Describe, Manage and Discover Research Software

Sue Cook (CSIRO)
Jens Klump (CSIRO)
Paola Petrelli (CLEX)
Margie Smith (GA)
Geoff Squire (CSIRO)
Lesley Wyborn (NCI)
Mingfang Wu (ARDC)

Outline

- Introduction, landscape of software citation and publish, changes in Research Data Australia (RDA) for promoting software (Mingfang Wu, ARDC)
- New requirement from publishers and funders for software citation (Lesley Wyborn, NCI)
- Lightning talks:
  - Software Citation and GA: Motivations, outcomes and future direction(Margie Smith, GA)
  - Software in the CSIRO DAP: Description (Sue Cook, CSIRO)
  - CLEX software publishing workflow (Paola Petrelli, CLEX)
  - Describing software for Virtual Laboratories (Geoff Squire, CSIRO)
- Q/A, group discussion and feedback (Jens Klump, CSIRO)

Why do we care

- Software is pervasive in research
  - >90% of researchers acknowledge software is important for their own research
  - ~70% say their research would not be possible without it.
  - Of 40 papers examined in Nature Jan-March 2016, 32 contain 211 mentions of distinct pieces of software, for an average of 6.5 mentions per paper

Hettrick. S. J., et al. (2014). UK Research Software Survey 2014 [Data set]. doi:10.5281/zenodo.14809
Nangia 2017b] Nangia, Udit; Katz, Daniel S. (2017): Understanding Software in Research: Initial Results from Examining Nature and a Call for Collaboration. https://arxiv.org/abs/1706.06527

12 scientific software challenges

Open Research and Scholarly Communication

- Intellectual property
- Publication and peer review
- Software dissemination, catalogues, search, and review

Sustainable Software

- Training and education
- Software engineering
- Portability
- Multidisciplinary science
- Reproducibility
- *Reusability*

Sustainable community

- Incentives, citation/credit models, and metrics
- Career paths
- Software communities and sociology
- Sustainability and funding models

Daniel S. Katz: Software in Research: Underappreciated and underrewarded. Keynote speech from 2017 eRA.

The FAIR Data Principles

Findable, Accessible, Interoperable, Reusable

The FORCE11 Software Citation Principles

Importance, Credit and attribution, Unique identification, Persistence, Accessibility, Specificity

The OSS Recommendations

Make source code publicly accessible from day one

Make software easy to discover by providing software metadata via a popular community registry

Adopt a license and comply with the license of third-party dependencies

Define clear and transparent contribution, governance and communication processes

Open research & Scholarly communication

Sustainable software

Sustainable community

Jiménez RC, Kuzak M, Alhamdoosh M *et al.* Four simple recommendations to encourage best practices in research software [version 1; referees: 3 approved]. *F1000Research* 2017, 6:876 (doi: 10.12688/f1000research.11407.1)

Who and What (Internationally)

For more info: https://bit.ly/2IQspUy

Open Research and Scholarly Communication

- FORCE11 Software Citation Implementation WG
- RDA Research Software Source Code IG

- Nature software submission guidelines (2018)
- Journal of Open Source Software
- Elsevier – Why publish a software
  SoftwareX, Science of Computer Program, Neurocomputing

Sustainable software

- US Research Software Sustainability Institute (URSSI)
- UK Software Sustainability Institute
- Working Towards Sustainable Software For Science (WSSSPE)

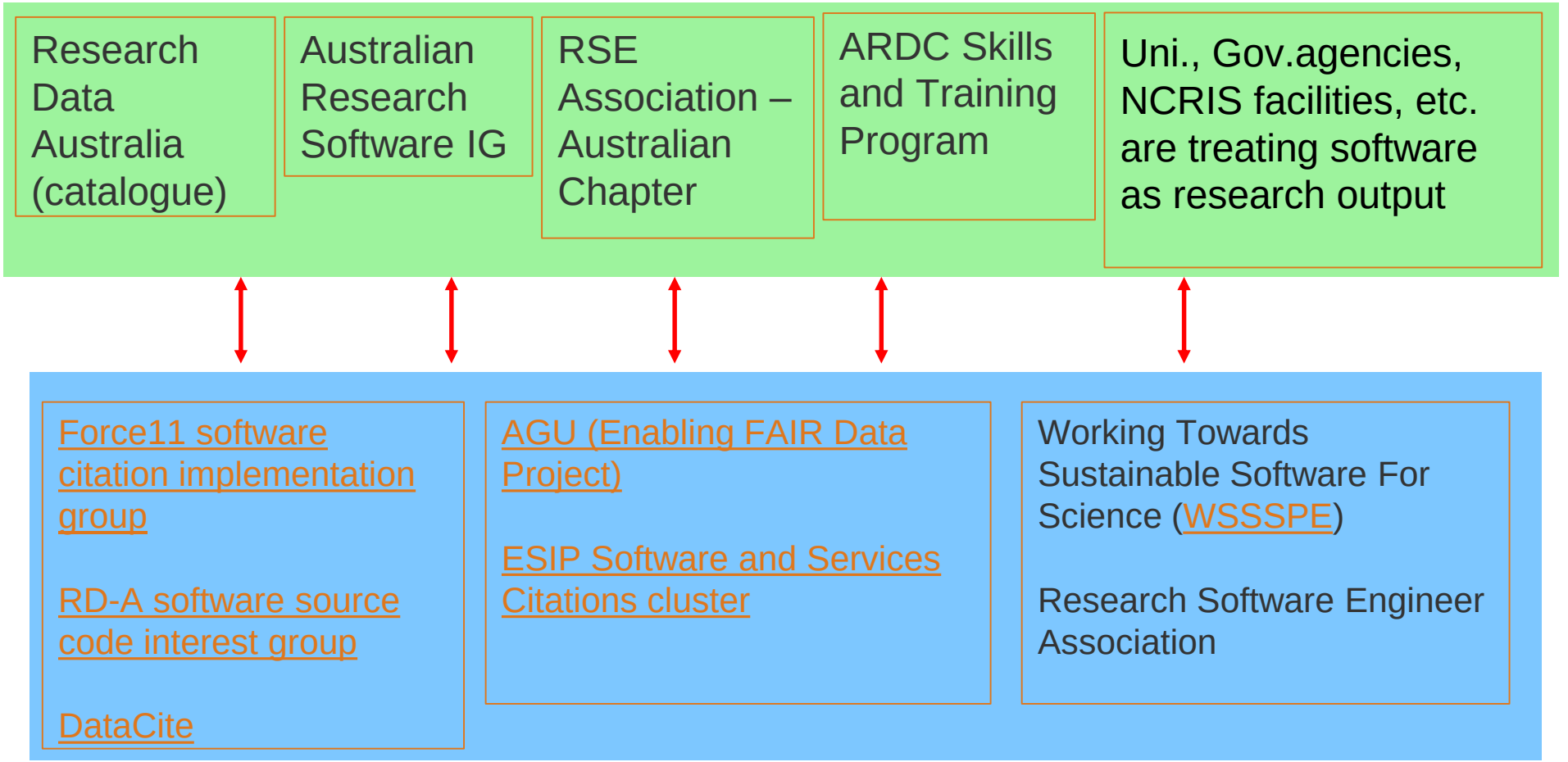
Sustainable community

- Research Software Engineer Association

Support from disciplines and organisations

- ESIP: Software Guidelines
- AGU: Enabling FAIR Data Project
- Astrophysics: AAS Journals, Astrophysics Source Code Library
- ...

Australian activities supporting research software



Supporting catalogue/repository

General repository

- DataCite
- Zenodo
- Code Ocean
- Code.gov
- Figshare

...

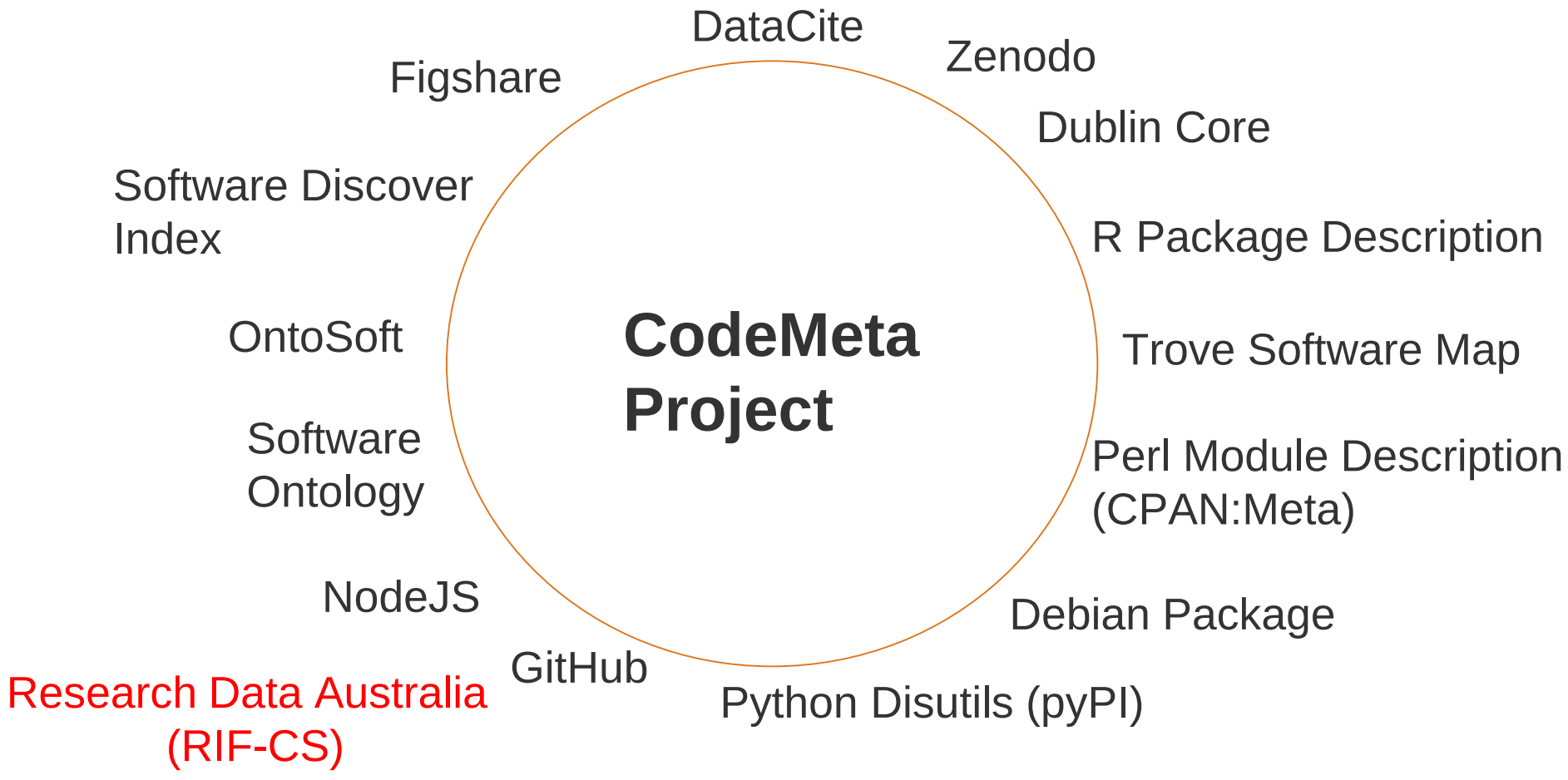
Software code archive:
Software Heritage

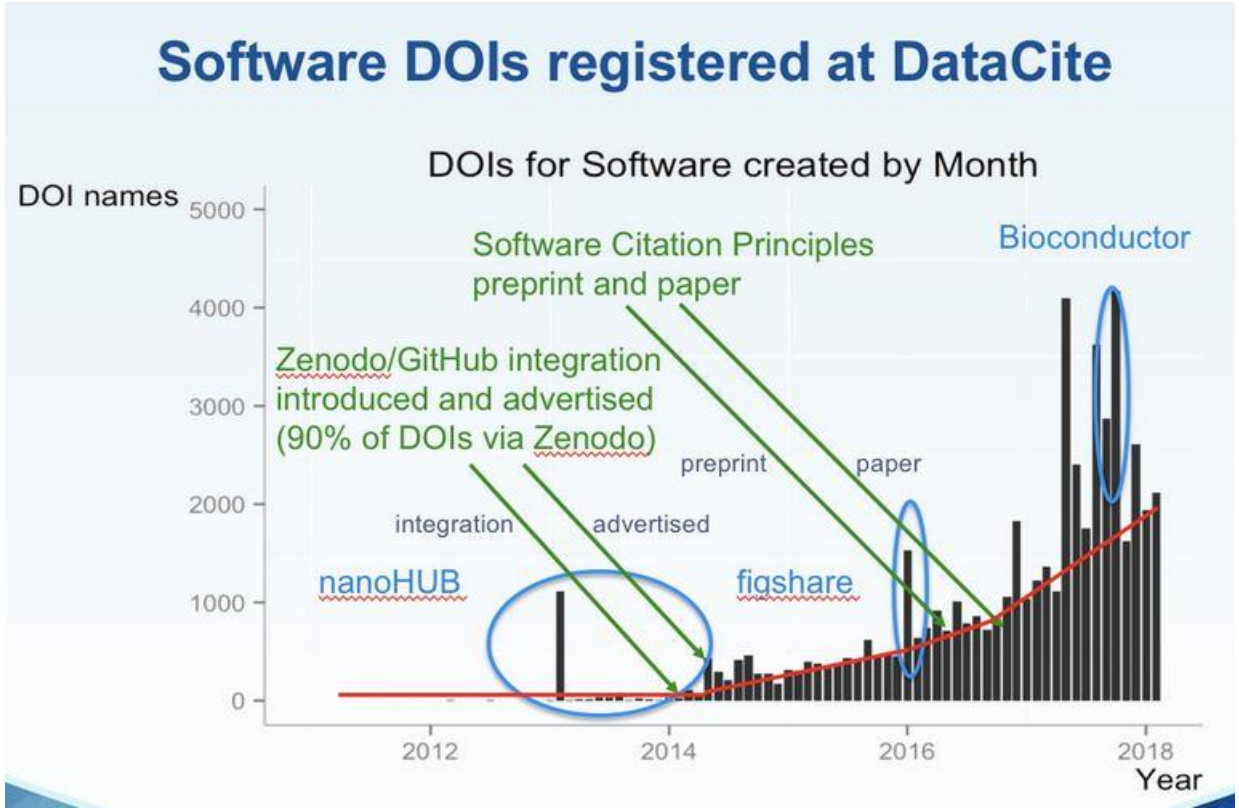
Domain specific software repository

- Astrophysics Source Code Library (http://ascl.net/)
- OMICStools (https://omictools.com/)
- Bio.tools (https://bio.tools/)
- Bioconductor (https://www.bioconductor.org/)

...

