FORCE11
The Future of Research Communications and e-Scholarship

RDA
RESEARCH DATA ALLIANCE

https://tinyurl.com/qpg7n7m

Use Cases and Software Source Code Identification

SCID WG

research data sharing without barriers
rd-alliance.org

27th March 2020 - RDA 15th Plenary Virtual Meeting

Contributors (alphabetical order by name)

https://tinyurl.com/qpg7n7m

- Alice Allen, Astronomy Source Code Library & U. Maryland, USA
- Anita Bandrowski - University of California San Diego, USA
- Roberto Di Cosmo - Software Heritage, Inria and University of Paris, France
- Martin Fenner - DataCite, Germany
- Morane Gruenpeter - Inria, Software Heritage, France
- Daniel S. Katz - University of Illinois at Urbana-Champaign, USA
- John Kunze - California Digital Library, University of California, USA
- Moritz Schubotz - swMATH, FIZ Karlsruhe, Germany

Agenda

https://tinyurl.com/qpg7n7m

- Introduction
  - Objectives, Outputs, Connections to other WG
- Use cases (Archiving, Referencing, Describing, Citing, etc.)
  - Audience may suggest additional use cases
- Identifiers schemas
  - DOIs, Hashes, SWH-ID,Wikidata entities, ARKS, ASCL-ID, RRID, swMATH-ID
- Small group discussion
  - documenting the use case : challenges, pros, and cons of different identifiers per use case
- Report-back and discussion
- Wrap-up

Introduction

Software Source Code Identification Working Group

Co-chairs

- Roberto Di Cosmo
- Martin Fenner
- Daniel S. Katz

Web page
https://www.rd-alliance.org/groups/software-source-code-identification-wg

Repository
https://github.com/force11/force11-rda-scidwg

Chronology...

Spawned at RDA **P11** in Berlin from

- the RDA SSC IG &
- the FORCE11 SCIWG

10/2018 - TAB endorsement

4/2019 - RDA **P13**, Philadelphia

- **WG kick-off**
- **ASCL & SWH presentation**

10/2019 - **FORCE2019**, Edinburgh
Full day hackathon on research software

Goals

https://tinyurl.com/qpg7n7m

- Bring together people involved/interested in software identification
  - Talk about why this is an issue
  - Talk about different types of identifiers
  - Talk about use cases
  - Discuss pros and cons of different identifiers for different use cases
  - Document discussions
- Produce concrete recommendations for the academic community

Expected outputs

https://tinyurl.com/qpg7n7m

Medium-term goals (M12)

- An initial collection of software identification **use cases** and software **identifier schemas**.
- An overview of the different contexts in which software artifact identification is relevant, including:
  - Scientific **reproducibility**
  - Fine grained **reference** to specific code fragments from scientific articles or documentation
  - Description of **dependency** information
  - Citation of software projects for proper **credit attribution**

Long-term goals (M18)

- Call out other RDA groups, in particular those working on citation and versioning issues, for consultation on the draft guidelines
- A set of guidelines for persistent software artifact identification, in each of the above contexts

Output due June 2020

Related Project - FORCE11 Software Citation

FORCE11 Software Citation Implementation Working Group
(co-chairs: N. Chue Hong, M. Fenner, D. S. Katz)

Following-on from FORCE11 Software Citation Working Group and the Software Citation Principles it developed

Objective: Produce concrete guidelines for software citation, and implement them within the scholarly research community (software developers, repositories and registries, journals and conference and publishers, indexers, institutions)

