We took a quartzite sample (**IGSN: GMY00007W**) from the Stack of Glencoul in the Moine thrust, and cut 3 thin sections. We measured c-axis orientations (**doi:10.6084/m9.figshare.786887**) using a petrographic microscope. We rotated to a common reference frame (**doi:10.6084/m9.figshare.798887**) using Duyster's StereoNett program (**doi:10.5281/zenodo.18954**). We plotted the data on lower hemisphere, equal area projections (**doi:10.6084/m9.figshare.798887**) using Duyster's StereoNett program (**doi:10.5281/zenodo.18966**), shown in Figure 4. **The provenance is shown in Fig 5**. […]





Goals of this Section

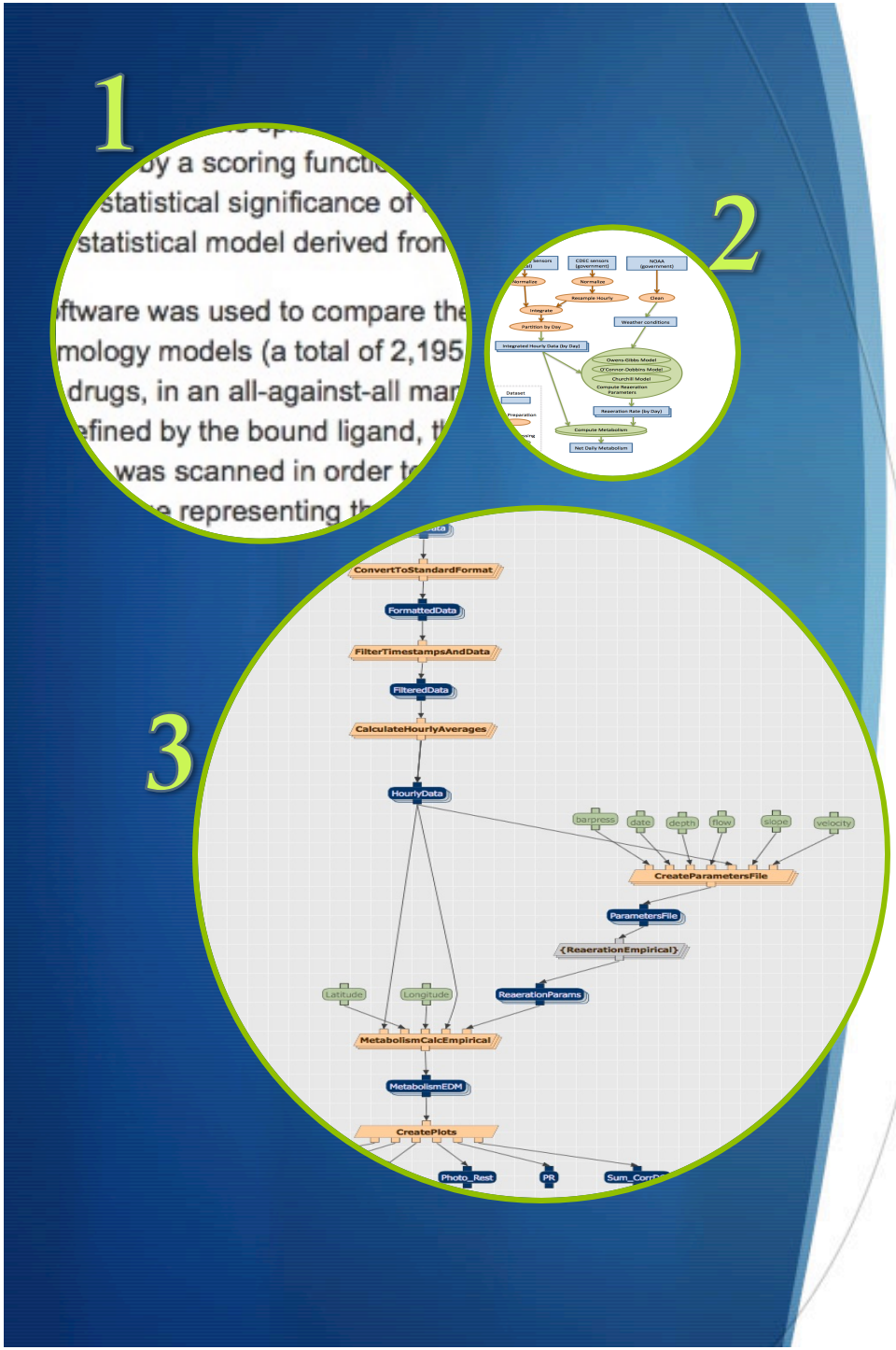
1. Understand what are methods and provenance is in a scientific article
2. Understand how to document methods and provenance properly in an article



Documenting Provenance and Methods:

Simplest Approach

1. Describe the workflow in text
   - Data + software + workflow
   - Specify unique identifiers for data and software, versions, credit all sources
2. Develop a workflow sketch
   - Capture high-level dataflow across components
3. For provenance, include a summary or an execution trace



Documenting Provenance and Methods:

Ideal Approach

1. Describe the workflow in text
   - Data + software + workflow
   - Specify unique identifiers for data and software, versions, credit all sources
2. Develop a workflow sketch
   - Capture high-level dataflow across components
3. Specify the formal workflow using a workflow system, electronic notebook, etc.
   - Command lines + parameter values
   - Dataflow across components
4. Include the provenance record
   - If generating it automatically, preferably using a standard (e.g., PROV)
5. Publish the workflow and provenance record in a publicly accessible repository (eg figshare, myExperiment, etc)
6. Get a unique persistent identifier for the workflow, the provenance, or both

Documenting Provenance and Methods:

How to show provenance and workflow in the article

- Describe the workflow in text
  - In the "Methods" section
- Include your workflow sketch
  - As a figure in the article
- Include your provenance summary or trace
- If available as formal workflow and provenance record, cite them in the paper (use a format analogous to data and software citation)

The Scientific Paper of the Future:
Improving Author Citation Profile and Researcher Impact

Part 6

Author Carpentry Training

Gail Clement

NSF ICER-1440323
ICER-1343800

http://www.scientificpaperofthefuture.org

∀uthorCarpєntry
RETOOLING AUTHORSHIP,
PUBLISHING, IMPACT & CREDIT

Establishing Your ORCID Profile & Researcher Impact

Gail Clement

Head of Research Services, Caltech Library

http://orcid.org/0000-0001-5494-4806

gperetsm@caltech.edu

AAAI -17 Tutorial | 4 Feb 2017 | San Francisco

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How to build your profile,
establish your reputation,
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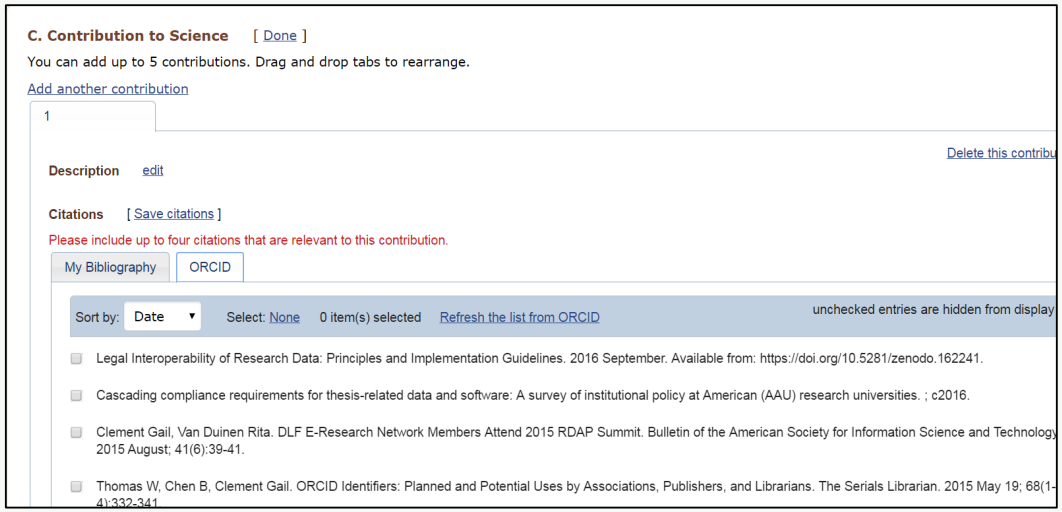
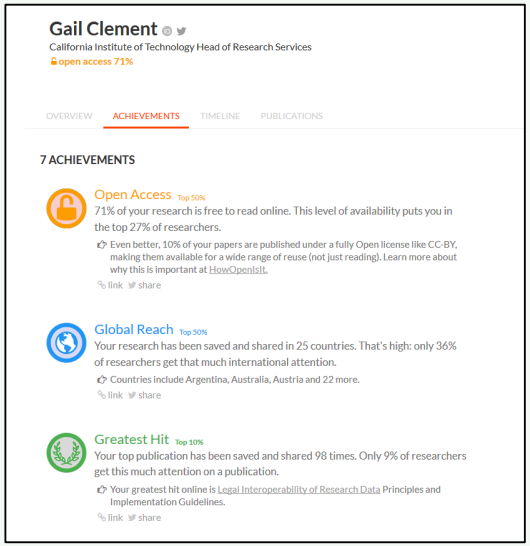
U.S. Funding Agencies – *SciENcv*
Science Experts Network Curriculum Vitae
https://www.ncbi.nlm.nih.gov/sciencv/



Research Institutions or Universities
Researcher Profile Systems,
e.g, VIVO
http://vivoweb.org/

Scholarly Sharing repositories and Researcher Networking Sites
e.g., ImpactStory
https://impactstory.org/



Citation

Surrogate of the work

ORCiD

Creator of work

DOI

Locator of the work

This 5-step lesson teaches how to apply these 3 standards to establish & maintain your scholarly identity and reputation with

Efficiency * Trust * Openness * Sustainability

5 Steps in a Nutshell

1. Start with the citation to a work you have created and link it to a persistent Web-resolvable unique identifier (DOI)
2. Establish your unique identity and authoritative profile with a persistent Web-resolvable unique identifier (ORCiD)
3. Link your works with their DOI's to your ORCiD profile – manually
4. Link your works with their DOI's to your ORCiD profile – automagically
5. Link your ORCiD profile with a scholarly impact service to generate metrics of use and attention

Step 1. Overview

Represent your work as an **open citation** with a **digital object identifier (DOI)** so it is machine readable and actionable

Copyright and Publication Status of Pre-1978 Dissertations: A Content Analysis Approach

Gail Clement and Melissa Levine

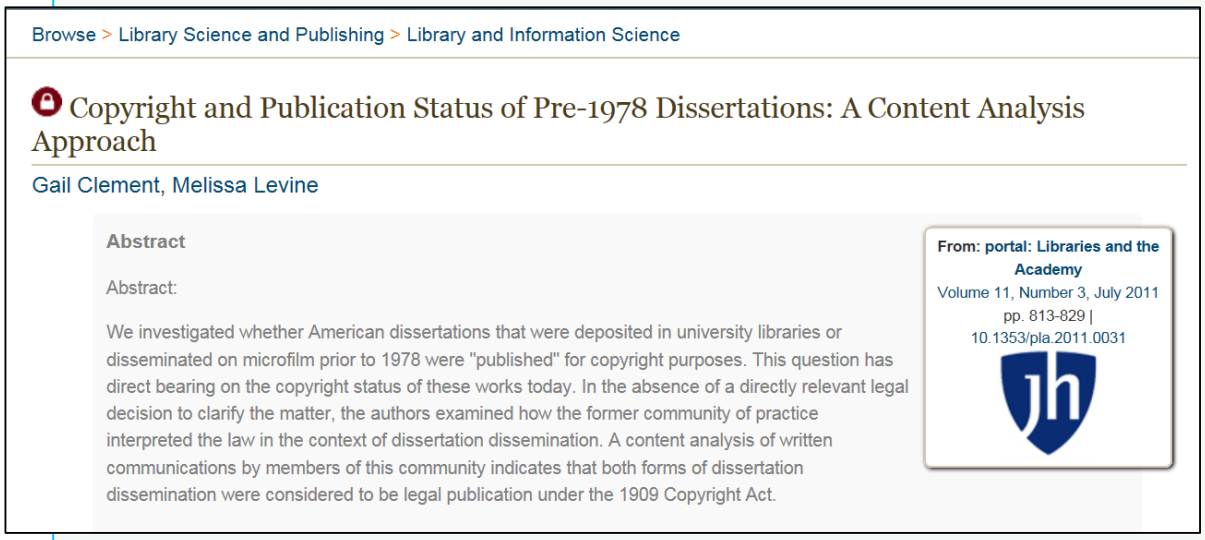
abstract We investigated whether American dissertations that were deposited in university libraries or disseminated on microfilm prior to 1978 were "published" for copyright purposes. This question has direct bearing on the copyright status of these works today. In the absence of a directly relevant legal decision to clarify the matter, the authors examined how the former community of practice interpreted the law in the context of dissertation dissemination. A content analysis of written communications by members of this community indicates that both forms of dissertation dissemination were considered to be legal publication under the 1909 Copyright Act.

Introduction

In this study, we examine the publication and copyright status of American dissertations produced before 1978. Our particular focus is the subset of dissertations that were not distributed through formal channels such as books and journals. Rather, their only means of public access was as typescript copies shelved in the library or as microfilm reproductions available from a third-party distributor. We are interested in this particular set of dissertations because of its potential to yield public domain works, not subject to copyright restrictions and thus suitable for digital access and other scholarly uses. With an estimated 520,000 works in this category, the possibility that some portion could be made available for free public access with relative administrative ease would be a significant boon for digital library development and scholarship across the disciplines.[1]

Why would some mid-20th century dissertations be in the public domain? The answer comes from an understanding of earlier copyright law enacted in 1909 and

portal: Libraries and the Academy, Vol. 11, No. 3 (2011), pp. 813–829.
Copyright ©2011 by The Johns Hopkins University Press, Baltimore, MD 21218.