Software metadata/ontology/vocabulary





Martin Fenner, Daniel S. Katz, Lars Holm Nielsen, and Arfon Smith, DOI Registration for Software, May 17, 2018, **https://doi.org/10.5438/1nmy-9902**

What do we (ARDC) do

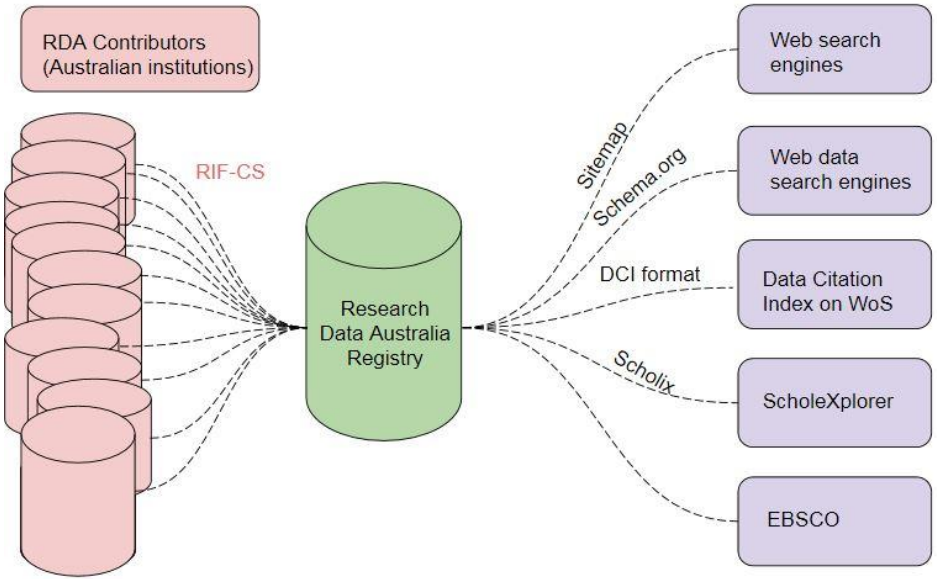
- Software citation guide: https://www.ands.org.au/working-with-data/citation-and-identifiers/software-citation

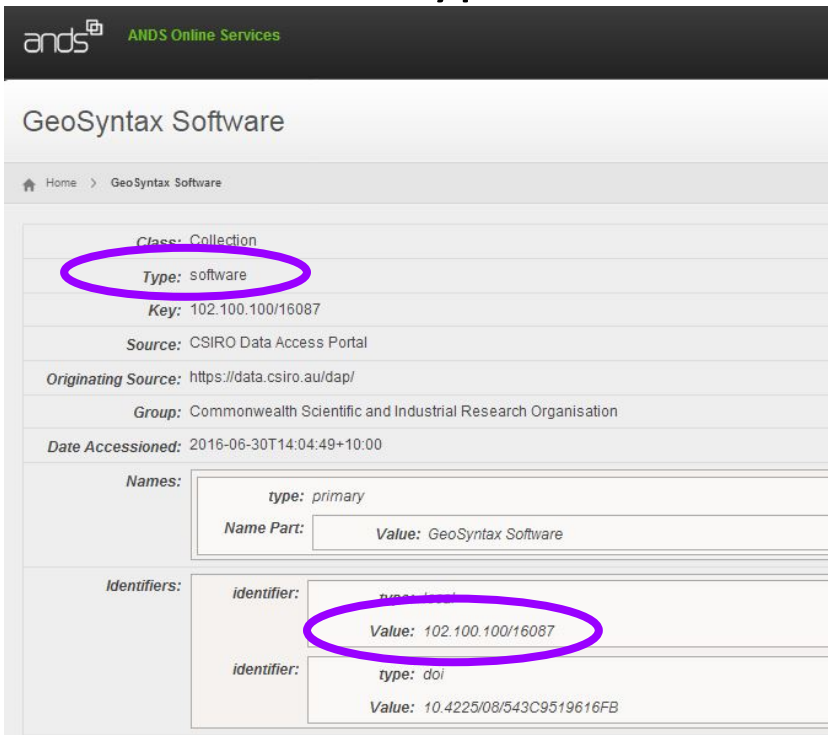
- Recommended software citation format

  Creator (PublicationYear): Title. Version No. Publisher. [resourceTypeGeneral]. Identifier.

What do we (ARDC) do

- Amended Research Data Australia (RDA) registry schema (RIF-CS) for describing software as a distinct resource type



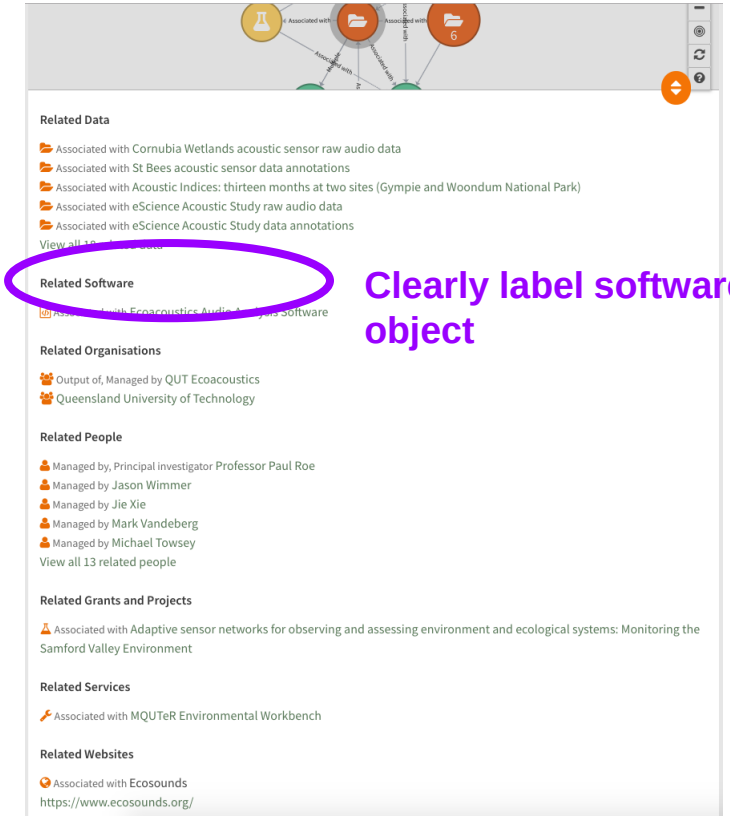


What do we (ARDC) do

- 212 registered software records from RDA (was 173 in Nov. 2017)
  - Commonwealth Scientific and Industrial Research Organisation 87
  - Geoscience Australia 70
  - Australian Ocean Data Network 34
  - Monash University 15
  - The University of Adelaide 4
  - ARC Centre of Excellence for Climate System Science 1
  - National Archives of Australia 1

  108 of them have minted DOI

Enhance software discoverability in RDA



Related Data

Associated with Cornubia Wetlands acoustic sensor raw audio data
Associated with St Bees acoustic sensor data annotations
Associated with Acoustic Indices: thirteen months at two sites (Gympie and Woondum National Park)
Associated with eScience Acoustic Study raw audio data
Associated with eScience Acoustic Study data annotations
View all 10 related data

Related Software

Associated with Ecoacoustics Audio Analysis Software

Related Organisations

Output of, Managed by QUT Ecoacoustics
Queensland University of Technology

Related People

Managed by, Principal investigator Professor Paul Roe
Managed by Jason Wimmer
Managed by Jie Xie
Managed by Mark Vandeberg
Managed by Michael Towsey
View all 13 related people

Related Grants and Projects

Associated with Adaptive sensor networks for observing and assessing environment and ecological systems: Monitoring the Samford Valley Environment