Browse > Library Science and Publishing > Library and Information Science

Copyright and Publication Status of Pre-1978 Dissertations: A Content Analysis Approach

Gail Clement, Melissa Levine

Abstract

Abstract:

We investigated whether American dissertations that were deposited in university libraries or disseminated on microfilm prior to 1978 were "published" for copyright purposes. This question has direct bearing on the copyright status of these works today. In the absence of a directly relevant legal decision to clarify the matter, the authors examined how the former community of practice interpreted the law in the context of dissertation dissemination. A content analysis of written communications by members of this community indicates that both forms of dissertation dissemination were considered to be legal publication under the 1909 Copyright Act.

From: portal: Libraries and the Academy
Volume 11, Number 3, July 2011
pp. 813-829 |
10.1353/pla.2011.0031

Open Citation 101

scholarly citation data which provides -- in an openly licensed, structured format -- accurate citation information (bibliographic references) harvested from the scholarly literature

Adapted from the Open Citations Project
http://opencitations.net/

@article{Clement_2011, title={Copyright and Publication Status of Pre-1978 Dissertations: A Content Analysis Approach}, volume={11}, ISSN={1530-7131}, url={http://dx.doi.org/10.1353/pla.2011.0031}, DOI={10.1353/pla.2011.0031}, number={3}, journal={portal: Libraries and the Academy}, publisher={Johns Hopkins University Press}, author={Clement, Gail and Levine, Melissa}, year={2011}, pages={813–829}}

DOI 101

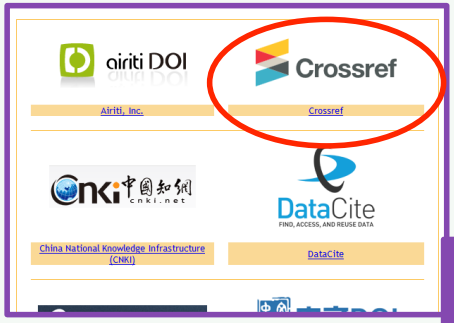
A DOI string will always resolve to a web page containing information about the work

Code '10' assigned to all DOIs by International DOI Federation

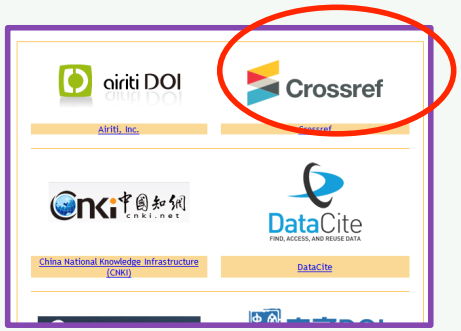
Suffix assigned to the work by its Publisher

https://doi.org/10.1353/pla.2011.0031

Prefix assigned to publisher by DOI Registration Agency



10 DOI Registration Agencies worldwide; CrossRef used for scholarly pubs



https://www.crossref.org/

CrossRef 101

- One of 10 DOI Registration Agencies worldwide
- Most published articles and proceedings get their DOIs from CrossRef
- Conform to all DOI Federation requirements for assigning DOI's *plus*
- They apply additional requirements for metadata deposit and types of works eligible and these can be picky
- They offer free services to find, cite, link and assess scholarly works