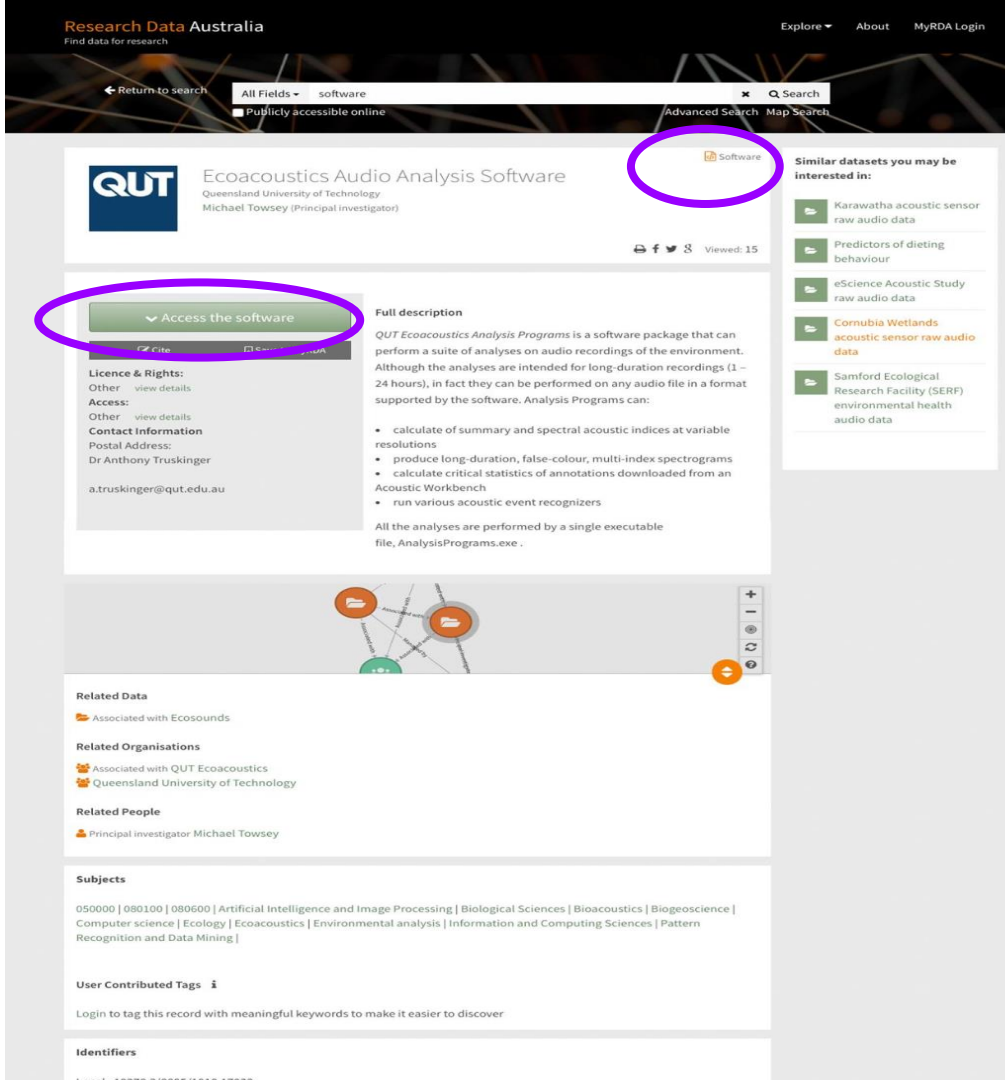
Related Services

Associated with MQUTeR Environmental Workbench

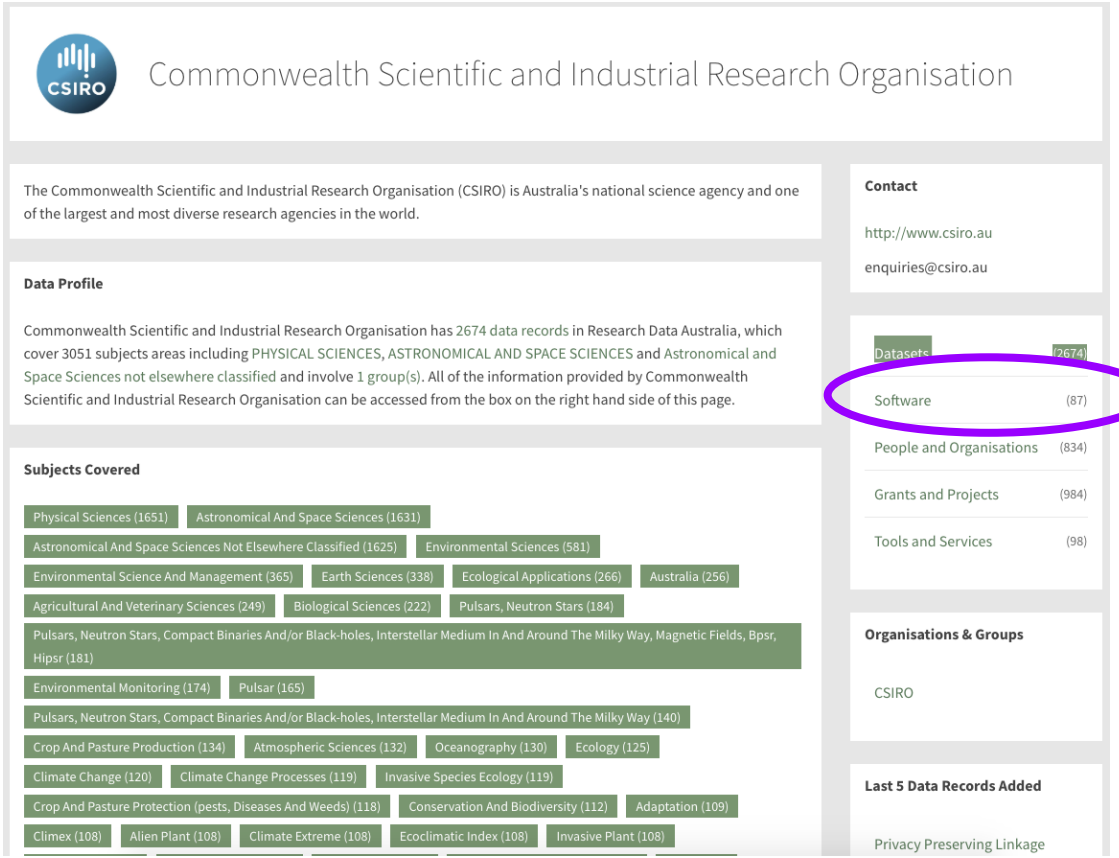
Related Websites

Associated with Ecosounds
https://www.ecosounds.org/

Clearly label software object

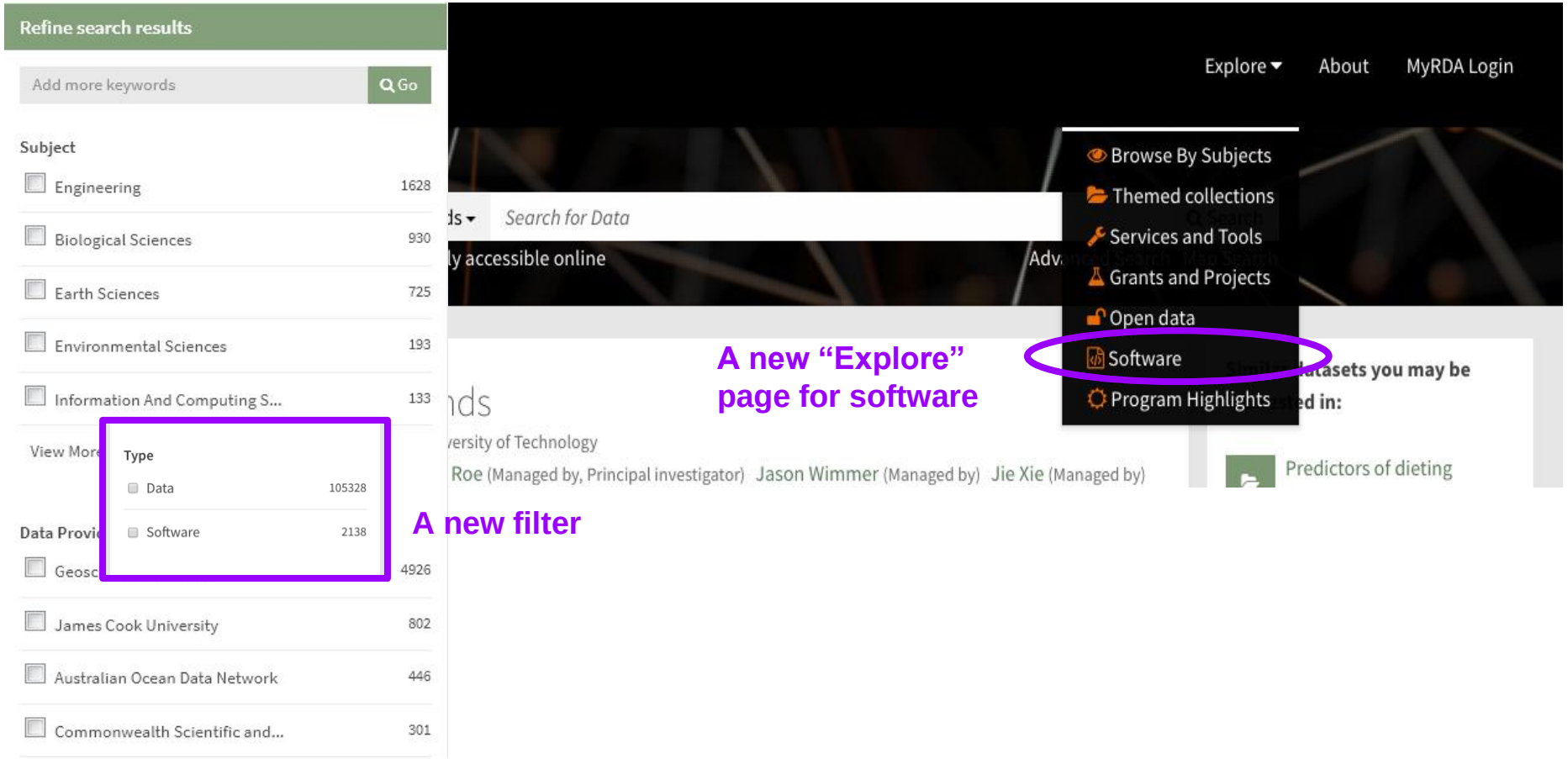


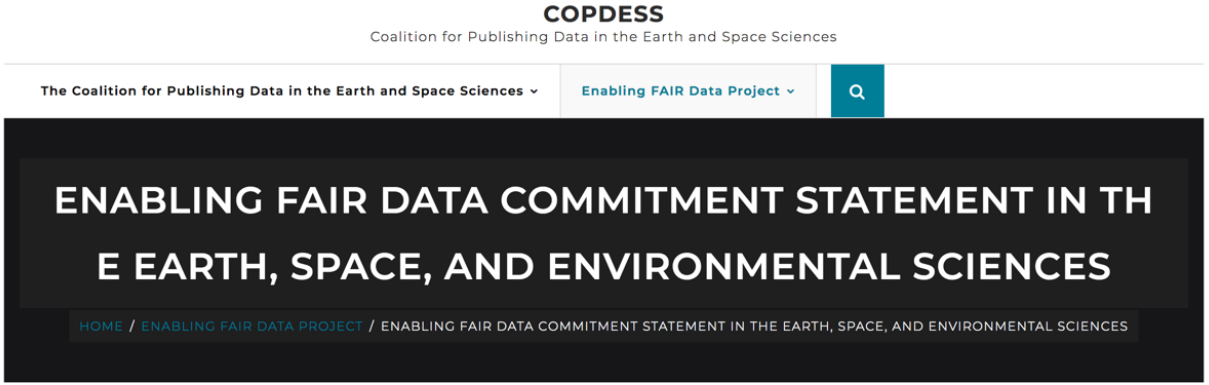
Enhance software discoverability in RDA



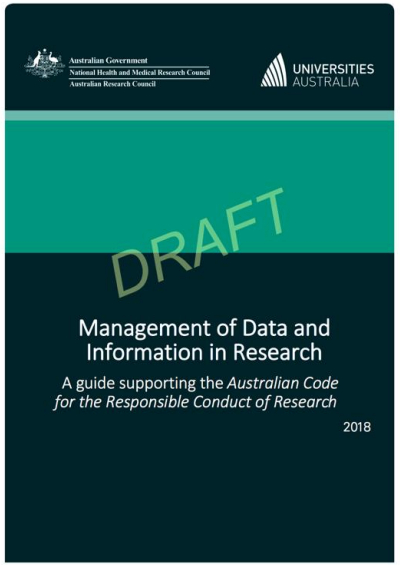
A new software link from this Contributor page

Enhance software discoverability in RDA





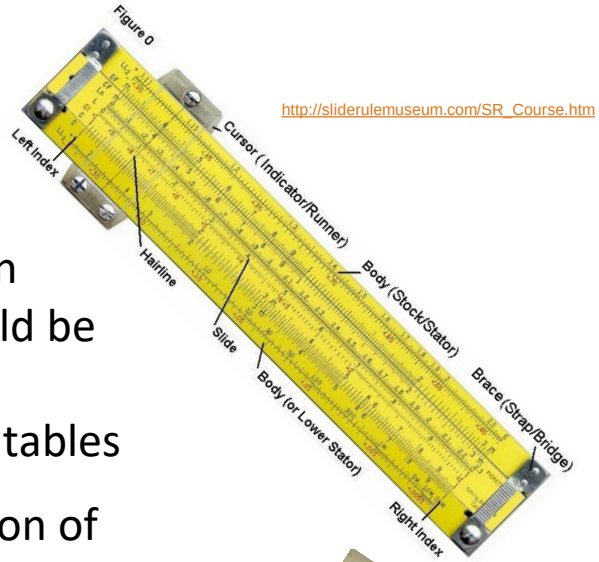
https://docs.google.com/presentation/d/1jBxFowB03p9hmkx1Cq08m5ObABvwIDVIVkjM3c3y0dk/edit#slide=id.g433aff2eb8_0_75



New requirements from Publishers (and the ARC/NHMRC/Universities Australia)

Lesley Wyborn
National Computational Infrastructure

The Drivers for Change



http://sliderulemuseum.com/SR_Course.htm

- Fifty years ago, most data that underpinned a publication could be represented in typeset tables and methods could be described in text.
  - Most calculations were done using slide rules and log tables
- With the advent of the digital age and the computerisation of instruments, volumes of data collected became too large to process manually and publish as tables: computer code became integral to modern scientific research.
- Increasingly data and software became included as a supplement in the research paper, accessible by contacting the journal, or else ‘by contacting the author’.

https://ia800803.us.archive.org/zipview.php?zip=/22/items/olcovers571/olcovers571-L.zip&file=5712066-L.jpg

The Problem

- The inability to access primary data, samples, and software limits the ability to test the veracity and reproducibility of any publication
- They do not guarantee accessibility and persistence of input research artefacts (data, software and samples in particular)

https://thelifeididntchoose.com/2018/08/14/life-is-absolutely-not-fair /

How do we fix it?

1. In 2017, a grant from the Laura and Arnold Foundation was awarded to the American Geophysical Union (AGU) and other partners to significantly improve the interconnection of data, software and samples in the literature in the Earth and environmental sciences, based around the FAIR guiding principles.
2. A coalition of Earth and environmental science publishers, disciplinary data repositories, and supporting organizations joined forces to work together to a commitment statement on FAIR publishing.
3. AuScope, ARDC and the NCI were all partners in the project and various members participated in stakeholder meetings and made contributions to final outcomes.

The Commitment Statement

This states that publication of scholarly articles in the Earth environmental science communities is conditional upon the concurrent availability of underpinning data and **software**.

These should, to the greatest extent possible, be shared, open, and stored in community-approved FAIR-aligned repositories.

This has been signed by publishers, repositories, professional societies, institutions, research data infrastructures and individuals (including AuScope, NCI, ARDC)

Available on: http://www.copdess.org/enabling-fair-data-project/

What does this mean for the Earth and environmental sciences?

For The Publishers?

Publishers are now working towards following consistent policies for sharing and citing data, samples and **software** and will move from having these as supplements to using trusted repositories for publishing supporting research artefacts

For Repositories?

Repositories will need to move towards be able to provide persistent identifiers, rich metadata, and related services for the data, **software** and samples they hold.

For Researchers?