Step 1 to do

```
$ curl -LH "Accept: text/bibliography; style=bibtex"
https://doi.org/10.1353/pla.2011.0031 >
clement2011.bib
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Step 1 to do

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Publication Status of Pre-1978 Dissertations: A Content
Analysis Approach}, volume={11}, ISSN={1530-7131},
url={http://dx.doi.org/10.1353/pla.2011.0031},
DOI={10.1353/pla.2011.0031}, number={3},
journal={portal: Libraries and the Academy},
publisher={Johns Hopkins University
 Press}, author={Clement, Gail and Levine, Melissa},
year={2011}, pages={813–829}}
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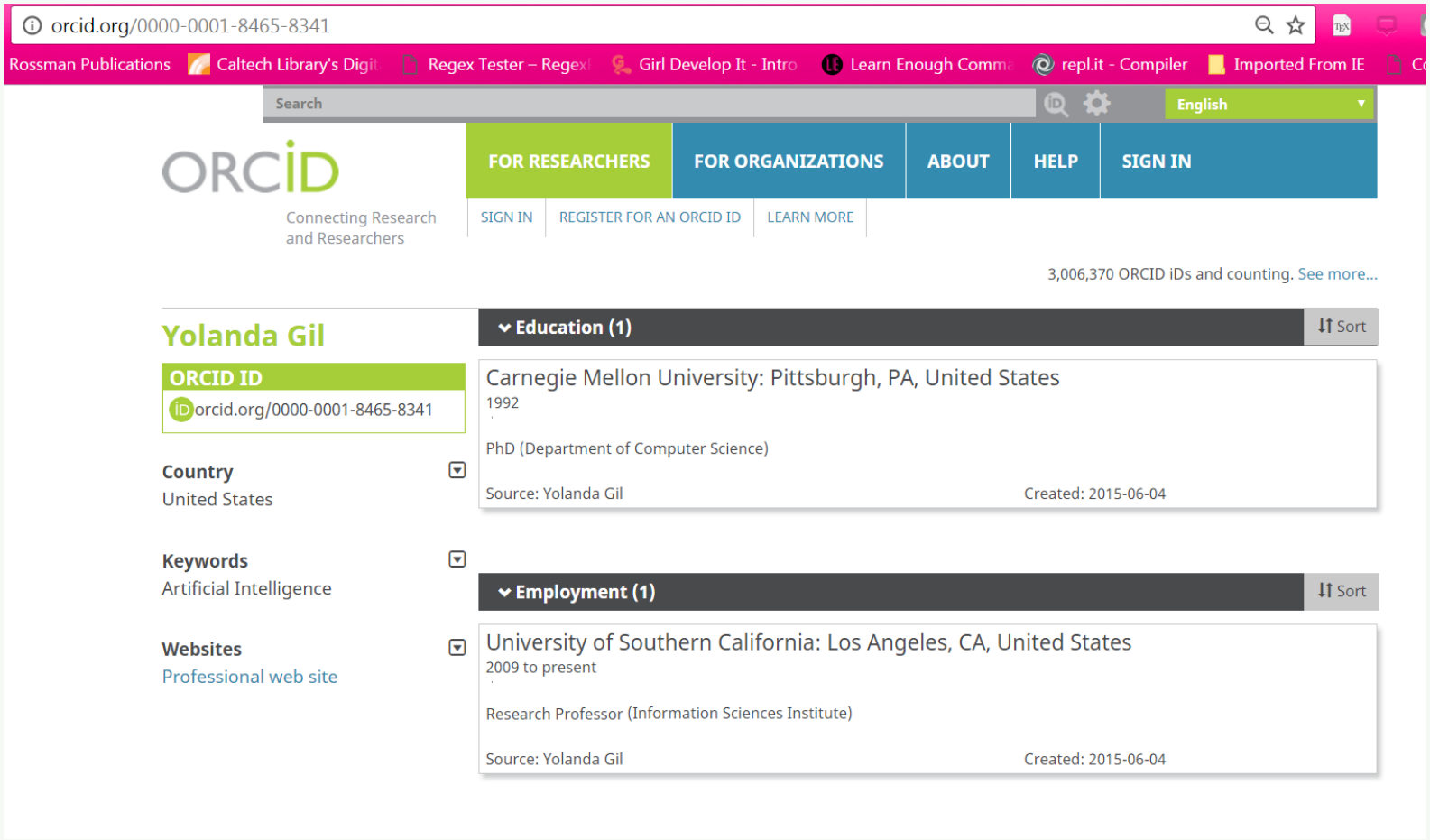
Step 2. Overview

Represent your identity as a unique number using ORCiD so it is machine readable and actionable

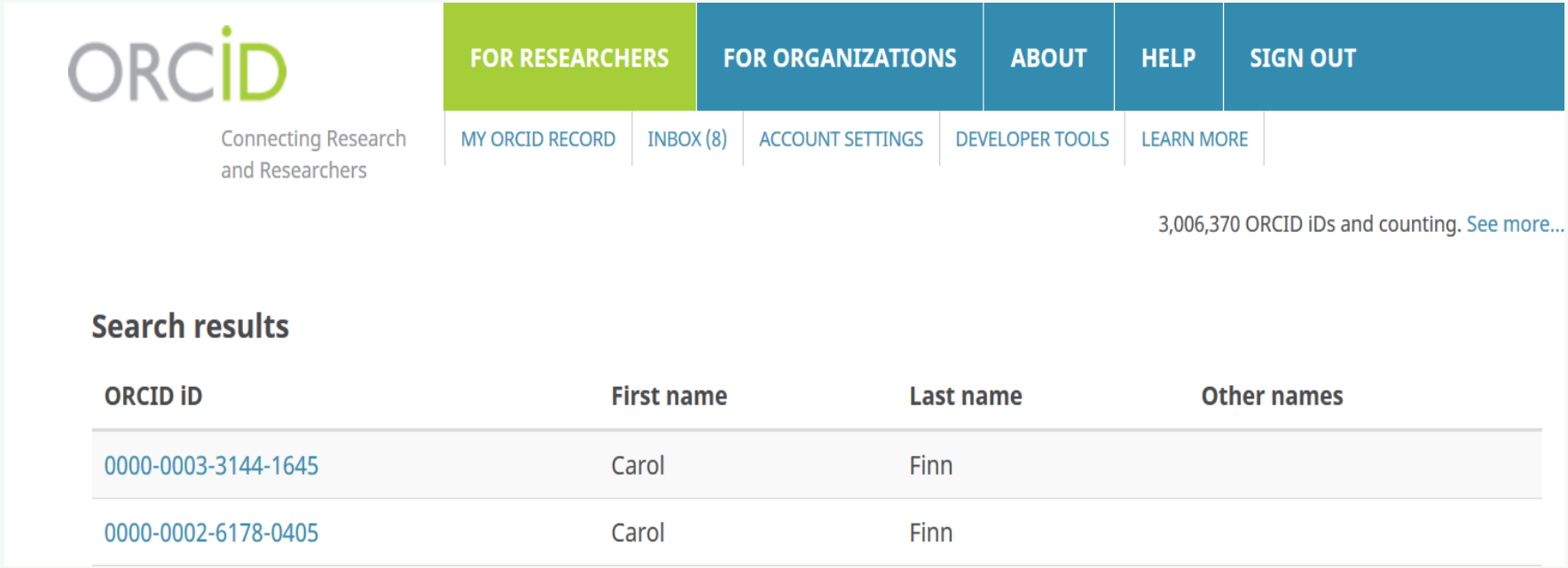


ORCiD 101

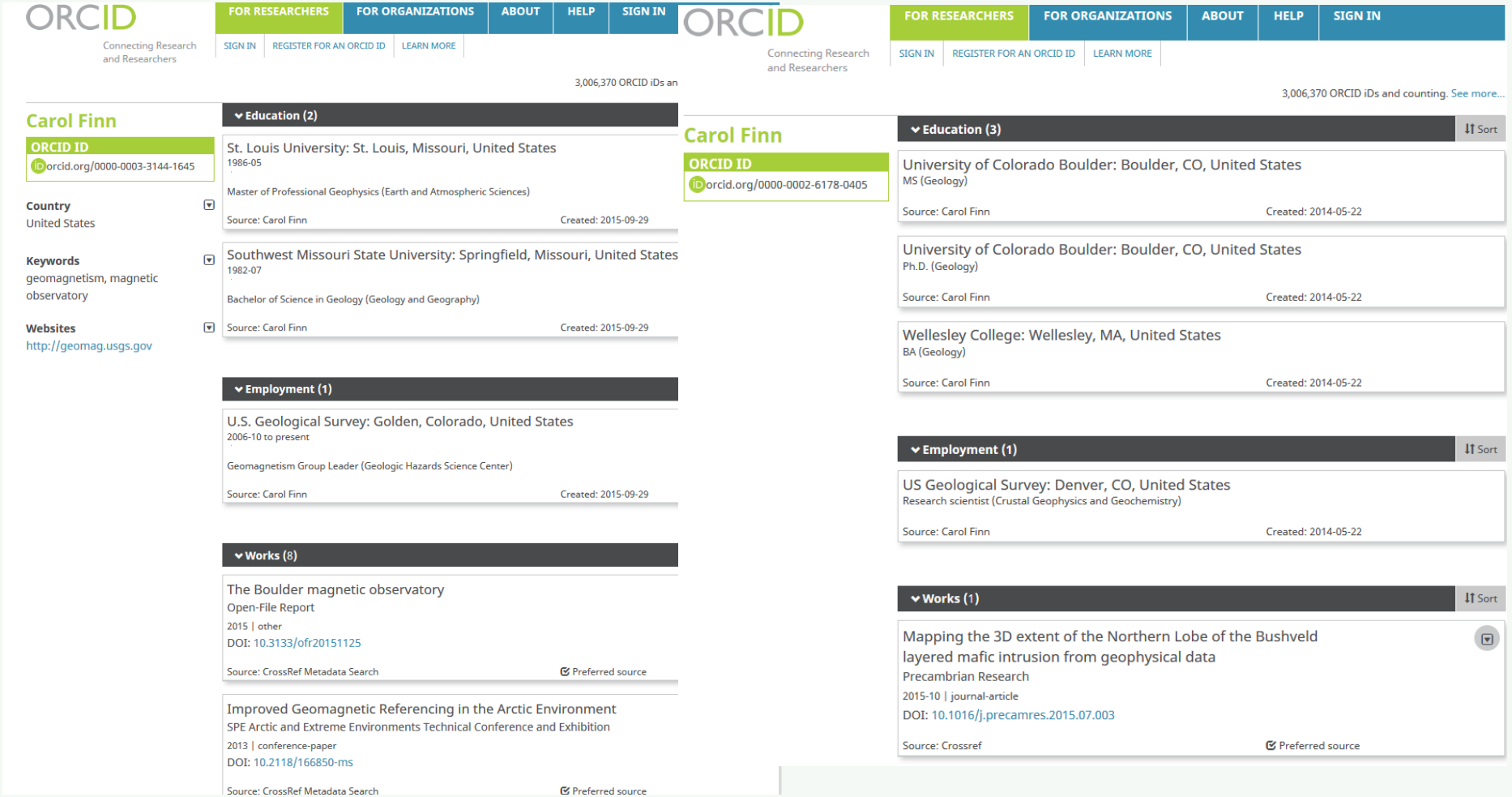
- Open Researcher and Contributor ID (ORCID) is three things:
  (1) A membership organization; (2) a standard; (3) a profile system
- The non-profit, membership organization to solving the long-standing name ambiguity problem in scholarly communication
- The profile system maintains a central registry of unique identifiers for individual researchers
- The system supports an open, transparent linking mechanism between ORCID and other current author identifier schemes (ISO's International Standard Name Identifier (ISNI);Thomson Reuter's ResearcherID; Elsevier's SCOPUS ID)
- The ORCID itself is a unique,16-digit identifier expressed a URL link. i.e. **http://orcid.org/5412-3652-8965-8745**
- The ORCID URL links to the owner's profile on the ORCID website.

ORCiD 101

ORCiD == Online Research Contributor iD ==
Global standard that solves Author Name Ambiguity Problems



ORCiD 101


ORCID
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FOR RESEARCHERS
FOR ORGANIZATIONS
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HELP
SIGN IN
SIGN IN
REGISTER FOR AN ORCID ID
LEARN MORE
3,006,370 ORCID iDs an
Carol Finn
ORCID ID
orcid.org/0000-0003-3144-1645
Country
United States
Keywords
geomagnetism, magnetic observatory
Websites
http://geomag.usgs.gov
Education (2)
St. Louis University: St. Louis, Missouri, United States
1986-05
Master of Professional Geophysics (Earth and Atmospheric Sciences)
Source: Carol Finn
Created: 2015-09-29
Southwest Missouri State University: Springfield, Missouri, United States
1982-07
Bachelor of Science in Geology (Geology and Geography)
Source: Carol Finn
Created: 2015-09-29
Employment (1)
U.S. Geological Survey: Golden, Colorado, United States
2006-10 to present
Geomagnetism Group Leader (Geologic Hazards Science Center)
Source: Carol Finn
Created: 2015-09-29
Works (8)
The Boulder magnetic observatory
Open-File Report
2015 | other
DOI: 10.3133/ofr20151125
Source: CrossRef Metadata Search
Preferred source
Improved Geomagnetic Referencing in the Arctic Environment
SPE Arctic and Extreme Environments Technical Conference and Exhibition
2013 | conference-paper
DOI: 10.2118/166850-ms
Source: CrossRef Metadata Search
Preferred source
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Connecting Research and Researchers
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ABOUT
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REGISTER FOR AN ORCID ID
LEARN MORE
3,006,370 ORCID iDs and counting. See more...
Carol Finn
ORCID ID
orcid.org/0000-0002-6178-0405
Education (3)
Sort
University of Colorado Boulder: Boulder, CO, United States
MS (Geology)
Source: Carol Finn
Created: 2014-05-22
University of Colorado Boulder: Boulder, CO, United States
Ph.D. (Geology)
Source: Carol Finn
Created: 2014-05-22
Wellesley College: Wellesley, MA, United States
BA (Geology)
Source: Carol Finn
Created: 2014-05-22
Employment (1)
Sort
US Geological Survey: Denver, CO, United States
Research scientist (Crustal Geophysics and Geochemistry)
Source: Carol Finn
Created: 2014-05-22
Works (1)
Sort
Mapping the 3D extent of the Northern Lobe of the Bushveld layered mafic intrusion from geophysical data