Researchers will need to know how to consistently share, document, and reference data, samples and **software** and use globally persistent identifiers to uniquely identify their research outputs

How can Australians Comply?

ARDC has developed guidelines for citing software based on international recommendations of FORCE 11 software citation principals, DataCite, CodeMeta, and others.

https://www.ands.org.au/working-with-data/citation-and-identifiers/software-citation.

Australian Government
Geoscience Australia

Software Citation and Geoscience Australia

Motivations, outcomes and future direction

Margie Smith

Data Policy and Informatics

Main motivations

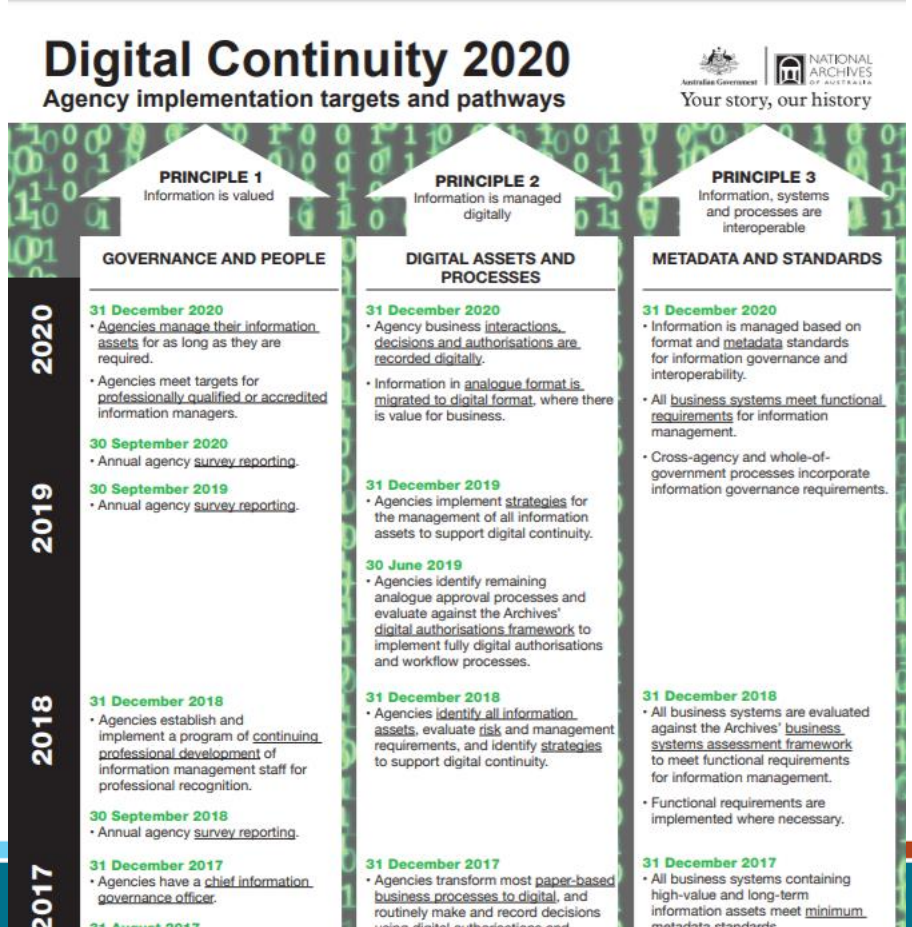
1. Government Policy and Legislation
    a) Digital Continuity 2020
    b) The Archives Act 1983
2. Geoscience Australia Data Strategy
3. Geoscience Australia's Science Principles
4. Geoscience Australia's Strategic Priorities
5. …

Government policy considerations

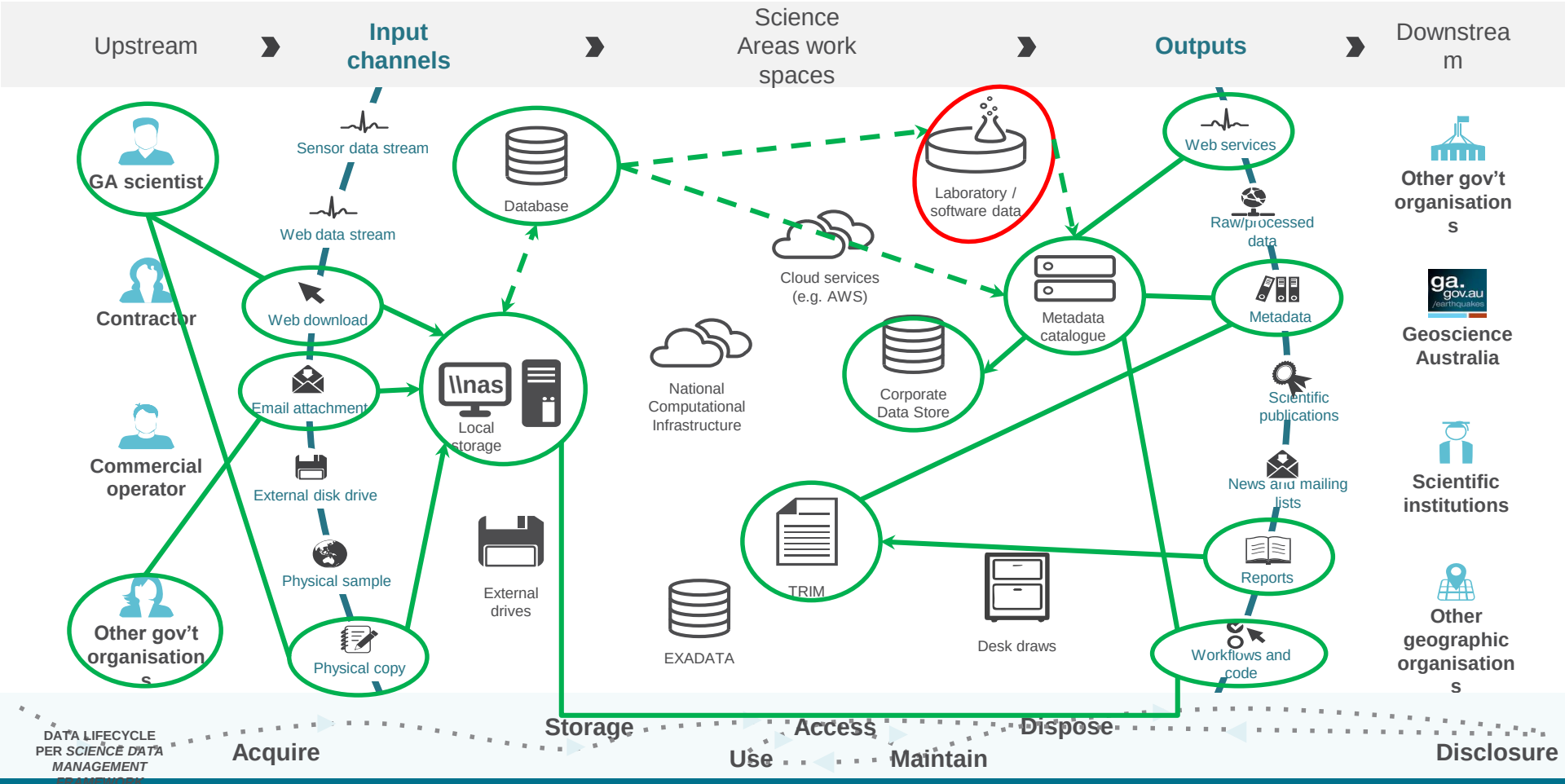
Government Data /
digital transformation agenda
through the DC2020

http://www.naa.gov.au/information-management/digital-transition-and-digital-continuity/index.aspx

and the Archives Act 1983 requiring provenance of method as described in the Records Disposal Authority.



Data management planning considerations



GA Data Strategy

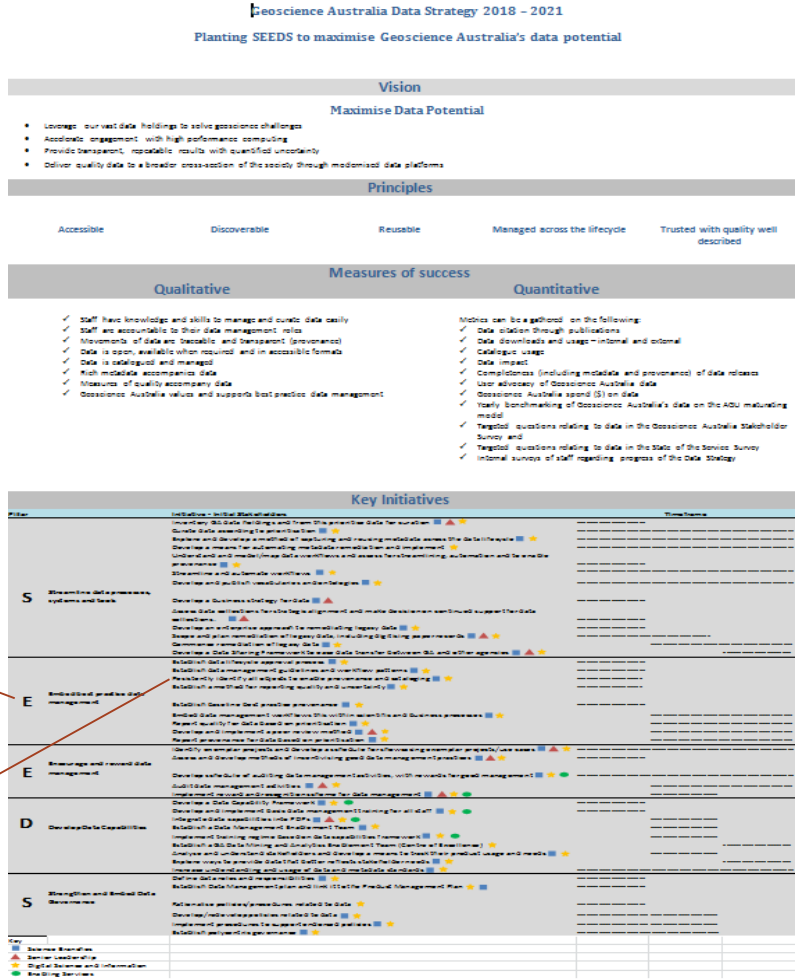
Australian Government
Geoscience Australia

Data Strategy 2018–21

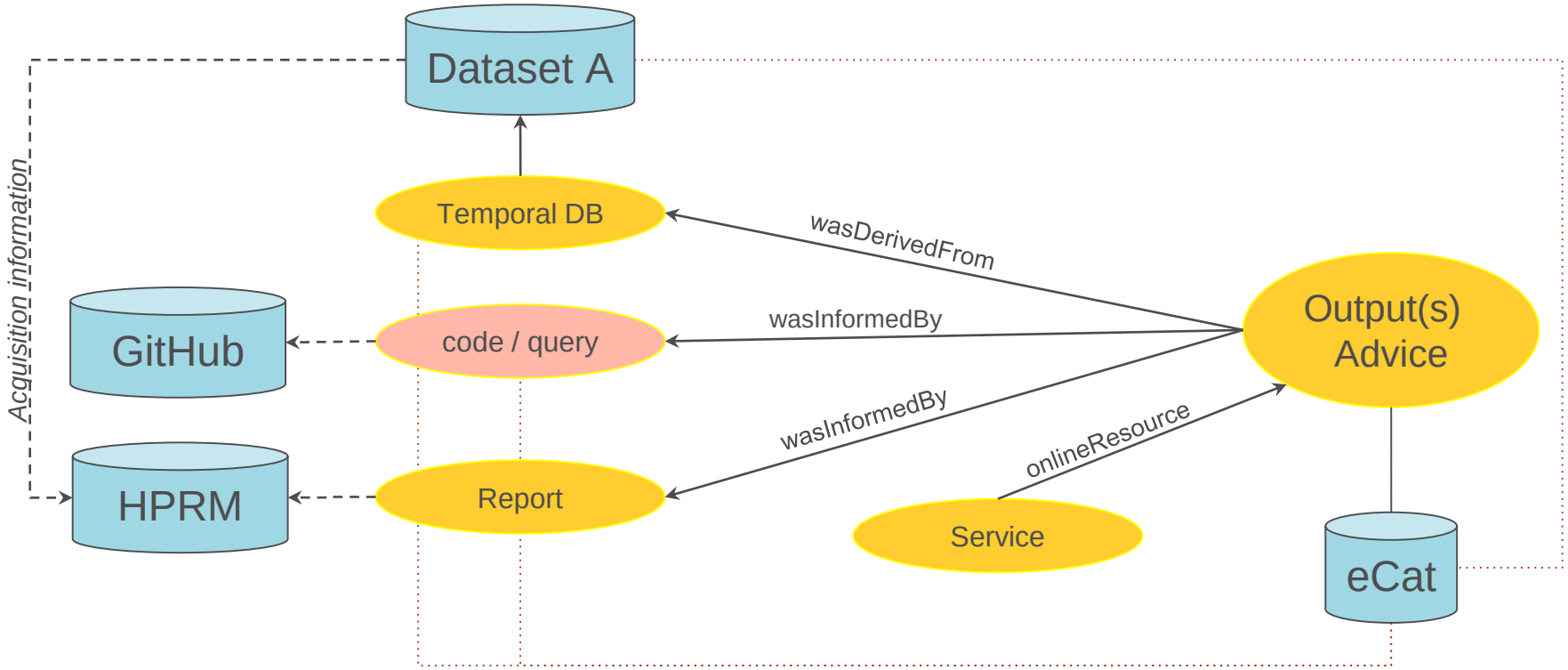
PLANTING SEEDS TO MAXIMISE DATA POTENTIAL