Precambrian Research
2015-10 | journal-article
DOI: 10.1016/j.precamres.2015.07.003
Source: Crossref
Preferred source

More and More Publishers Requiring ORCID iDs

American Chemical Society
eLife
PLOS
The Royal Society
American Geophysical Union & Wiley generally
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Faculty of 1000
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Author Name Ambiguity Problems

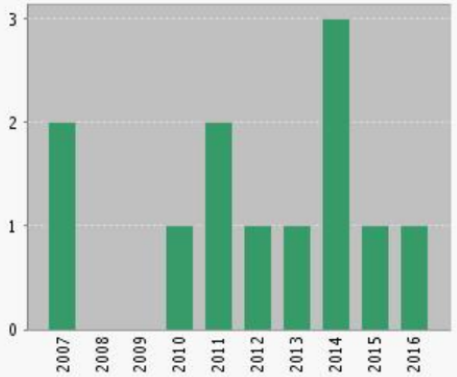
Citation Report: 12

(from Web of Science Core Collection)

You searched for: **AUTHOR:** (finn carol) **...More**

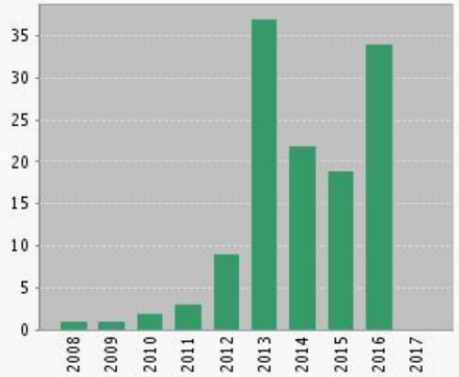
This report reflects citations to source items indexed within Web of Science Core Collection. Perform a Cited Reference Search to include citations to items not indexed within Web of Science Core Collection.

Published Items in Each Year



The latest 20 years are displayed.

Citations in Each Year



The latest 20 years are displayed.

Results found:	12
Sum of the Times Cited [?] :	128
Sum of Times Cited without self-citations [?] :	122
Citing Articles [?] :	118
Citing Articles without self-citations [?] :	113
Average Citations per Item [?] :	10.67
h-index [?] :	4

Is this Author getting credit where due?

Is this Author self-citing her own work?

Is this Author accruing accurate citation metrics?

Is this Author editing or reviewing her own papers?

Is this researcher double-dipping across funding agencies?

Step 2 to do

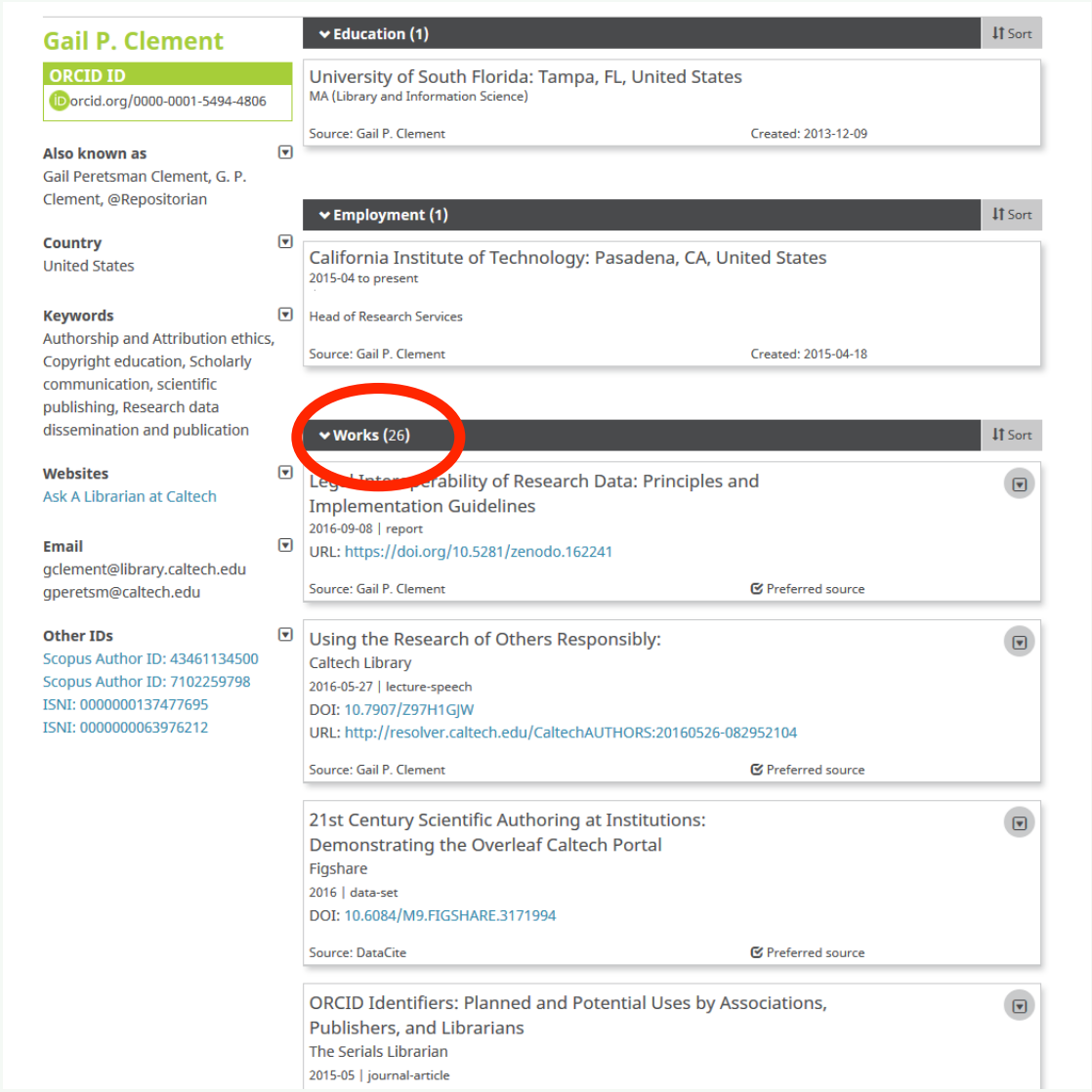
Point your browser to https://orcid.org/

Click on Register now! to sign up with your email

Check your email and click through the link provided

Steps 3 + 4 Overview

Connect your citations with DOIs to your ORCiD works

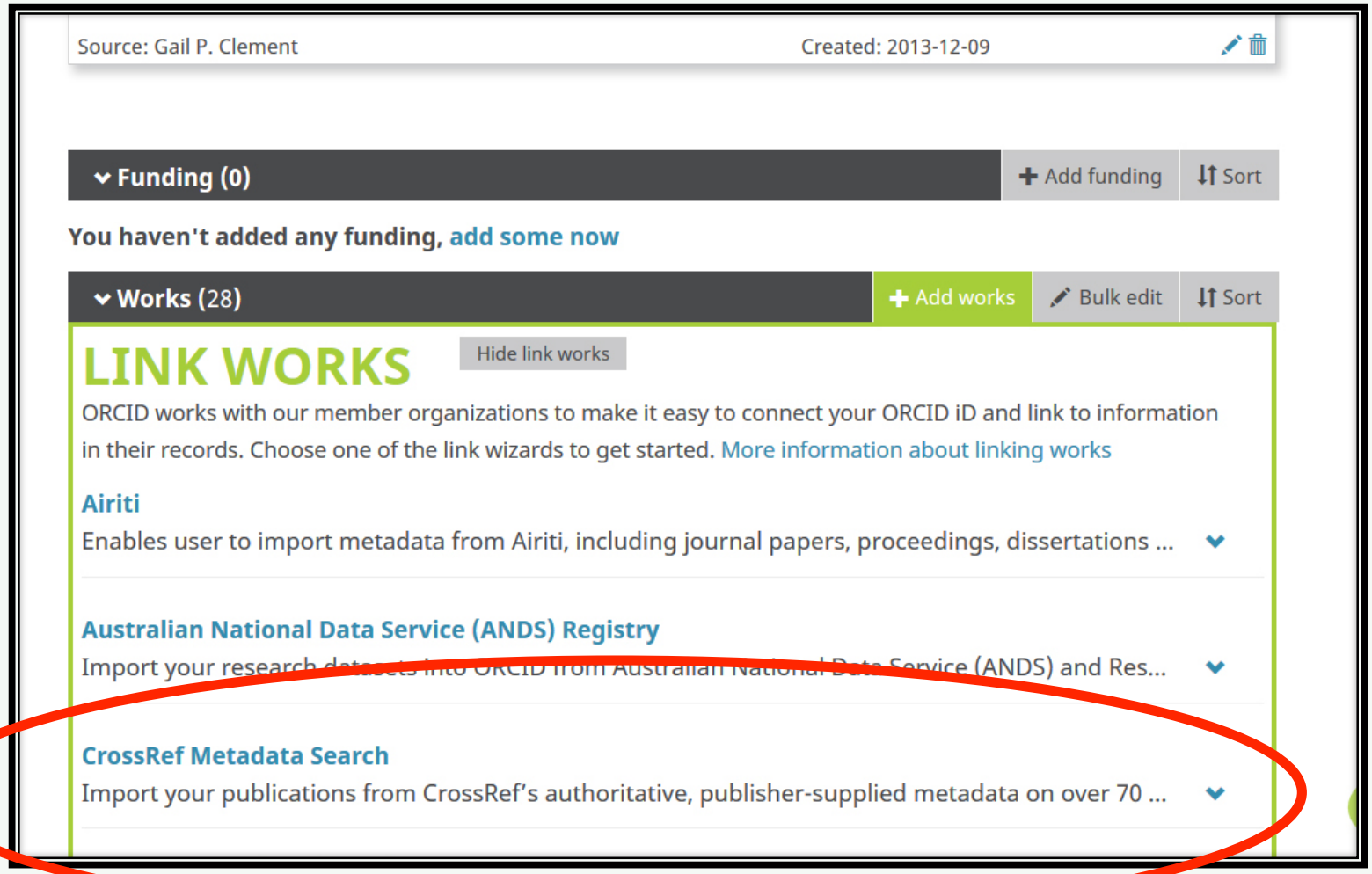


Step 3 to do

Connect your citations with DOIs to your ORCiD works, manually

Step 4 to do

Connect your citations with DOIs to your ORCiD works, auto-magically



Step 4 to do

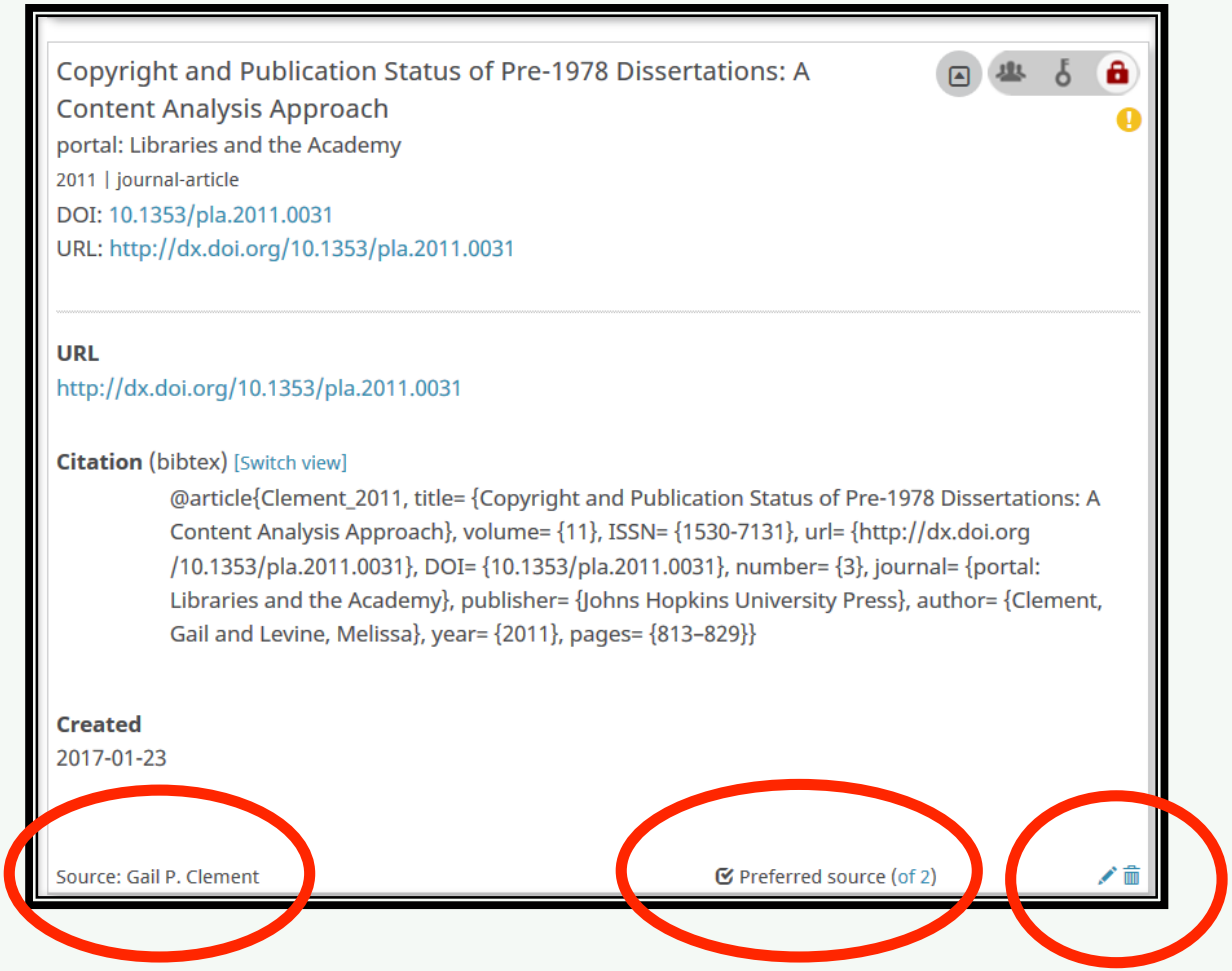

ORCID
Gail P. Clement
http://orcid.org/0000-0001-5494-4806
(Not You?)
CrossRef Metadata Search
has asked for the following access to your ORCID Record
Add works
Read your ORCID record
This application will not be able to see your ORCID password, or other private info in your ORCID Record. Privacy Policy.
Deny
Authorize

Step 4 to do


Crossref
Gail Clement
Status
API
Help
Gail Clement
TYPE
Journal Article (2,346)
YEAR
2011 (2,346)
PUBLICATION
PLoS ONE (41)
Physics Letters B (36)
Journal of High Energy Physics (35)
Physical Review Letters (34)
Cancer Research (17)
The European Physical Journal C (17)
Physical Review D (15)
ChemInform (11)
Genetic Engineering & Biotechnology News (11)
SORT BY: RELEVANCE PUBLICATION YEAR
PAGE 1 OF 2,346 RESULTS
Copyright and Publication Status of Pre-1978 Dissertations: A Content Analysis Approach
Journal Article published 2011 in portal: Libraries and the Academy volume 11 issue 3 on pages 813 to 829
Authors: Gail Clement, Melissa Levine
https://doi.org/10.1353/pla.2011.0031
Actions
IN YOUR PROFILE
The Basis of Differential Responses to Folic Acid Supplementation
Journal Article published 2011 in Journal of Nutrigenetics and Nutrigenomics volume 4 issue 2 on pages 99 to 109
Authors: Ioana Cotlarciuc, Toby Andrew, Tracy Dew, Gail Clement, Raj Gill, Gabriela Surdulescu, Roy Sherwood, Kourosh R. Ahmadi
https://doi.org/10.1159/000327768
Actions
ADD TO ORCID

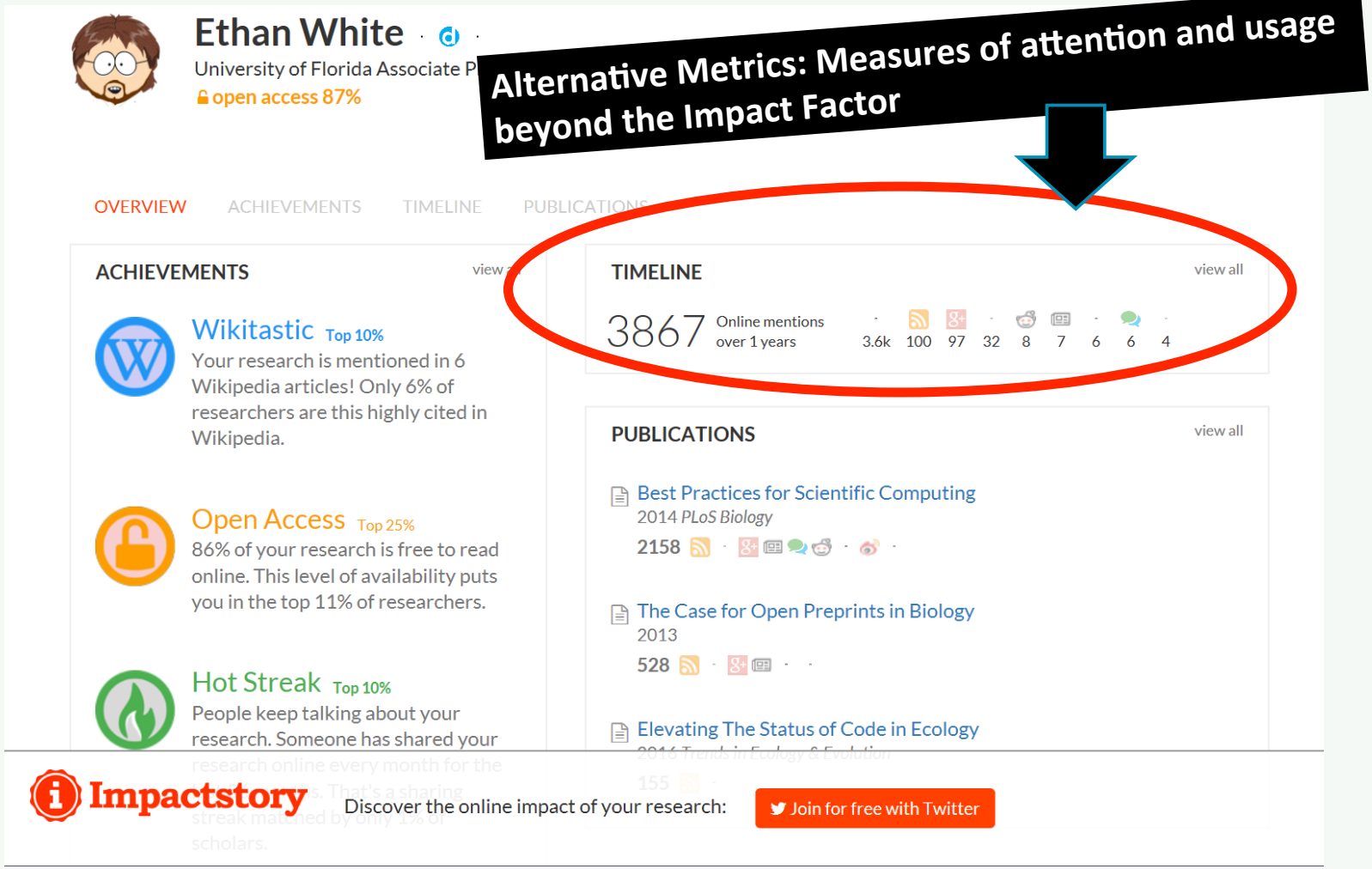
Step 4 to do

Manage duplicate entries in your ORCiD works



Step 5 Overview

Connect your citations, DOI's and ORCiD profile to a scholarly impact service to generate metrics



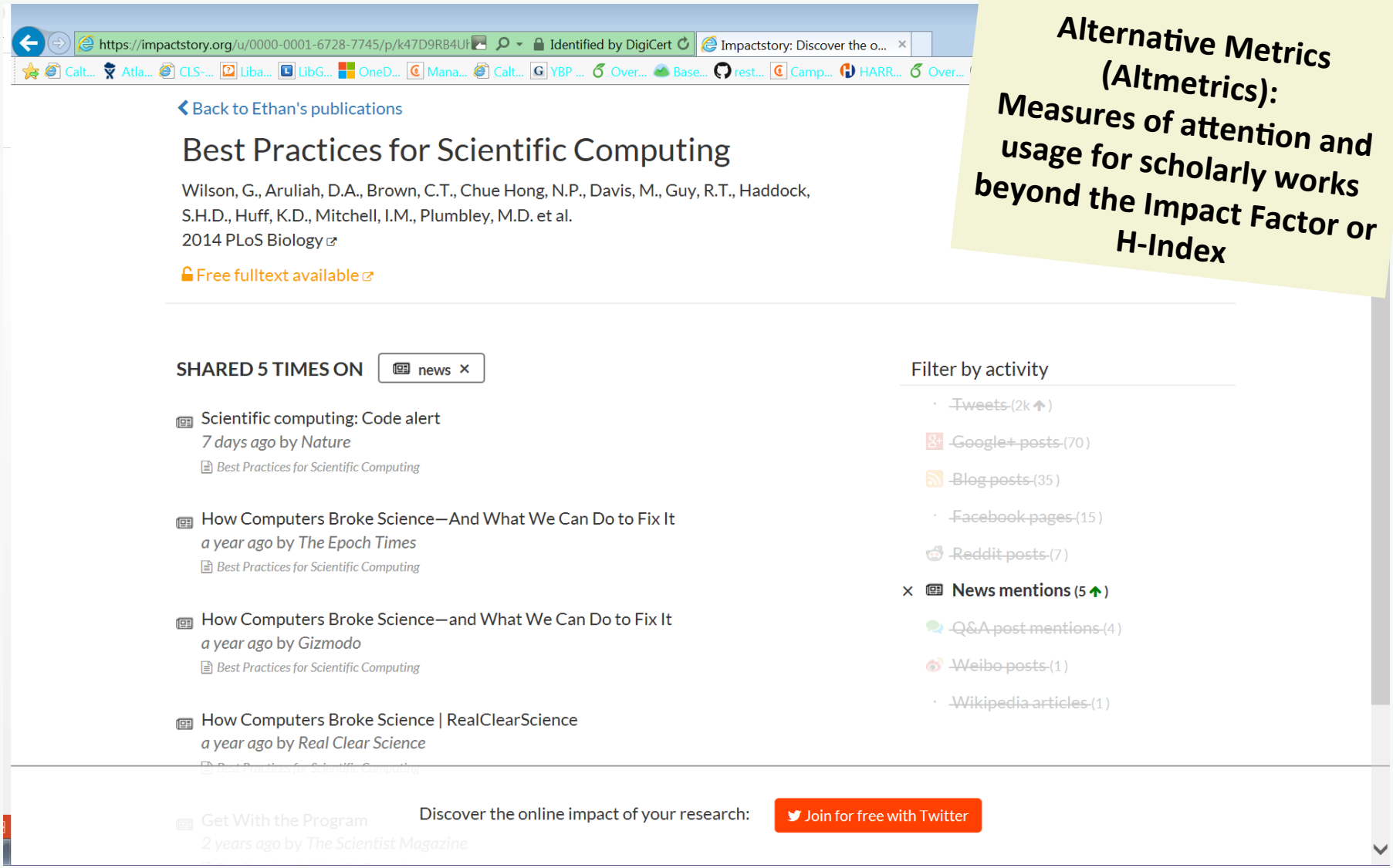
https://www.impactstory.org/

ImpactStory 101

- A non-profit web service by and for researchers
- Provides alternative measures of attention and usage for scholarly works ("Altmetrics")
- Awarded a $297,500 EAGER grant from the National Science Foundation to study how automatically-gathered impact metrics can improve the reuse of research software.
- Integrates with ORCiD for citation and author data 