Embed best practice data management

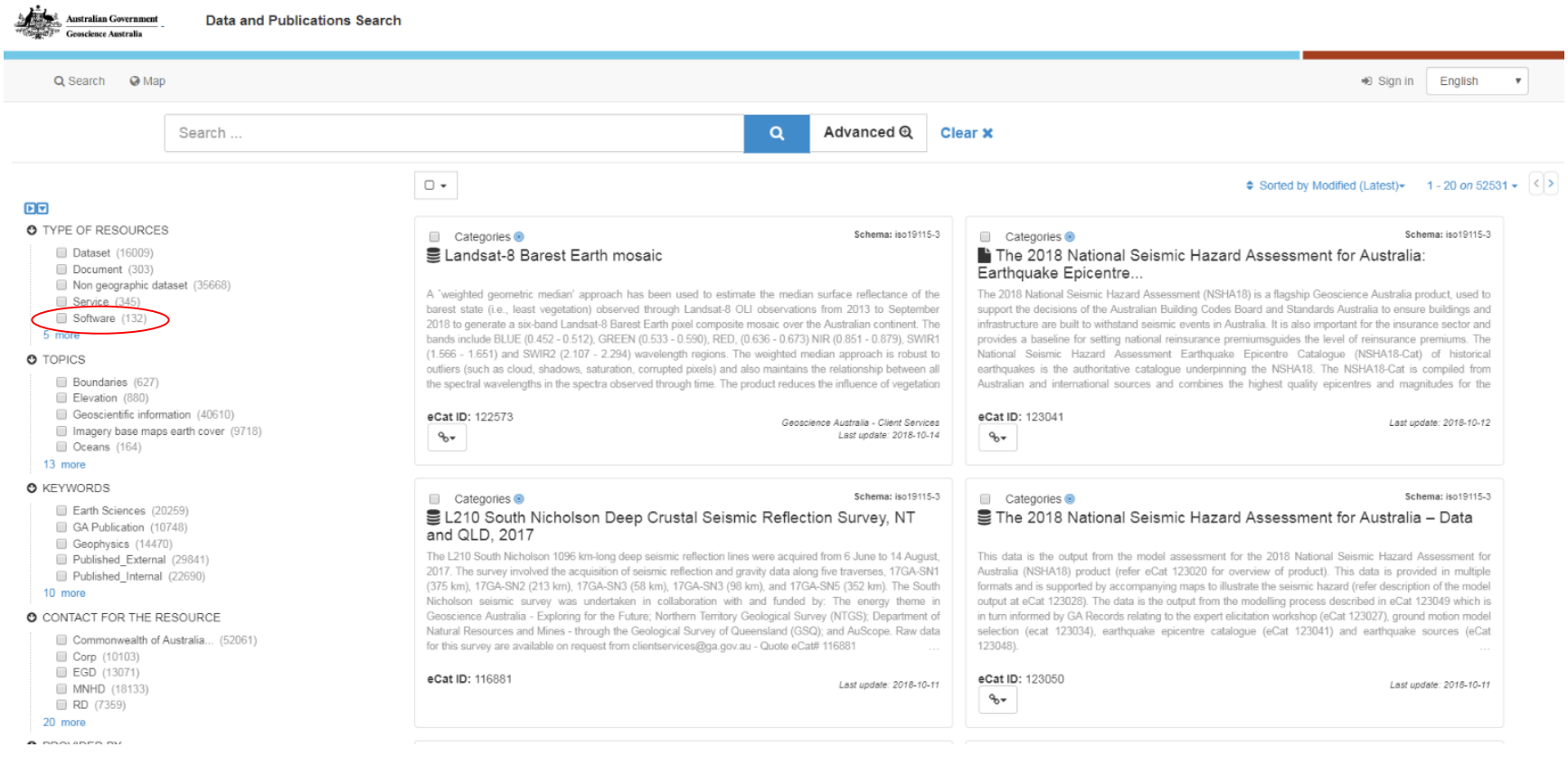
Persistently identify all objects to enable provenance and cataloguing



Outcomes – tracking provenance through the standard



Current eCat search is not granular



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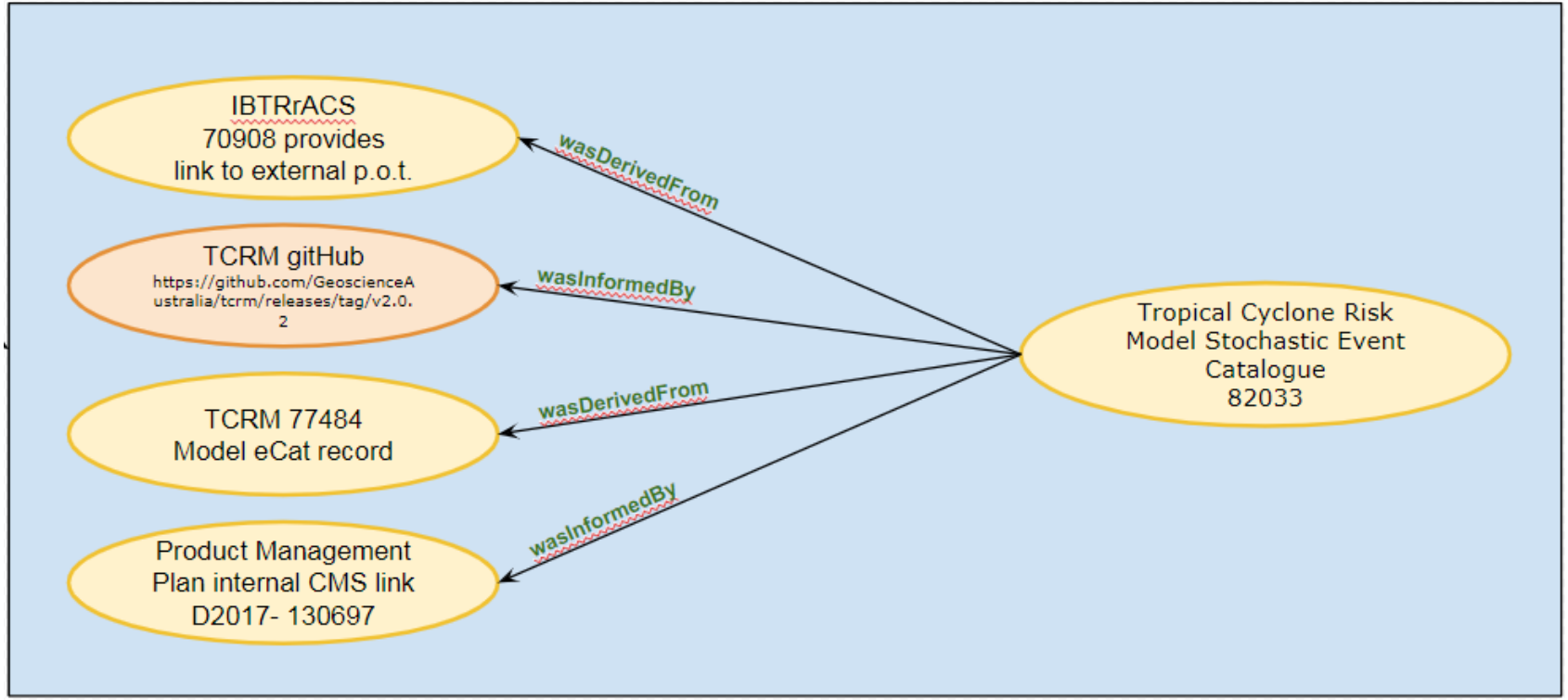

Machine discoverable (?) but not people friendly

Moving towards correct citation for advice

Citation cases 1. (proposed workflow tool N. Car 2017-05-11)

•{AUTHORS} ({YEAR}) *{TITLE}*. {TOOL_TYPE {REPO_BRANCH}[0,1]}. {PUBLISHER}. {DOI | URI}. {ACCESSED_DATE}[0,1]

What we hope to have in eCat for provenance against advice generated:

•Arthur, W.C. (2014) *tcrm*. Git code repository, Branch: v2.0.2. Geoscience Australia. accessed 2018-09-28. http://pid.geoscience.gov.au/dataset/ga/77484

Future direction – discovery and linkage improvement

Back to search ‹ Previous page Next ›

Tropical Cyclone Risk Model Stochastic Event Catalogue

The TCRM Stochastic Event Catalogue contains artificially generated tropical cyclone tracks and wind fields representing 10000 years of tropical cyclone activity. The catalogue is stored by year, with a track file and wind field file. The wind field file contains the maximum wind speed from all events occuring in the corresponding track file (i.e. it represents annual maximum wind speeds).

About this resource

Scope Code	dataset
Categories	Climatology, meteorology, atmosphere
other	• Data Package • DC2020 • Published_Internal
Australian and New Zealand Standard Research Classification (ANZSRC)	• Natural Hazards
Legal constraints	Creative Commons Attribution 4.0 International Licence
Author	Arthur, W.C.
Contact for the resource	Custodian **CSEMD** Owner **Commonwealth of Australia (Geoscience Australia)**

Back to search ‹ Previous page Next ›

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Legal constraints	Creative Commons Attribution 4.0 International Licence
Author	Arthur, W.C.
Contact for the resource	Custodian **CSEMD** Owner

Future direction – discovery and linkage improvement

Slowly improving compliance

Status of GA's GitHub Repo's metadata

Totals

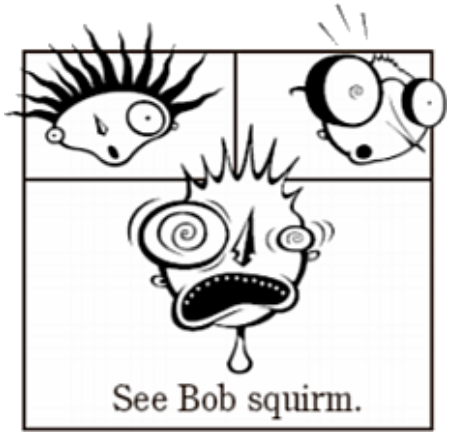
- Total: 195
- Passed: 36
- Failed: 159

Previously
- Total: 155
- Passed: 2
- Failed: 153

Repos failing tests

DefinitelyTyped	repo_must_contain_readme	passed
	readme_must_start_with_title	passed
	repo_must_have_license_file	passed
	readme_must_contain_license_section	passed
	readme_must_contain_contacts_section	README does not contain a subsection titled 'Contacts' README does not contain any GA email addresses for contact people
GeodePy	repo_must_contain_readme	passed
	readme_must_start_with_title	passed
	repo_must_have_license_file	passed
	readme_must_contain_license_section	passed
	readme_must_contain_contacts_section	README does not contain a subsection titled 'Contacts' README does not contain any GA email addresses for contact people

Thank you

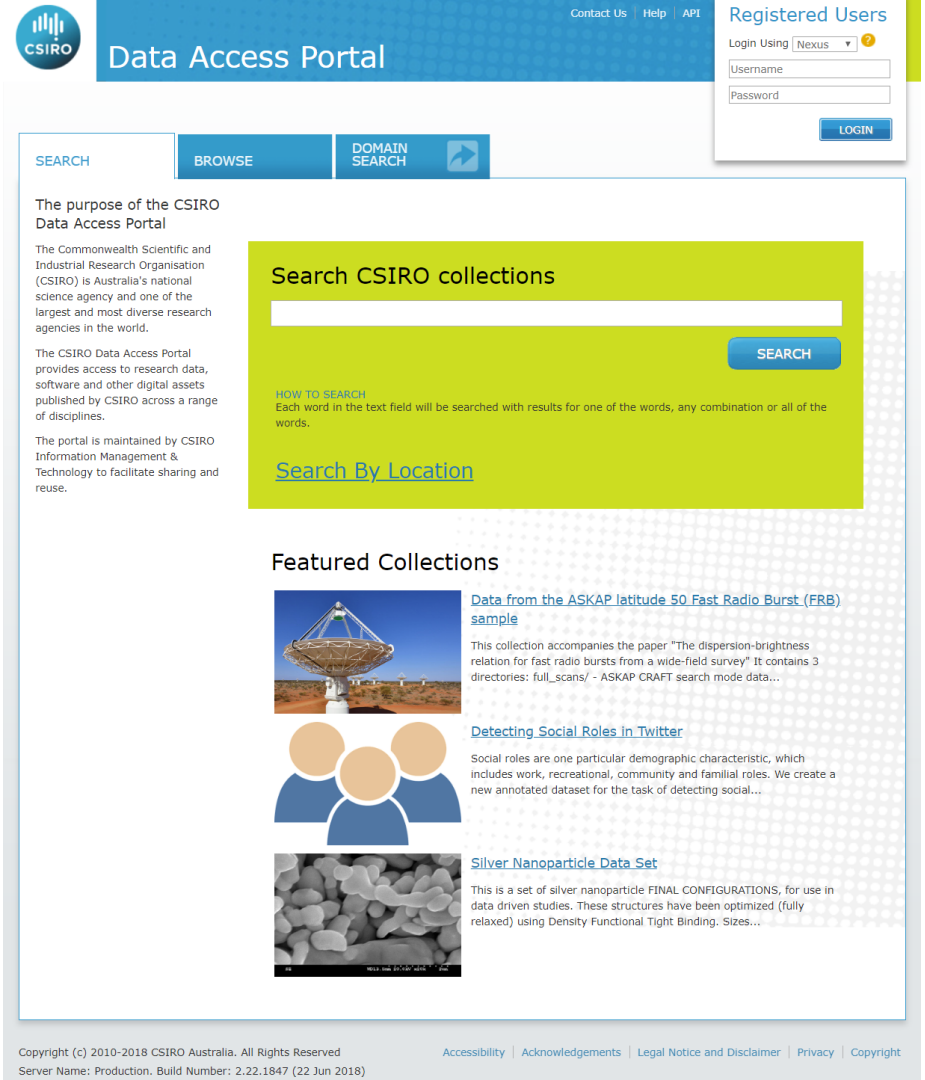


data@ga.gov.au

Software in the CSIRO DAP: Description

Sue Cook| Data Librarian

17 October 2018



https://data.csiro.au/dap

Search Results

REFINE RESULTS

Published date:
All

Clear all filters

Show ONLY:

- [ ] Files I can access (1999)

Collection type:

- [ ] Data (2523)
- [x] Software (90)
- [ ] Service (7)

Clear

Licence type:

- [ ] Creative Commons Attribution 4.0

Showing results for: SEARCH

Found: **90** results Display: 10|**25**|50 results Sort by: Relevance | **Recent** | Title

indicates that access to files within this collection is restricted

Privacy Preserving Linkage Software

A set of software tools for privacy preserving entity linkage. * anonlink: A library for carrying out the low level hash comparisons required server side * entity-service: Our linkage server implemen... more

Confidential Computing - - Published 05 Oct 2018

AusFarm Decision Support Software

AusFarm modelling tool built using the Common Modelling Protocol.

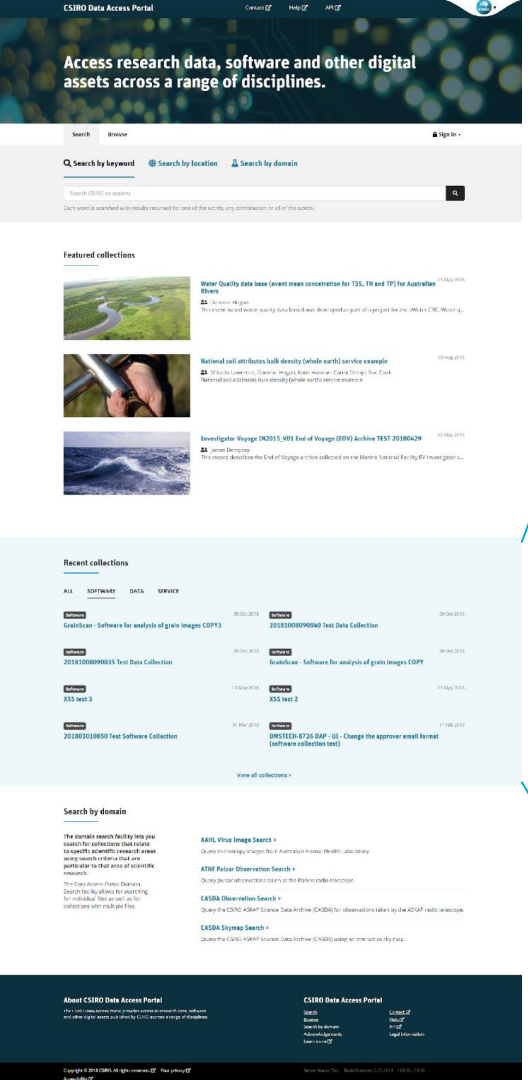
One CSIRO Rural Decision Support - Software development - Published 13 Sep 2018

PorosityPlus

The PorosityPlus code can be used to calculate the surface area, volume and pore size distribution (PSD) of particle networks. These particles can be multiscale ranging from atoms, to nanoparticles to... more

MMM Research & Applications - MMM Software - Published 04 Sep 2018

cuda-fixnum



https://data.csiro.au/collections/

Recent collections

ALL | SOFTWARE | DATA | SERVICE

Software — 09 Oct 2018
GrainScan - Software for analysis of grain images COPY3

Software — 09 Oct 2018
20181008090840 Test Data Collection

Software — 09 Oct 2018
20181008090835 Test Data Collection

Software — 08 Oct 2018
GrainScan - Software for analysis of grain images COPY

Software — 23 May 2018
XSS test 3

Software — 23 May 2018
XSS test 2

Software — 01 Mar 2018
201803010850 Test Software Collection

Software — 14 Feb 2018
DMSTECH-8726 DAP - UI - Change the approver email format (software collection test)

View all collections >

Refine results clear all

Published date
- within last year (475)
- within last month (27)
- within last week (20)
- within last day (9)

clear

Files I can access
- Files I can access (1278)

clear

Collection type
- Data (1339)
- Software (140)
- Service (60)

clear

Licence type

Page 1 of 140 results View 25 per page Sort by Relevance Subscribe to RSS

Software Oct 09, 2018

GrainScan - Software for analysis of grain images COPY3

Alex Whan, Matt Bolger, Leanne Bischof

This collection is to accompany the publication of the paper "GrainScan: A low cost, fast method for grain size and colour measurements". It contains the software version that is referred to in that publication.

Software Oct 09, 2018

20181008090840 Test Data Collection

Suresh Palaniyandi

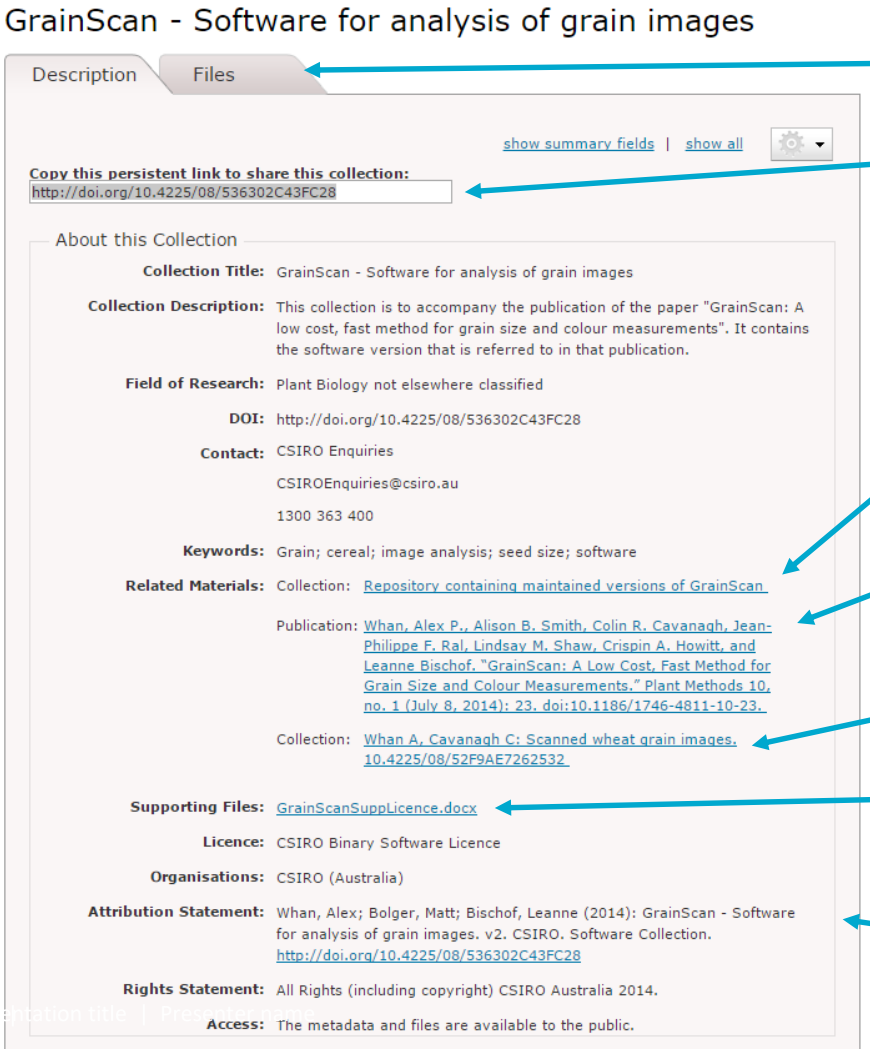
20181008090835 Test Data Collection

Software Oct 09, 2018

20181008090835 Test Data Collection

Suresh Palaniyandi

20181008090835 Test Data Collection



Files- code or executable

DOI (for this version)

Link to code repository for updates and development

Link to the related publication

Link to the data

Licence and supplement

Attribution including collection type

Workspace: Scientific Workflow Platform

Description | Files

show summary fields | show all

Copy this persistent link to share this collection:
https://doi.org/10.25919/5b3c1dc633cd3

About this Collection

Collection Title: Workspace: Scientific Workflow Platform

Collection Description: Workspace is a powerful software platform designed to address two specific user scenarios: 1) Scientists who want to create and share scientific workflows in one coherent, simple environment where much of the "heavy lifting" has already been developed and proven over a number of years 2) Developers who want to make their software avail... more

Field of Research: Software Engineering

DOI: https://doi.org/10.25919/5b3c1dc633cd3

Contact: CSIRO Enquiries
CSIROEnquiries@csiro.au
1300 363 400

Keywords: scientific workflow platform

Related Links: Publication: Workspace: A Platform for Delivering Scientific Applications
Publication: Workspace: scientific workflow platform
Website: Workspace website at CSIRO
Publication: Workspace - a Scientific Workflow System for enabling Research Impact
Publication: Opportunities for workflow tools to improve translation of research into impact

Supporting Files: workspace.license

Licence: CSIRO Binary Software Licence

Organisations: CSIRO (Australia)

Attribution Statement: CSIRO; Cleary, Paul; Hetherton, Lachlan; Bolger, Matt; Rucinski, Chris; Sankaranarayanan, Nirupama; Thomas, David; Watkins, Damien; Zhang, Zikai; Subramanian, Rajesh; Nguyen, Dang Quan; McNally, Matt (2018): Workspace: Scientific Workflow Platform. v14. CSIRO. Software Collection. https://doi.org/10.25919/5b3c1dc633cd3

Rights Statement: All Rights (including copyright) CSIRO 2018.

Access: The metadata and files (if any) are available to the public.

show all

Access: The metadata and files (if any) are available to the public.

show all

More about this Collection

Environment Requirements: Windows/Linux/Mac

Language (Programming): C++

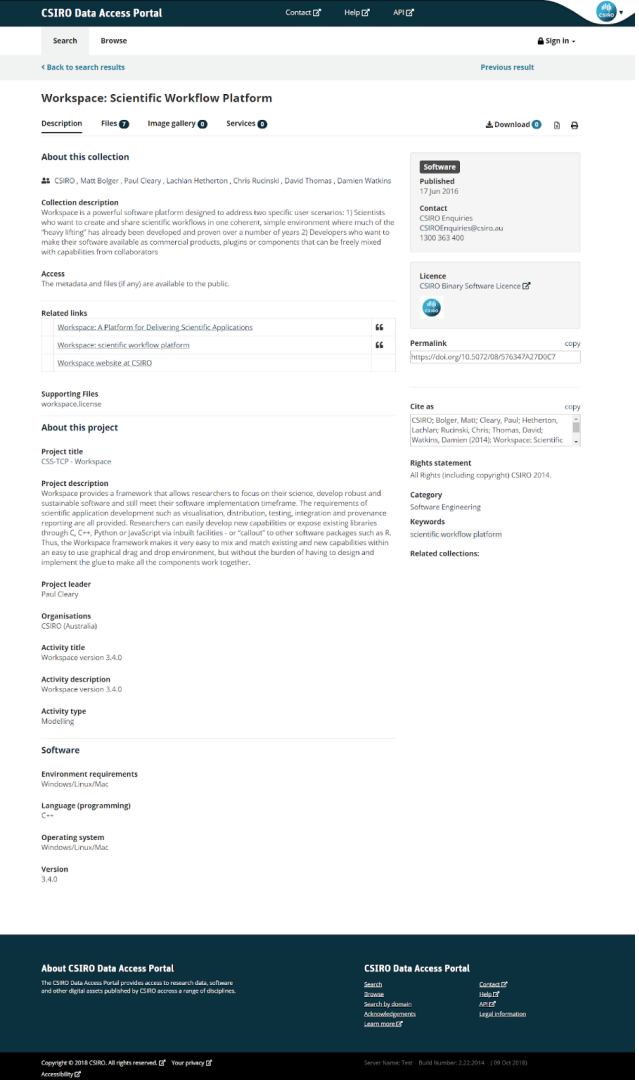
Operating System: Windows/Linux/Mac

Version: 5.4.0

About this Project

Project Title: Industrial Transformation and Situational Awareness

Project Description: Workspace is a powerful software platform designed to address two specific user scenarios: 1) Scientists who want to create and share scientific



Workspace: Scientific Workflow Platform

Description | Files 7 | Image gallery 0 | Services 0 | Download 0

About this collection

CSIRO , Matt Bolger , Paul Cleary , Lachlan Hetherton , Chris Rucinski , David Thomas , Damien Watkins

Collection description

Workspace is a powerful software platform designed to address two specific user scenarios: 1) Scientists who want to create and share scientific workflows in one coherent, simple environment where much of the "heavy lifting" has already been developed and proven over a number of years 2) Developers who want to make their software available as commercial products, plugins or components that can be freely mixed with capabilities from collaborators

Access

The metadata and files (if any) are available to the public.