- Integrates with Elsevier/SCOPUS for citation data 

Step 5 Overview

Alternative Metrics (Altmetrics): Measures of attention and usage for scholarly works beyond the Impact Factor or H-Index

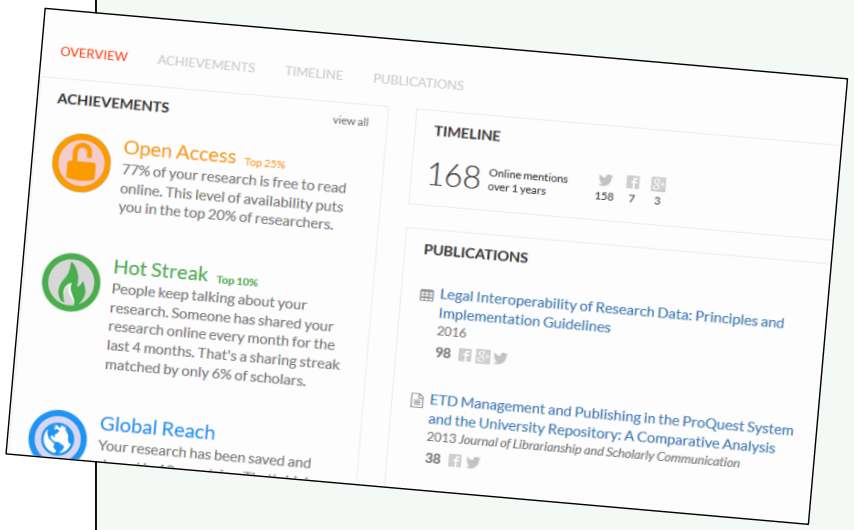


Step 5 to do

Point your browser to https://impactstory.org

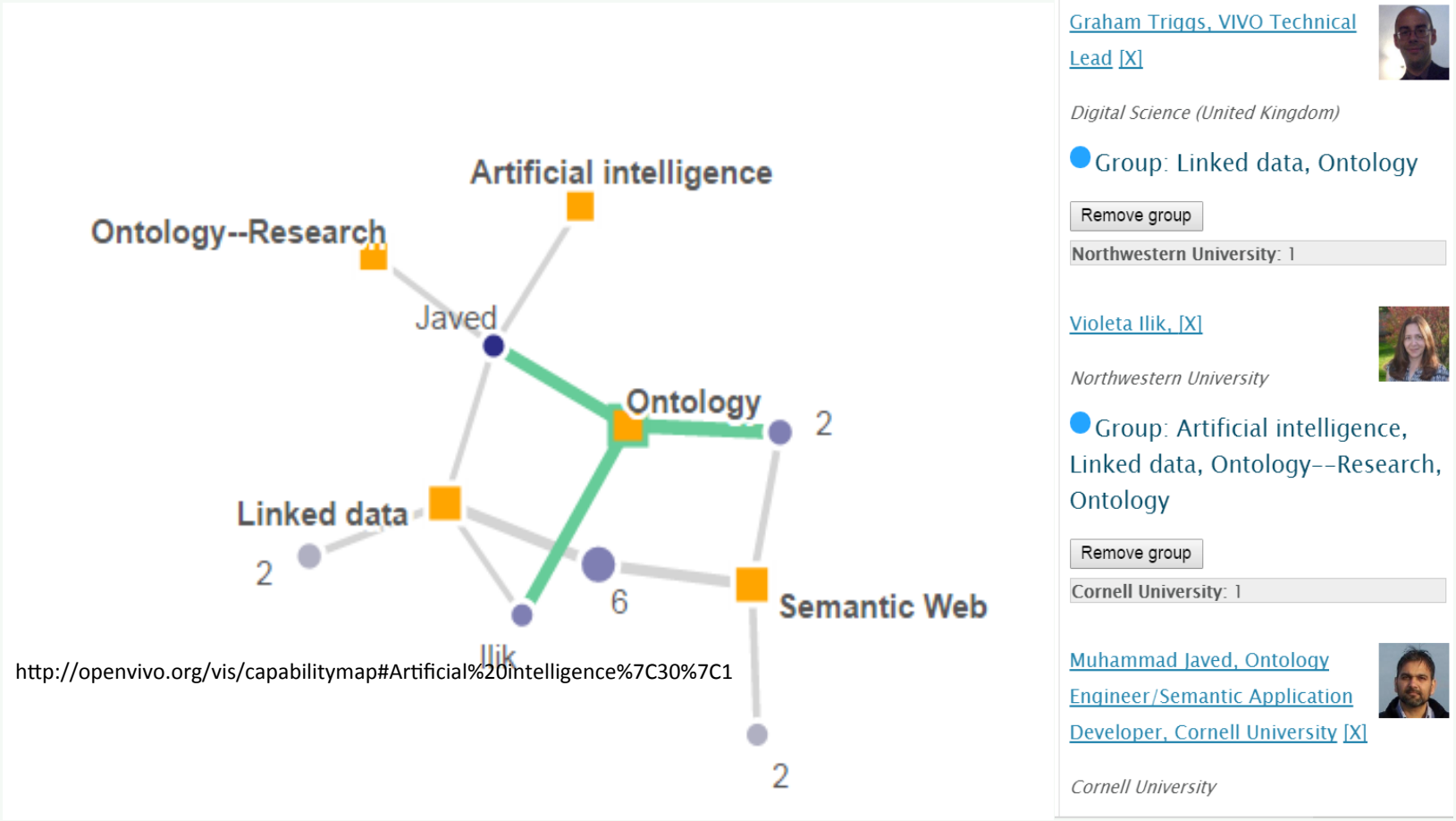
Click Login to sign up with your ORCiD

Voila! Watch your impact profile auto-populate thanks to linkages between those 3 standards (citation, DOI, ORCiD)



Next Steps?

Explore what other linkages and networks
you can generate with your 3 linked data building blocks



Welcome back, Gail Clement

OpenVIVO has found works for you to claim. For each work, you will have an opportunity to indicate your role in the work.

There are 3 works to claim.

Click the "Claim these works" to claim the works. Click Cancel if you do not wish to claim works at this time.

Claim these works Cancel

21st Century Scientific Authoring at Institutions: Demonstrating the Overleaf Caltech Portal
2016;
Miller, S ; **Clement, G**

- Unlisted Author
- Editor
- Other Contribution

Please indicate the contribution that you made to this work

Hide roles

Author

- Writing Original Draft
- Figure Development
- Editing and Proofreading
- Translator
- Background and Literature Search
- Conceptualization

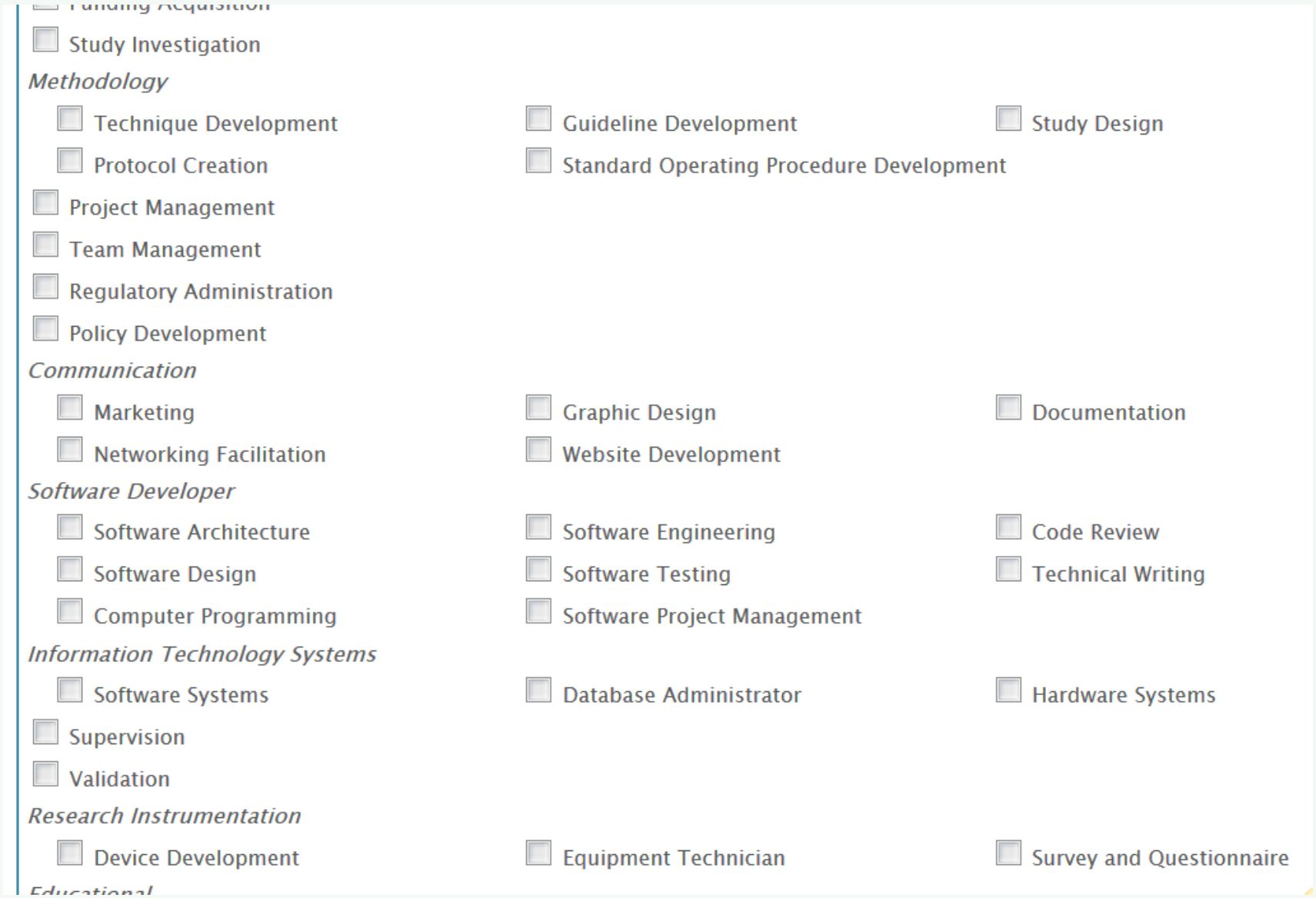
Preservation

- Archivist
- Digital Preservation

Data

- Data Curation
- Data Analysis
- Data Integration
- Metadata Application
- Statistical Data Analysis
- Data Quality Assurance
- Data Entry
- Data Collection
- Data Modeling

VIVO applies the Contributor Role taxonomy developed through Project CRediT



VIVO applies the Contributor Role taxonomy developed through Project CRediT

Recommended Resources

AuthorCarpentry | https://authorcarpentry.github.io

Contributor Roles Taxonomy (Project CRedIT) | http://docs.casrai.org/CRediT

CrossRef DOI Registration Agency | https://corssref.org/

CrossRef API Documentation | https://github.com/CrossRef/rest-api-doc/blob/master/rest_api.md

DOI Federation | https://www.doi.org/

ImpactStory | https://impactstory.org

Laure Haak's ORCiD Blog – Publishers Starting to Require ORCiDs, Jan 7, 2016
https://orcid.org/blog/2016/01/07/publishers-start-requiring-orcid-ids

Open Citations Project, http://opencitations.net/

SciENcv, National Library of Medicine, https://www.ncbi.nlm.nih.gov/sciencv/

SciENcv: Integrating with ORCID (video demo) https://www.youtube.com/watch?v=G_cKSRr7TJ4&feature=youtu.be

"Scientists Your Number is up". *Nature News* 485(7400) May 30 2012
http://www.nature.com/news/scientists-your-number-is-up-1.10740

VIVO Scholarly Networking System | http://vivoweb.org/


Thank you!
∀uthor ℂarp∈ntry

The Scientific Paper of the Future: An Author Checklist

OntoSoft Training

Part 7

http://dx.doi.org/10.5281/zenodo.15920

http://www.scientificpaperofthefuture.org

NSF ICER-1440323
ICER-1343800

What is a Scientific Paper of the Future

- **Data**: Available in a public repository, including documentation (metadata), a clear license specifying conditions of use, and citable using a unique and persistent identifier.
- **Software**: Available in a public repository, with documentation (metadata), a license for reuse, and citable using a unique persistent identifier.
  - Not only major software used, but also other ancillary software for data reformatting, data conversions, data filtering, and data visualization.
- **Provenance**: Documented for all results by explicitly describing the series of computations and their outcome with a provenance record of the execution traces and a workflow sketch (or formal workflow)
  - Possibly in a shared repository and with a unique and persistent identifier.

Scientific Paper of the Future

Modern Paper

Text:
Narrative of the method, some data is in tables, figures/plots, and the software used is mentioned

Data:
Include data as supplementary materials and pointers to data repositories

Open Science

Sharing:
Deposit data and software (and provenance/workflow) in publicly shared repositories

Open licenses:
Open source licenses for data and software (and provenance/workflow)

Metadata:
Structured descriptions of the characteristics of data and software (and provenance/workflow)

Reproducible Publication

Software:
For data preparation, data analysis, and visualization

Provenance and methods:
Workflow/scripts specifying dataflow, codes, configuration files, parameter settings, and runtime dependencies

Digital Scholarship

Persistent identifiers:
For data, software, and authors (and provenance/workflow)

Citations:
Citations for data and software (and provenance/workflow)

Review of Best Practices: Author Checklist

1. Data accessibility
2. Data documentation
3. Software accessibility
4. Software documentation
5. Provenance documentation
6. Methods documentation
7. Authors identification

1 Data accessibility

Simplest Approach

1. **Create a public entry for your dataset with a persistent unique identifier**
   - Go to a domain repository (use a general repository, e.g.., zenodo.org, if you cannot find one), create an account
   - Create an entry for your dataset
2. **Specify the metadata**
   - Including license -- choose from http://www.creativecommons.org/licenses
3. **Upload/point to the data**

Voilà! The repository will give you a data citation

1 Data accessibility

Ideal Approach

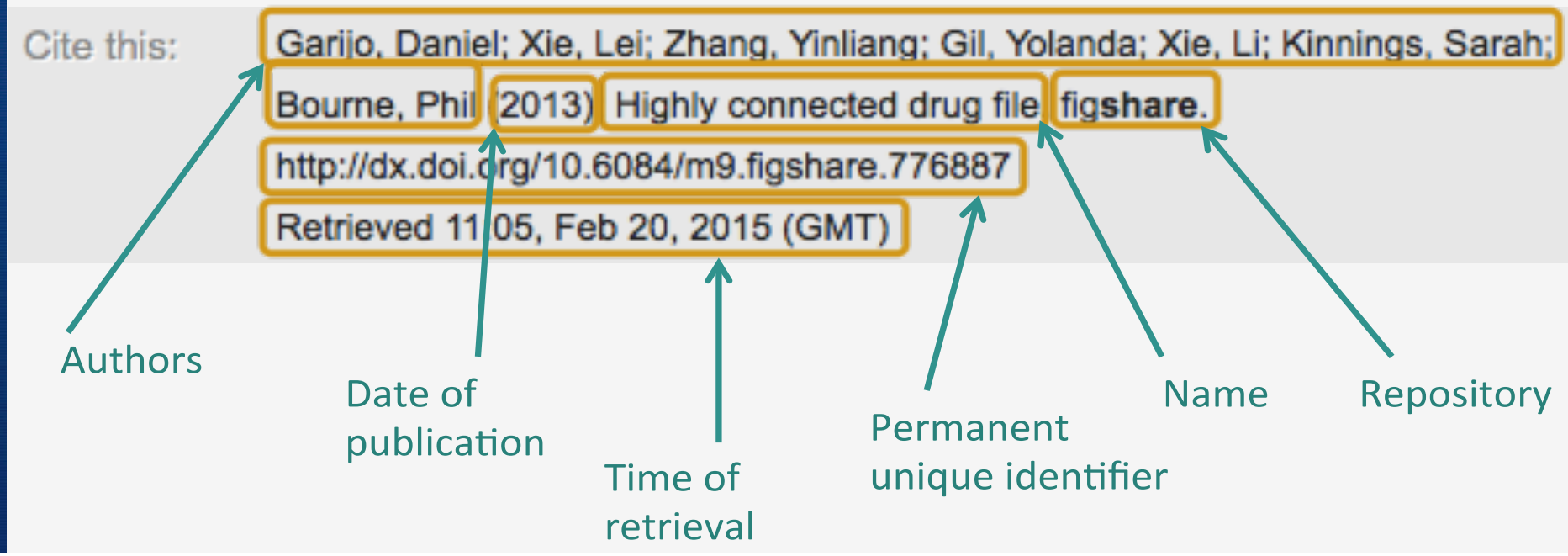
1. Find a repository that your community uses, if there is not one then organize one!
2. Create a public entry for your dataset with a persistent unique identifier
   - Create an entry for your dataset
3. Specify the metadata required by that repository using metadata standards for that community
   - Including license -- choose from http://www.creativecommons.org/licenses
4. Upload/point to the data
5. Get a data citation from the repository

1 Data accessibility

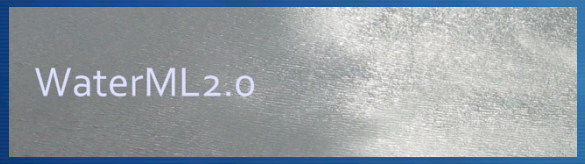
What to Show in the Paper

- ★ Cite each of your datasets like you would cite another paper
- ★ Citation includes publication date, date of retrieval, repository, and persistent identifier
- ★ If there is a data paper, cite it

Data Citation Format



ISO 19115



2 Data documentation

Simplest Approach

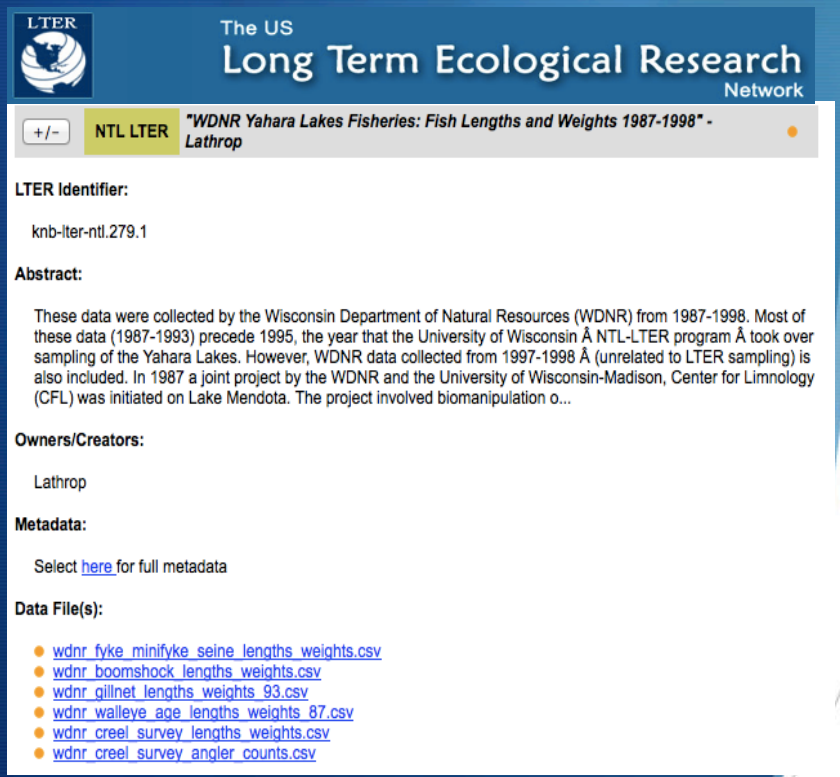
- ★ Datasets should have general-purpose metadata specified (creator, date, name, etc.)

Ideal Approach

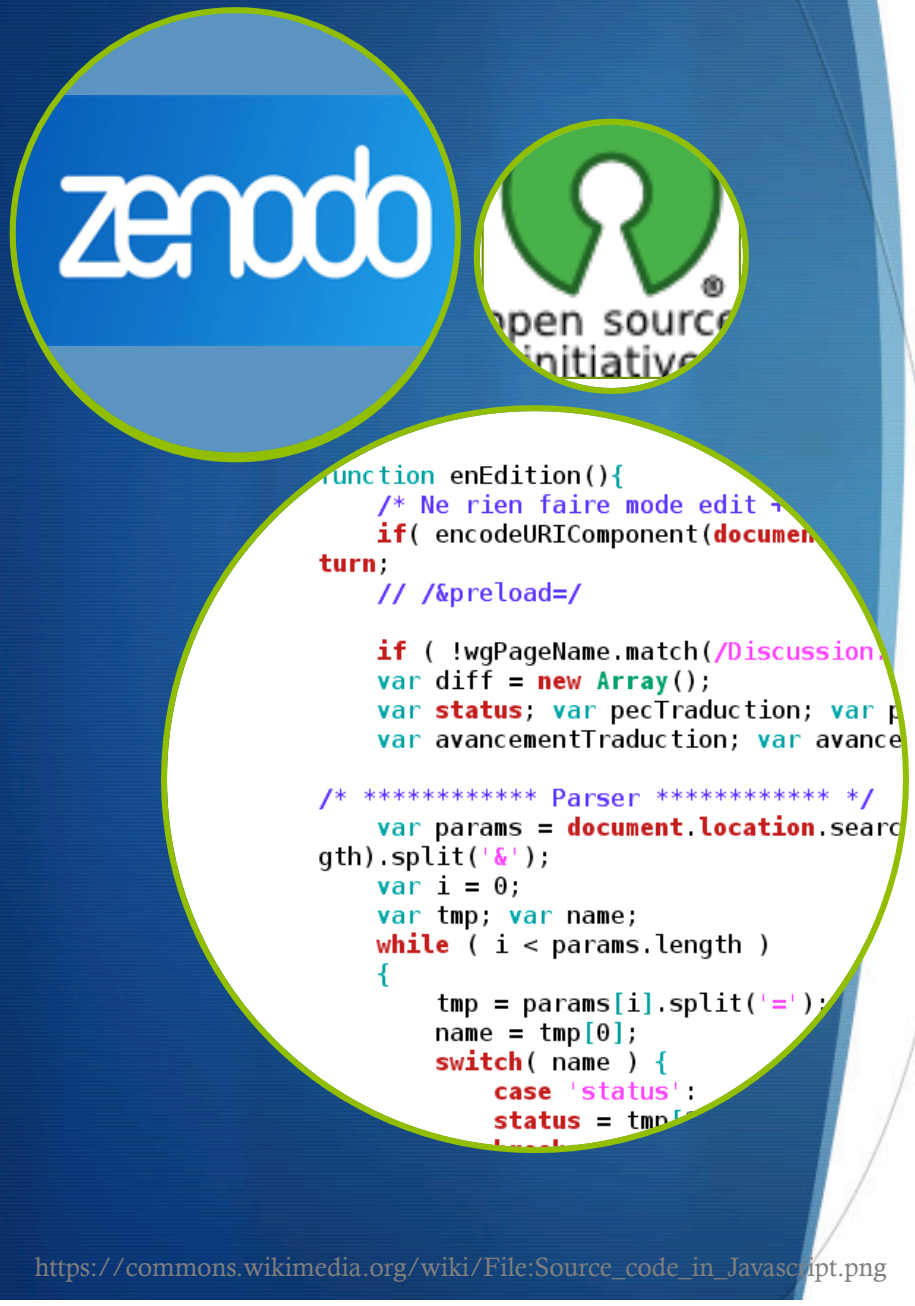
- ★ Dataset characteristics should be explained in detail
- ★ Domain-specific metadata should be documented
- ★ Availability of related datasets should be documented

2 Data documentation

What to Show in the Paper



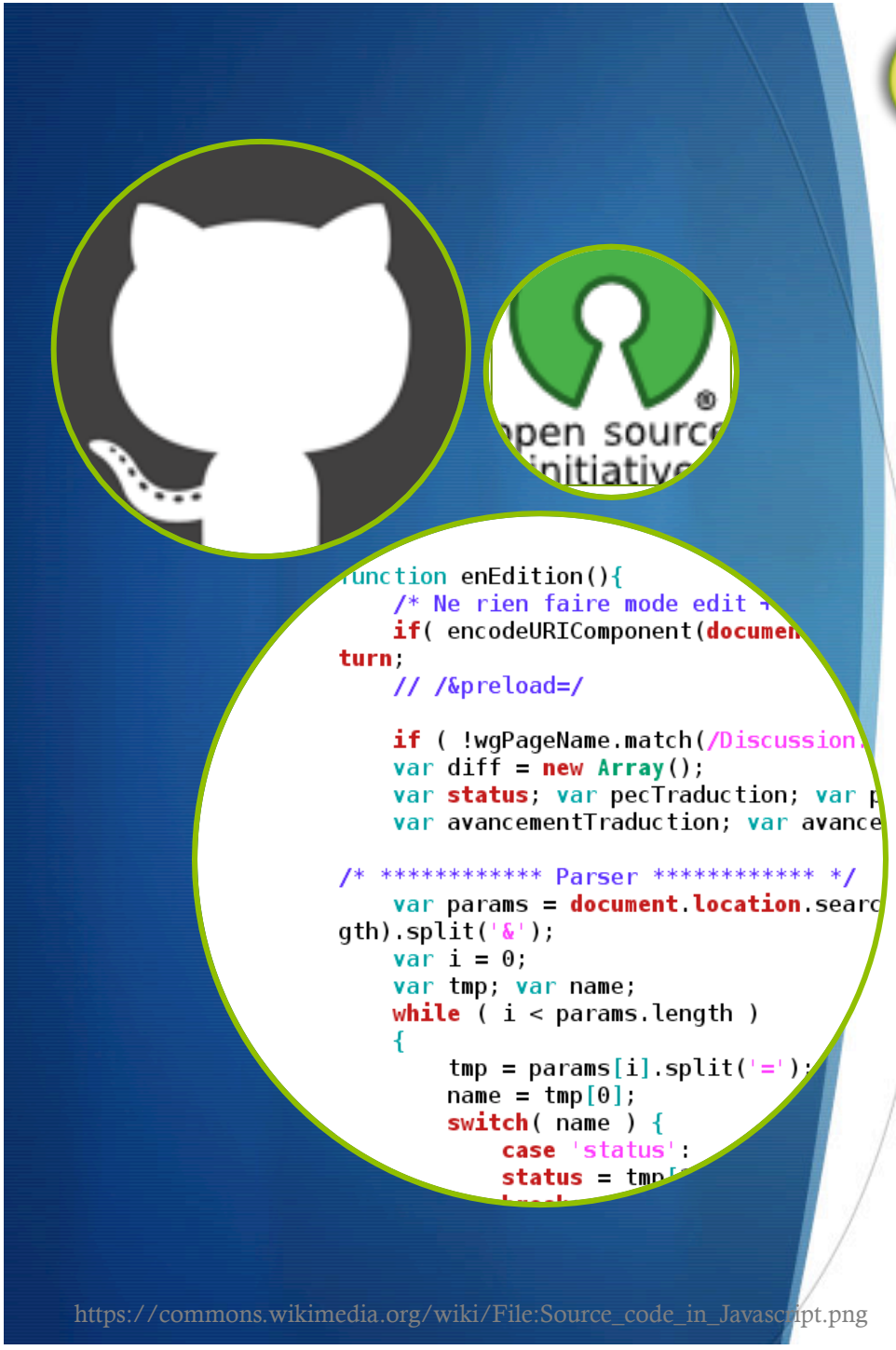
- ★ Mention that the persistent identifier for your data has pointers to its metadata and includes a detailed description of the data
- ★ Optionally, include the metadata also as supplemental material
- ★ If there is a data paper, cite it



https://commons.wikimedia.org/wiki/File:Source_code_in_Javascript.png

Simplest Approach

1. Create a public entry for your software with a persistent unique identifier
   - Upload to a data repository (e.g., Zenodo) as you would data, and get a DOI
     - Or post on your web site and use a PURL
2. Specify basic metadata
   - Including license -- choose from http://opensource.org/licenses, preferably Apache v2.0
3. Specify desired citation



https://commons.wikimedia.org/wiki/File:Source_code_in_Javascript.png

3 Software accessibility

Ideal Approach

1. Learn to use a code repository that allows version tracking and collaborative software development
   - GitHub, BitBucket, etc.
2. Create a public entry for your software with a persistent unique identifier
3. Specify the metadata
   - Including license -- choose from http://opensource.org/licenses, preferably Apache v2.0
4. Specify desired citation

3 Software accessibility

What to Show in the Paper

- Cite each piece of software that you use (preparation, analysis, visualization) like you would cite another paper
  - Citation similar to data but includes software version
- If there is a software paper, cite it