Related links

Publication	Workspace: A Platform for Delivering Scientific Applications	❝
Publication	Workspace: scientific workflow platform	❝
Website	Workspace website at CSIRO	

Supporting Files

workspace.license

About this project

Software

Published
17 Jun 2016

Contact
CSIRO Enquiries
CSIROEnquiries@csiro.au
1300 363 400

Licence
CSIRO Binary Software Licence

Permalink copy
https://doi.org/10.5072/08/576347A27D0C7

Cite as copy

CSIRO; Cleary, Paul; Hetherton, Lachlan; Bolger, Matt; Rucinski, Chris; Sankaranarayanan, Nirupama; Thomas, David; Watkins, Damien; Zhang, Zikai; Subramanian, Rajesh; Nguyen, Dang Quan; McNally, Matt (2018): Workspace: Scientific Workflow Platform. v14. CSIRO. Software Collection. https://doi.org/10.25919/5b3c1dc633cd3

Workspace: Scientific Workflow Platform

Description Files 7 Image gallery 6 Services 3 Download 8

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- Workspace website at CSIRO

Supporting Files
workspace.license

About this project

Project title
CSS-TCP - Workspace

Project description
Workspace provides a framework that allows researchers to focus on their science, develop robust and sustainable software and still meet their software implementation timeframe. The requirements of scientific application development such as visualisation, distribution, testing, integration and provenance reporting are all provided. Researchers can easily develop new capabilities or expose existing libraries through C, C++, Python or JavaScript via inbuilt facilities - or "callout" to other software packages such as R. Thus, the Workspace framework makes it very easy to mix and match existing and new capabilities within an easy to use graphical drag and drop environment, but without the burden of having to design and implement the glue to make all the components work together.

Project leader
Paul Cleary

Organisations
CSIRO (Australia)

Activity title
Workspace version 3.4.0

Activity description
Workspace version 3.4.0

Activity type
Modelling

Software

Environment requirements
Windows/Linux/Mac

Language (programming)
C++

Operating system
Windows/Linux/Mac

Version
3.4.0

Software
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Cite as copy
CSIRO; Bolger, Matt; Cleary, Paul; Hetherton, Lachlan; Rucinski, Chris; Thomas, David; Watkins, Damien (2014): Workspace: Scientific

Rights statement
All Rights (including copyright) CSIRO 2014.

Category
Software Engineering

Keywords
scientific workflow platform

Related collections:

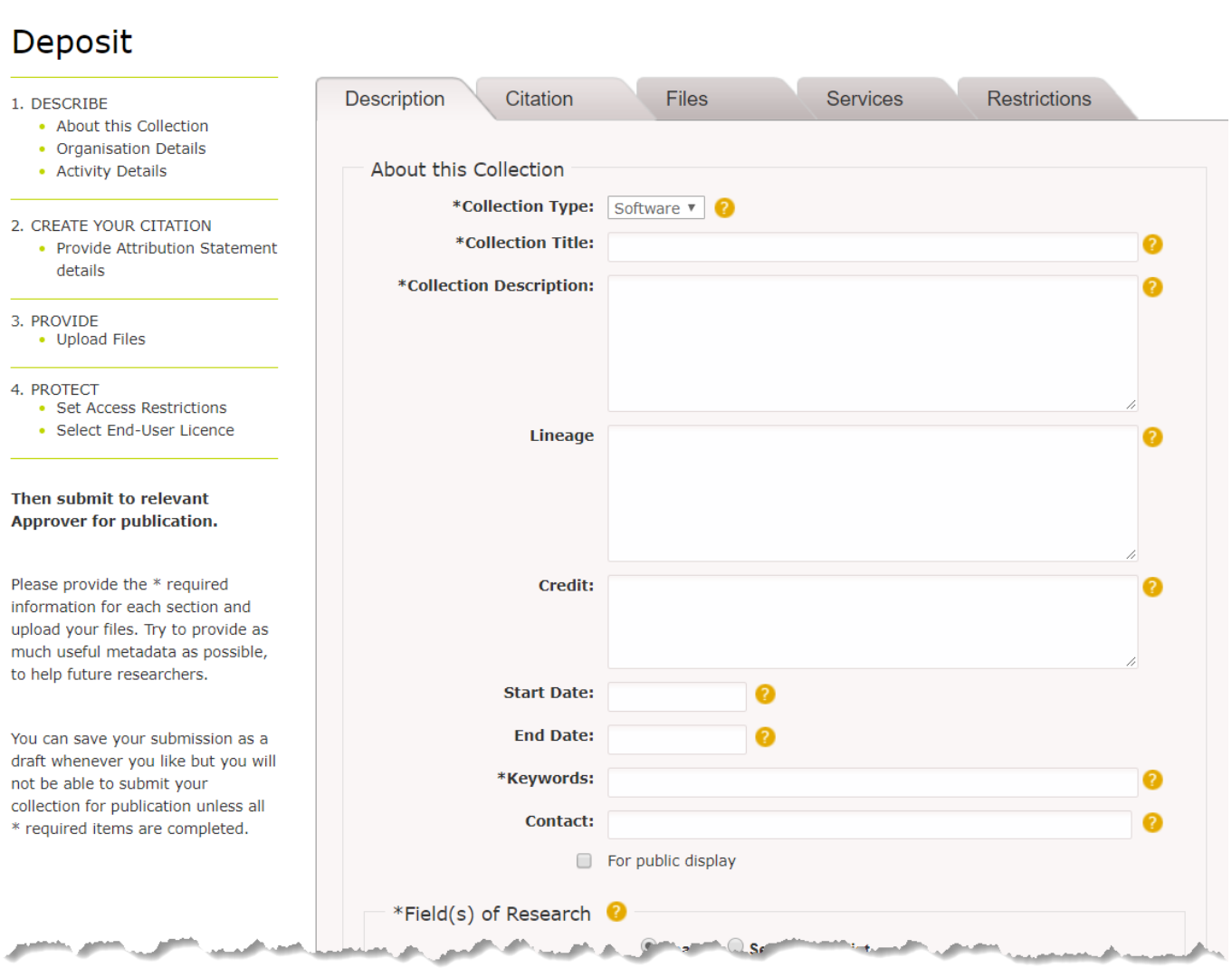
Software

Environment requirements
Windows/Linux/Mac

Language (programming)
C++

Operating system
Windows/Linux/Mac

Version
3.4.0



DAP common metadata: CSMD-CCLRC Core Scientific Metadata Model

More about this Collection

If you are entering software or data that requires specific research area fields, select extra descriptors to further search capabilities:

Metadata Schema: Software

- Select your metadata schema
- ANZLIC
- Darwin Core
- Marine Community Profile
- VO Resource
- Software
- Sensor

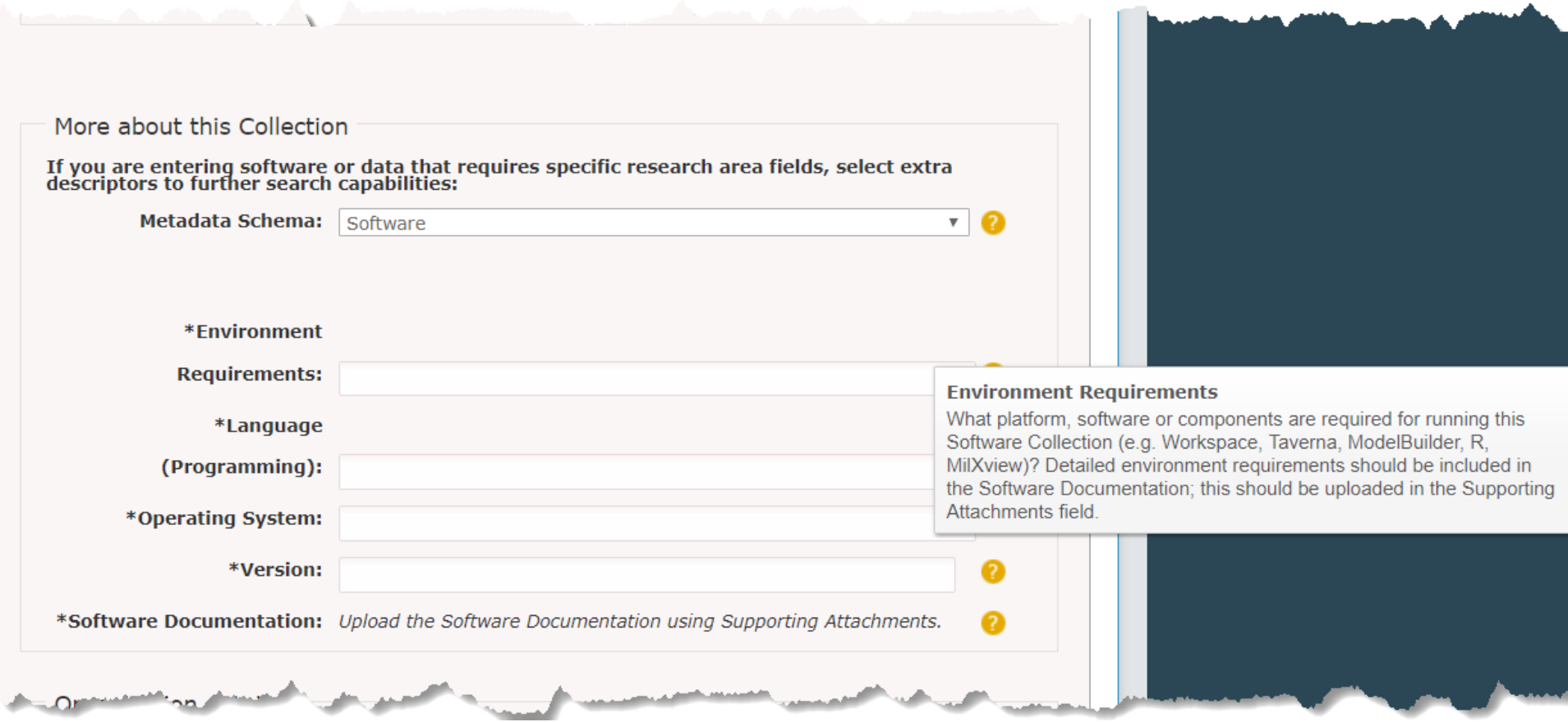
***Environment Requirements:**

***Language (Programming):**

***Operating System:**

***Version:**

***Software Documentation:** *Upload the Software Documentation using Supporting Attachments.*


More about this Collection
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Metadata Schema:
Software
*Environment
Requirements:
*Language
(Programming):
*Operating System:
*Version:
*Software Documentation:
Upload the Software Documentation using Supporting Attachments.
Environment Requirements
What platform, software or components are required for running this Software Collection (e.g. Workspace, Taverna, ModelBuilder, R, MilXview)? Detailed environment requirements should be included in the Software Documentation; this should be uploaded in the Supporting Attachments field.