Software Citation Format

Garijo, Daniel;Xie, Lei; Zhang, Yinliang; Gil, Yolanda; Xie, Li (2013) Tool for computing anomalies, GitHub. V.1 http://dx.doi.org/10.5281/zenodo.18765 Retrieved 11:05, Feb, 15, 2015 (GMT)

Authors

Date of publication

Time of retrieval

Permanent unique identifier

Name

Repository

Version

4 Software documentation

Simplest Approach

1. Describe as much metadata as you can in your software site
    1. Document the basic metadata discussed earlier
    2. If you use a code repository, there is some basic structure you can follow

Ideal Approach

1. Use software registry
   - http://www.ontosoft.org/portal, csdms.colorado.edu, etc.
   - Guides through questions to provide metadata
2. Save the metadata as HTML, XML,…
3. Post the metadata on your code site

4 Software documentation

What to Show in the Paper

- ★ Mention that the persistent identifier location for your software points to its metadata
- ★ Optionally, include the software metadata as supplemental material
- ★ If there is a software paper, cite it

PIHM [Christopher Duffy]

Identify

Locate - Unique description

What is the software called ?

- PIHM

What is a short description for this software ?

- PIHM is a multiprocess, multi-scale hydrologic model where the major hydrological processes are fully coupled using the semi-discrete finite volume method. PIHM is a physical model for surface and groundwater, â€œtightly-coupledâ€ to a GIS interface. PIHMgis which is open source, platform independent and extensible. The tight coupling between GIS and the model is achieved by developing a shared data-model and hydrologic-model data structure.

  Initial metadata was retrieved from http://csdms.colorado.edu/wiki/Model:PIHM

What are general categories (keywords, labels) for this software ?

- Hydrology
- Basins
- Continental

Is there a project website for the software ?

- http://www.pihm.psu.edu/pihm_home.html

Understand

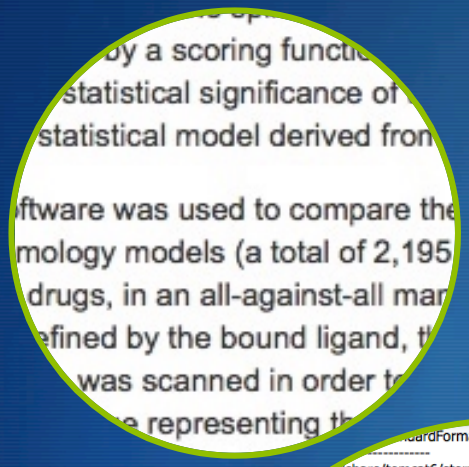
Trust - Quality and ratings

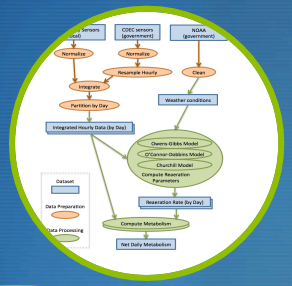
Who created this software? (Project, Organization, Person, Initiative, etc.)

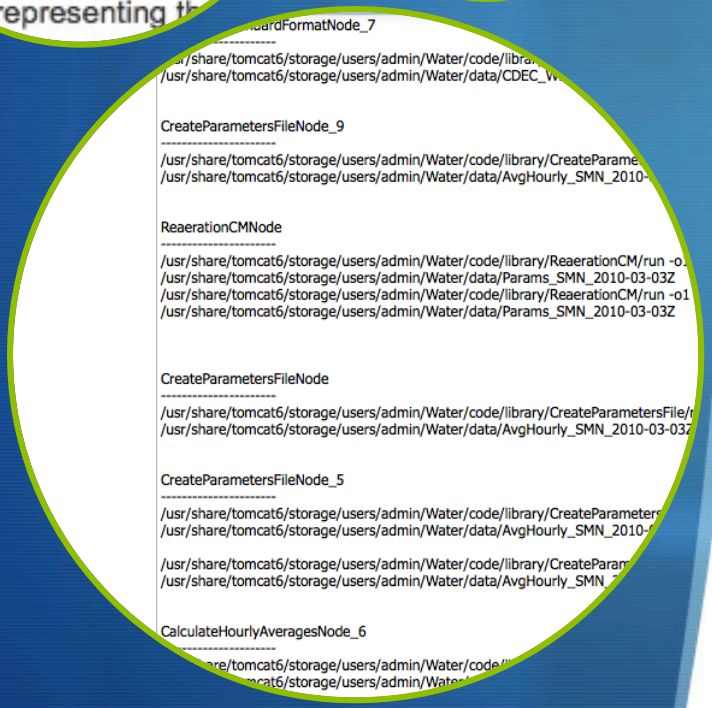
- Christopher Duffy

Are there any additional contributors of note for this software ?

- Mukesh Kumar
- Gopal Bhatt







5 Provenance documentation

6 Methods documentation

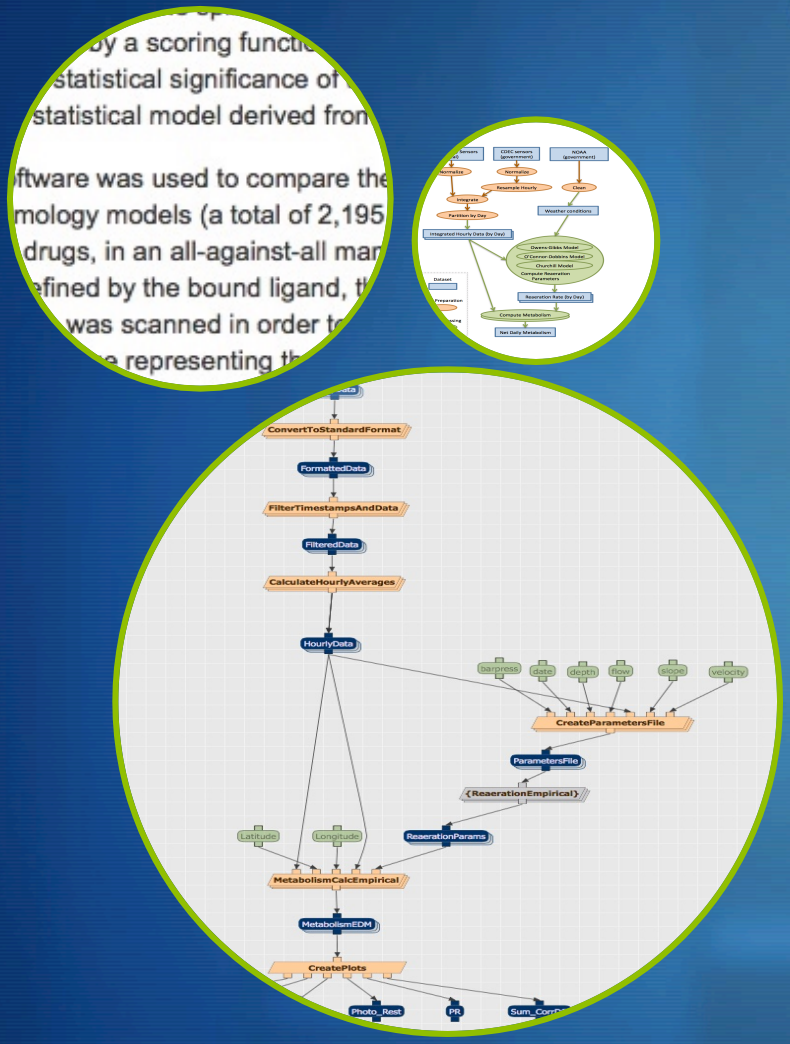
Simplest Approach

1. Describe the workflow in text
   - Data + software + workflow
   - Specify unique identifiers for data and software, versions, credit all sources
2. Develop a workflow sketch
   - Capture high-level dataflow across components
3. For provenance, include a summary or an execution trace

5 Provenance documentation

6 Methods documentation

Ideal Approach



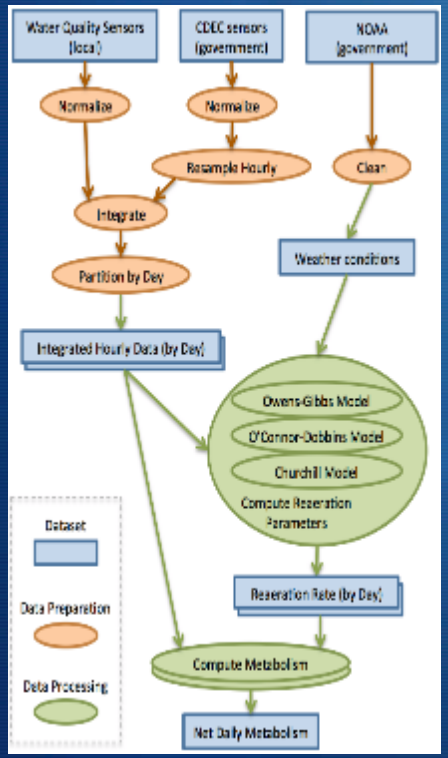
1. Describe the workflow in text
   - Data + software + workflow
   - Specify unique identifiers for data and software, versions, credit all sources
2. Develop a workflow sketch
   - Capture high-level dataflow across components
3. Specify the formal workflow using a workflow system, electronic notebook, etc.
   - Command lines + parameter values
   - Dataflow across components
4. Include the provenance record
   - If generating it automatically, preferably using a standard (e.g., PROV)
5. Publish the workflow and provenance record in a publicly accessible repository (eg figshare, myExperiment, etc)
6. Get a unique persistent identifier for the workflow, the provenance, or both

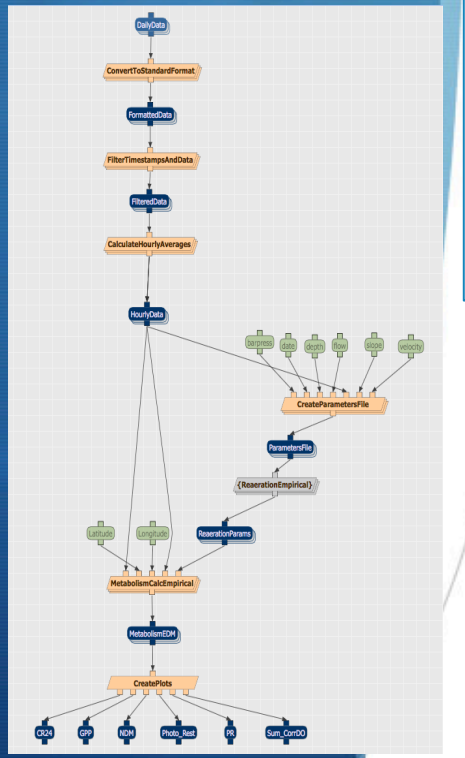
5 Provenance documentation

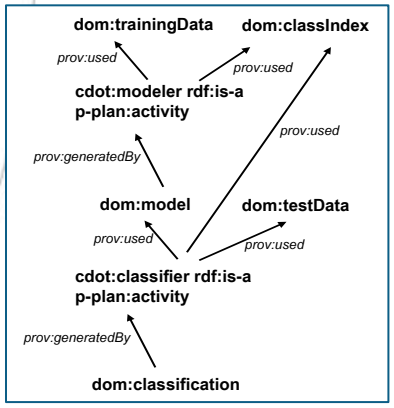
6 Methods documentation

What to Show in the Paper

- Describe workflow in text and provide a workflow sketch
  - Optionally, provide the formal workflow or lab notebook, use a persistent identifier, and cite it
- Include a summary of the execution traces as supplementary material, or use a persistent identifier and cite it
  - Optionally, include instead the provenance records using a standard like W3C PROV







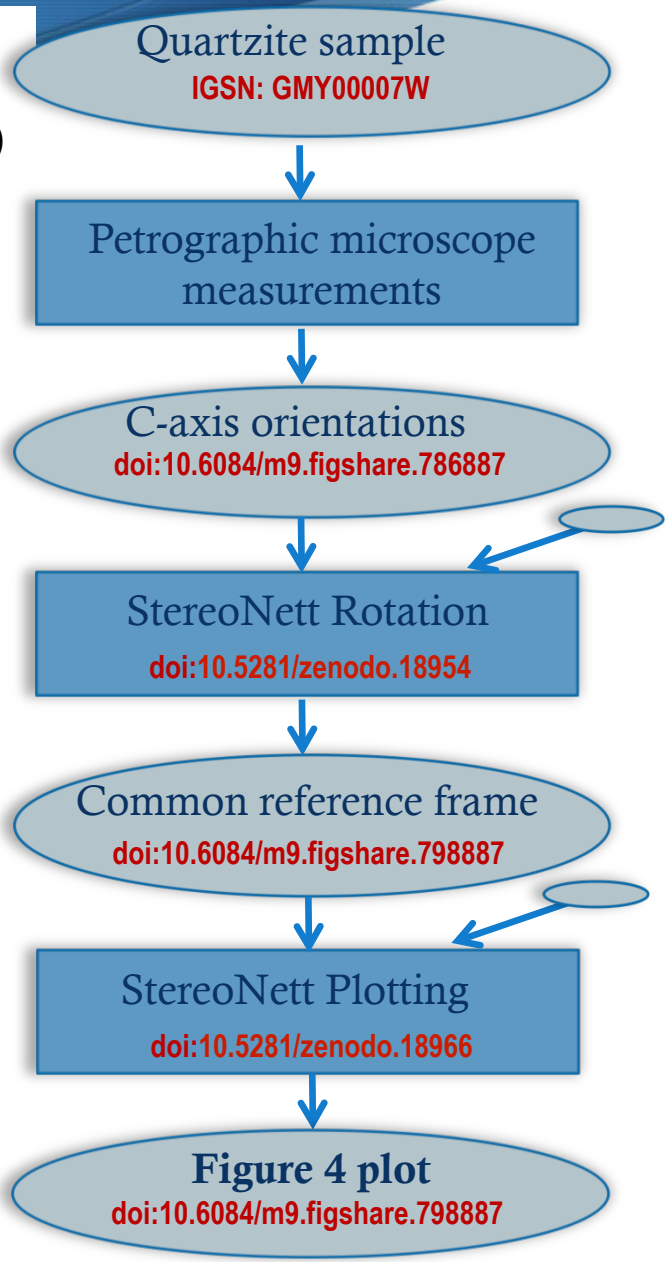

```
# Entities
ex:testData1 a prov:Entity .
ex:model1 a prov:Entity .
ex:classification1 a prov:Entity .
# Activities
ex:Classifier1 a prov:Activity .
# Usage and Generation relations between entities and activities
ex:Classifier1
    prov:used ex:testData1 ;
    prov:used ex:model1 .
ex:classification1
    prov:wasGeneratedBy
        ex:Classifier1 .
```

SPF authors should publish and cite the initial sample (or initial data), the intermediate data, the software, the final results, and the provenance of each figure or result

Understanding kinematic data from the Moine thrust zone (doi:10.1016/j.ess.2009.08.012)

Jade Silverstein (orcid.org/0000-0001-8455-8431)

[…] We took a quartzite sample (**IGSN: GMY00007W**) from the Stack of Glencoul in the Moine thrust, and cut 3 thin sections. We measured c-axis orientations (**doi:10.6084/m9.figshare.786887**) using a petrographic microscope. We rotated to a common reference frame (**doi:10.6084/m9.figshare.798887**) using Duyster's StereoNett program (**doi:10.5281/zenodo.18954**). We plotted the data on lower hemisphere, equal area projections (**doi:10.6084/m9.figshare.798887**) using Duyster's StereoNett program (**doi:10.5281/zenodo.18966**), shown in Figure 4. **The provenance is shown in Fig 5**. […]



7 Authors identification

What to Show in the Paper

https://pixabay.com/en/people-character-faces-real-305836/

- Authors have a persistent unique identifier
  - Use www.orcid.org

ORCID

Author Checklist

1. Data accessibility
2. Data documentation
3. Software accessibility
4. Software documentation
5. Provenance documentation
6. Methods documentation
7. Authors identification

- **For datasets**, the paper should include one or more citations, specifying the authors, the site where they are described and can be accessed, the repository, and the license.
- **For software**, the paper should include one or more citations, specifying the authors, the site where it is described and can be accessed, the repository, and the license.
- **For provenance and workflow**, the paper should include figures and traces, and if available the citations mentioning the authors, site to access them, the repository, and the license.
- **For authors**, there should be a unique identifier (e.g., ORCID)

What You Have Learned Today:
To Write a Scientific Paper of the Future and also to…

1. **Get credit** for all your research products
   - ★ Citations for software, data, samples, …
2. **Increase citations** of your papers
3. Write impressive **Data Management Plans**
4. **Extend your CV** with data and software sections
5. **Reproduce** your work from years ago
6. Comply with new **funder and journal requirements**

Training Goals

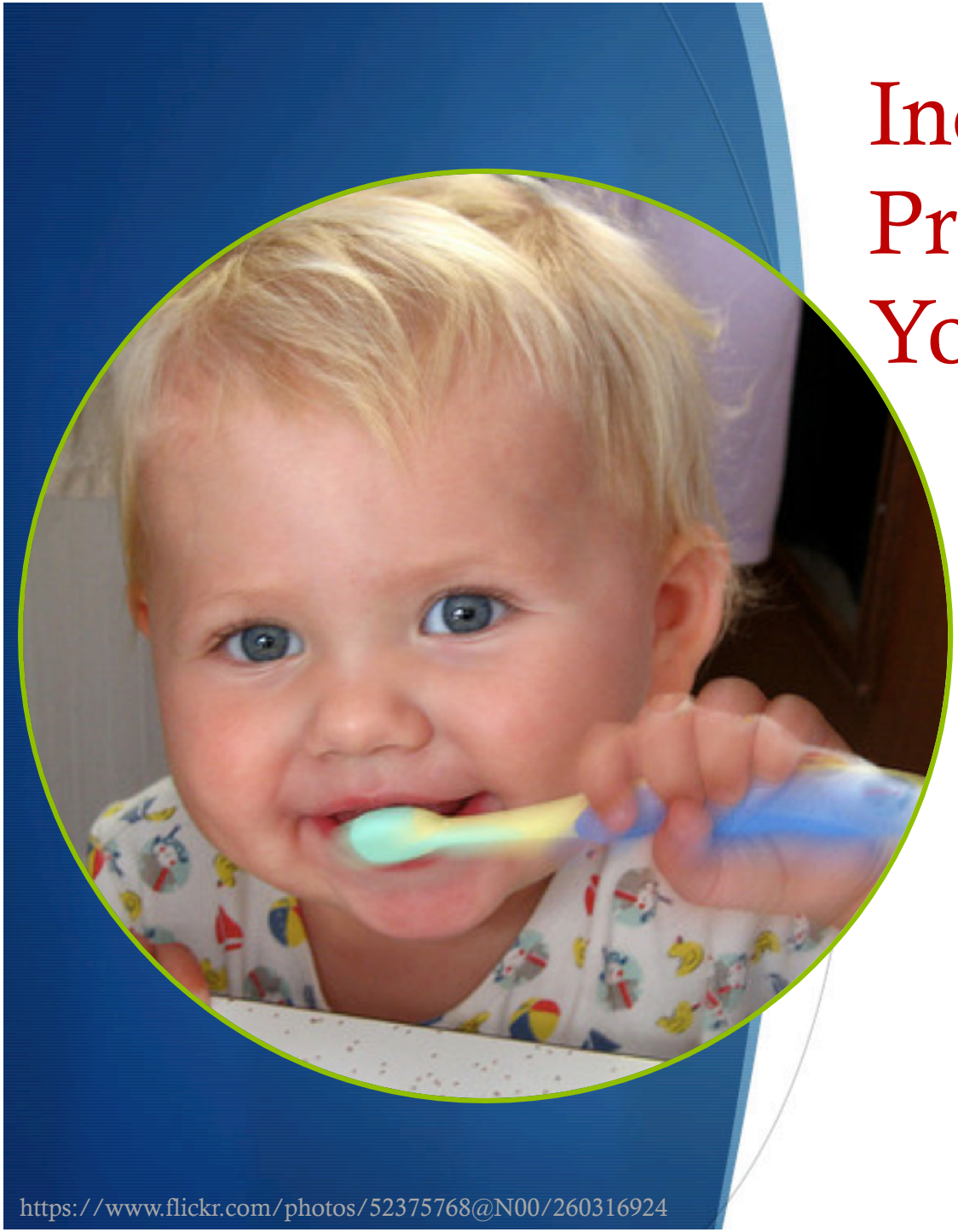
What Training Covers

- **Best practices**
  - Many are still being developed by the community
- **Major concepts and goals**, regardless of the platform, research area, or target journal
- **Mindful of effort**
  - How to implement best practices with simplest approach

What is Not Covered

- Metadata standards specific to particular research areas
- Improving software development skills
- Details of using code sharing sites

Incorporate Best Practices Into Your Work



https://www.flickr.com/photos/52375768@N00/260316924

- Easier to track research products, report to funders, get credit, etc.
- Making a paper into an SPF is then very straightforward

Author Support

- **Public mailing list for authors:**
  http://mailman.isi.edu/mailman/listinfo/spf-authors
  - **General questions**
  - **Approaches and tools used**
  - **Best practices in specific disciplines**
- **Public mailing list for announcements:**

  http://mailman.isi.edu/mailman/listinfo/spf-announce
  - **Training sessions**
  - **Formation of author groups**
  - **Special issues**

Acknowledgments

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ICER-1343800

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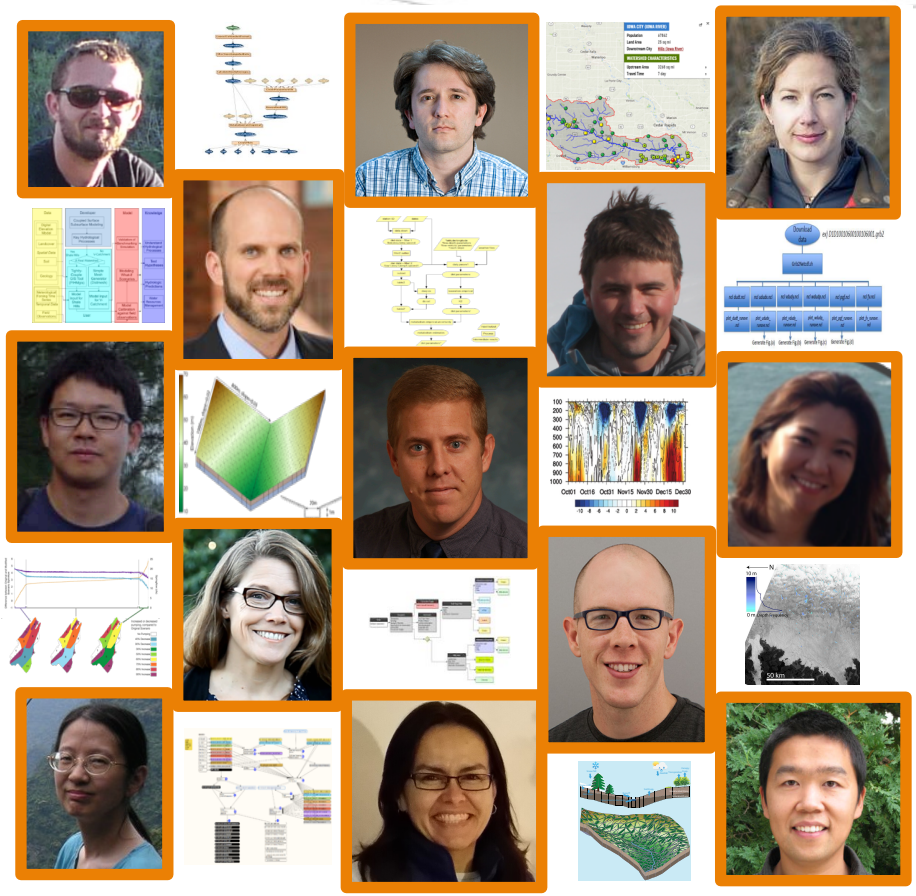
For More Information

http://www.scientificpaperofthefuture.org



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