Software Schema Usage

Metadata access	Used Software Schema?		Totals
	Yes	No	
Public	64	26	90
CSIRO Only	3	3	6
Specific Users	1	1	2
Totals	**68**	**30**	**98**

Schema.org tags


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        "datePublished": "2018",
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        "publisher" : "CSIRO",
        "temporalCoverage": "",
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        "identifier" : "DOI : 10.25919/5b3c1dc633cd3",
        "URL" : "https://doi.org/10.25919/5b3c1dc633cd3"

}
</script>
```

Next

Rest of 2018

- Tech debt and consolidation
  - Could address some of our gaps- eg collection types in DataCite and schema.org

2019/20

- New UI for depositor pages
- Greatly enhanced API for deposit

Vision

- Deposit API and CodeMeta could be mapped to pull in software from code repositories.

‹ More Library Services news

04 October 2018
Get to know Altmetrics ›

03 October 2018
Learn more about Library Services ›

02 October 2018
New Taylor and Francis eBooks in chemical engineering ›

27 September 2018
Cambridge University Press eBooks in Physics and Astronomy ›

25 September 2018
EndNote Training October ›

Make your research software citable

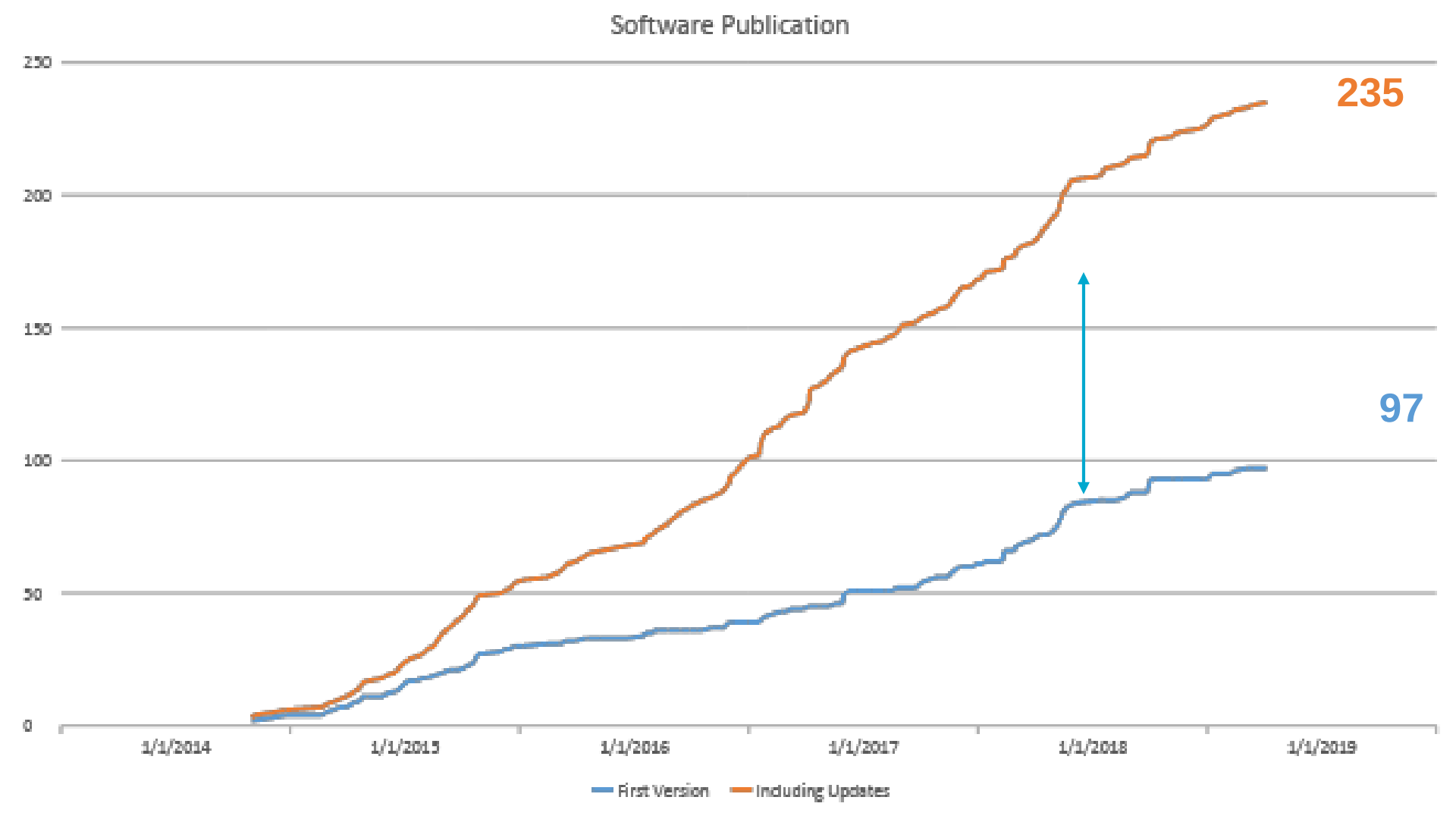
Did you know that you can make your research software citable?

More and more journals are adopting the FORCE 11 Software Citation principles and encouraging researchers to make the software that was used in their research available. The easiest way for people to find out about the availability of your research software is to cite it in your references.

The way to do this in CSIRO is to publish your software in the CSIRO Data Access Portal (DAP). This will create a snapshot of the version that you used and give you an attribution statement, including a DOI, which can be used as your citation. If you want to update your software later, you can simply update the existing record with the new release and the DAP will give you a new DOI and keep both versions preserved. See how other researchers have already created software records.

There is a Software Release Process that needs to be completed. This will help you to select the right licence for your software. Putting a record on the DAP will generate an approval process so you know your CSIRO compliance issues are taken care of.

See Using the DAP for software or contact researchdatasupport@csiro.au for more information.


Software Publication
250
200
150
100
50
0
235
97
1/1/2014
1/1/2015
1/1/2016
1/1/2017
1/1/2018
1/1/2019
First Version
Including Updates

Thank you

Thanks to:

Dom Hogan for the statistics and

Research Data Support team for feedback

CLEX software publishing workflow

Paola Petrelli - Climate data officer

ARC Centre of excellence for Climate Extremes

The Centre of Excellence for Climate Extremes (CLEX) is a major initiative funded by the Australian Research Council. The Centre is an international research consortium of five Australian universities and a network of outstanding national and international partner organizations.

What we’re trying to achieve

Encourage our community to share their codes

Provide a source of relevant and reliable code for our community

Supply a place to publish software in case our researchers want or have to

Starting point

We are not an institution we rely on others for services (mostly)

We need to act quickly: less than 6 yrs left

We have a “data source” with RDA

We work at NCI and so publish data with their services

We manage a github organization: https://github.com/coecms

We manage a DMP web tool based on the UK DCC roadmap/dmponline

Which software

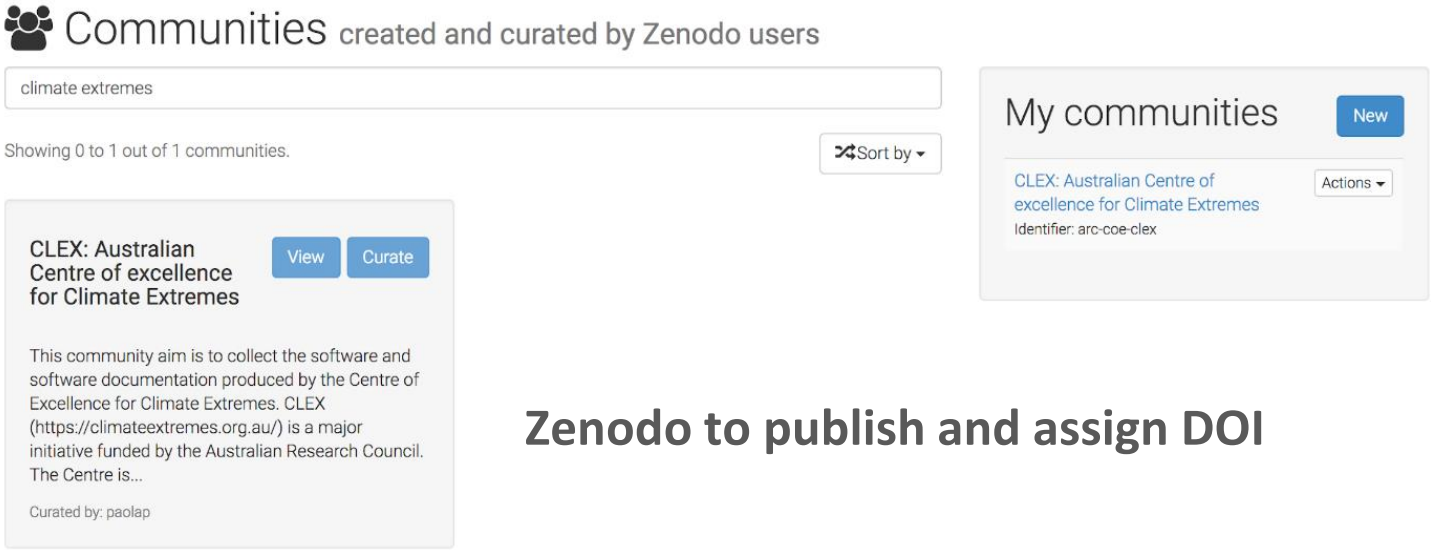
From github:

- Code produced by our team: manage data/model and analysis
- Code produced by student and researchers: for analysis, often used by the all research group, occasionally by a wider community

Lost somewhere:

- Model related combination of code and data, as: configurations, alterations of a model scheme, tutorials.

Proposed workflow



Zenodo to publish and assign DOI

Publishing also on RDA using existing data source

CleX Roadmap data plan tool to create metadata and/or keep track of records.

Proposed workflow

Version control

Most code already on github or bitbucket.

Model configurations? Probably provide some form of template to help collecting them

Add metadata

Collect information from repository and save as codemeta.json and zenodo.json files:

- harvest metadata from repository (python)
- template on Clex Roadmap

Upload json files to repository

Publish zenodo & RDA

Admin review records and publish to zenodo CleX community: python code using zenodo api.

Export record to RDA

If metadata harvested directly from repository, then harvest record from zenodo to CleX Roadmap.

Describing software for Virtual Labs

Geoffrey Squire

www.data61.csiro.au

Describing software for use

- Publishing software is easy
  - e.g. via GitHub, PyPI, download
  - Findable
  - Accessible
- But users want to Just Use It!

The goal is to make published software more useable by enabling automation.

Information Model

Applications run **Solutions** that use **Toolboxes** to solve Problems

- Machine-readable descriptions
- Metadata for searching, understanding, citation and provenance
- Sufficient to provision and run software automatically

Toolbox

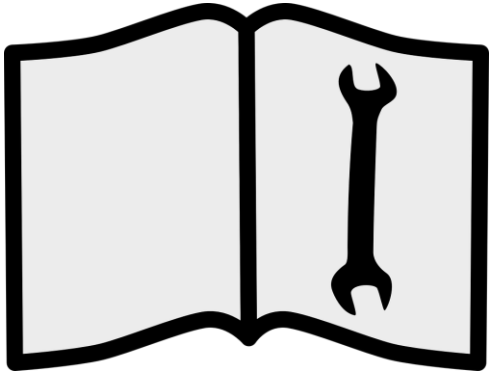
Describes a software environment that can run published software

- Links to the published software
- How to instantiate the environment
- Dependencies
  - python
  - puppet
  - toolbox
- Implementation
  - cloud image
  - HPC
  - puppet module
  - execute instructions

Solution

Describes a workflow that uses a Toolbox to solve a specific Problem

- Link to published artifact (e.g. python script)
- Link to the Problem it solves
- Dependencies
  - Toolbox (usually)
- How to implement the Solution
  - Specification of inputs and outputs
    - Name
    - Description
    - Type
    - Constraints



Making it all useful

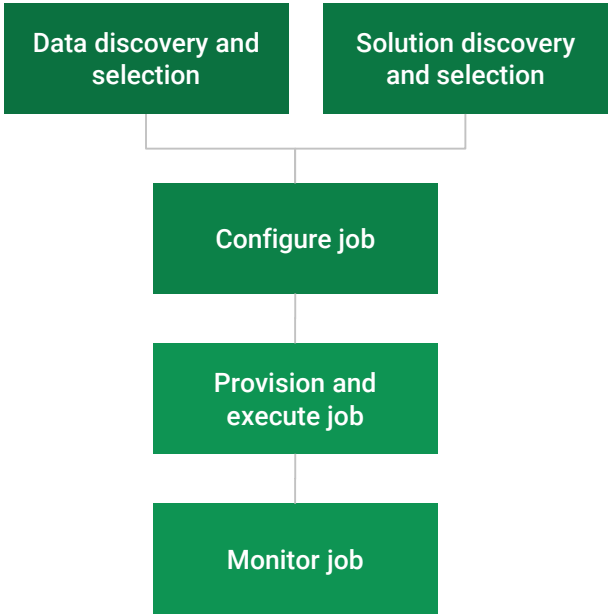
- A Solution Centre is a catalogue of Toolboxes and Solutions
- Developers (or others!) can publish descriptions of their software
- URIs for reference, citation and provenance
- Client apps can discover Solutions plus info to use them
- WIP on CodeMeta, RIF-CS and DOIs

https://sssc-vgl.geoanalytics.csiro.au

Making use of it all

- Virtual Laboratories (VLs) are clients
  - Data sets and services from registries
  - Solutions and toolboxes from the Solution Centre
- Users find relevant and **useable** data and solutions
- VL automates the job:
  - Generate UI to configure the Solution (parameters and inputs)
  - Assemble software environment
  - Wrangle input data
  - Execute and monitor the job
  - Store outputs and notify user when complete
  - Provide a provenance record

https://vgl.auscope.org



THANK YOU

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Software Engineer

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Q/A, Discussion

Thank you ...

Research software interest group:
https://www.ands.org.au/partners-and-communities/ands-communities/ascig-software-citation