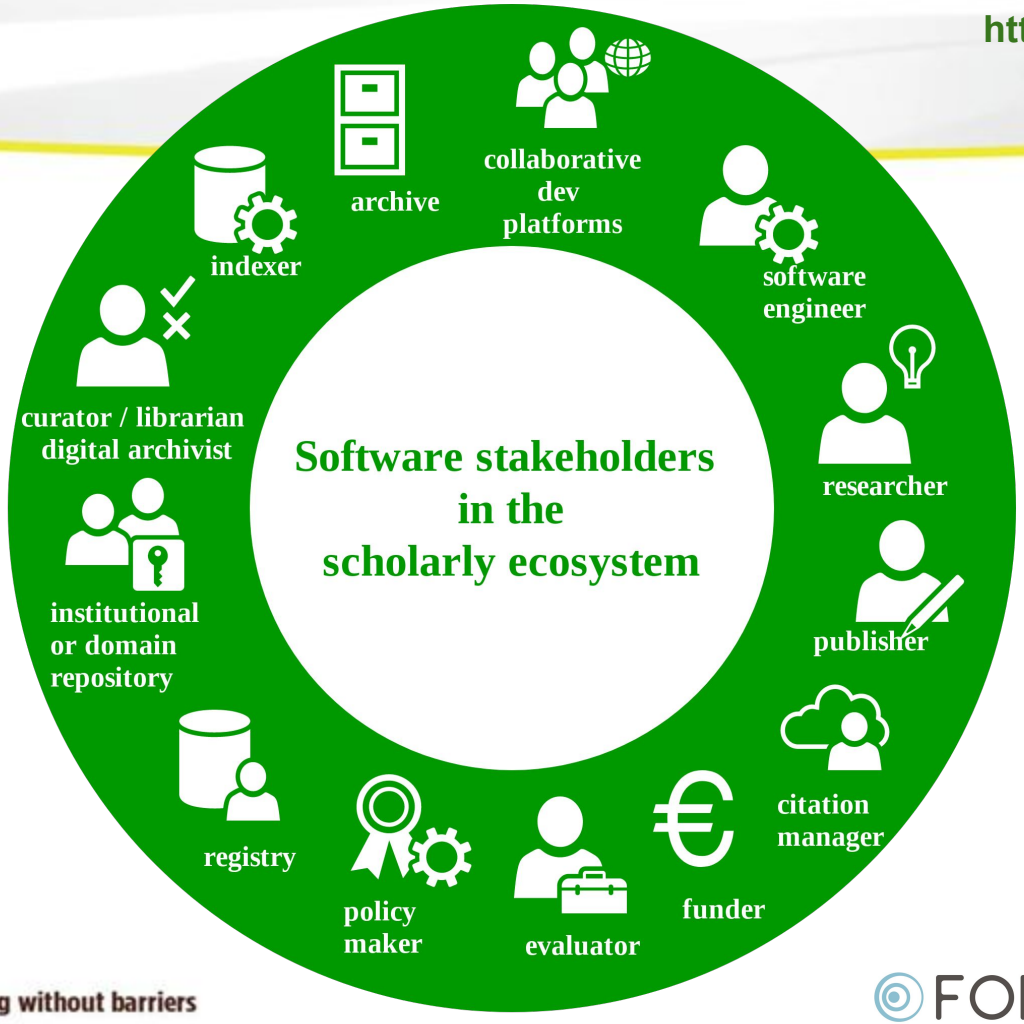
A community with monthly calls to discuss challenges and progress in implementing software citation, with task forces for

- **CodeMeta** - standardizing metadata for software, moving towards merging into schema.org
- **Guidance** - developing documents for developers, authors, and reviewer
- **Journals** - coordinating editors and publishers to simplify and implement guidance
- **Repositories** - developing best practices document for handling software

Use cases

Actors

https://tinyurl.com/qpg7n7m



Partly taken from the
Software Citation Principles
https://peerj.com/articles/cs-86/

What is at stake

[Archive]

ensure (research) software artifacts *are not lost*

[Reference]

ensure (research) software artifacts *can be precisely identified*

[Describe]

make it easy to *discover / find* (research) software artifacts

[Credit]

ensure *proper credit* is given *to authors*

Use cases

https://tinyurl.com/qpg7n7m

researcher *:*

- **access and use** SSC *no longer available* on a collaborative platform [**Archive**]
- **reproduce** an experiment detailed in an article (replication studies) [**Reference**]
- **reference** SSC used in an article (SageMath algorithm example) [**Reference**]
- **search and find** appropriate SSC using rich metadata [**Describe**]
- **give and get credit** for research SSC via correct *citations* to articles and data [**Credit**]

Let's see some concrete examples

Use case: replication studies

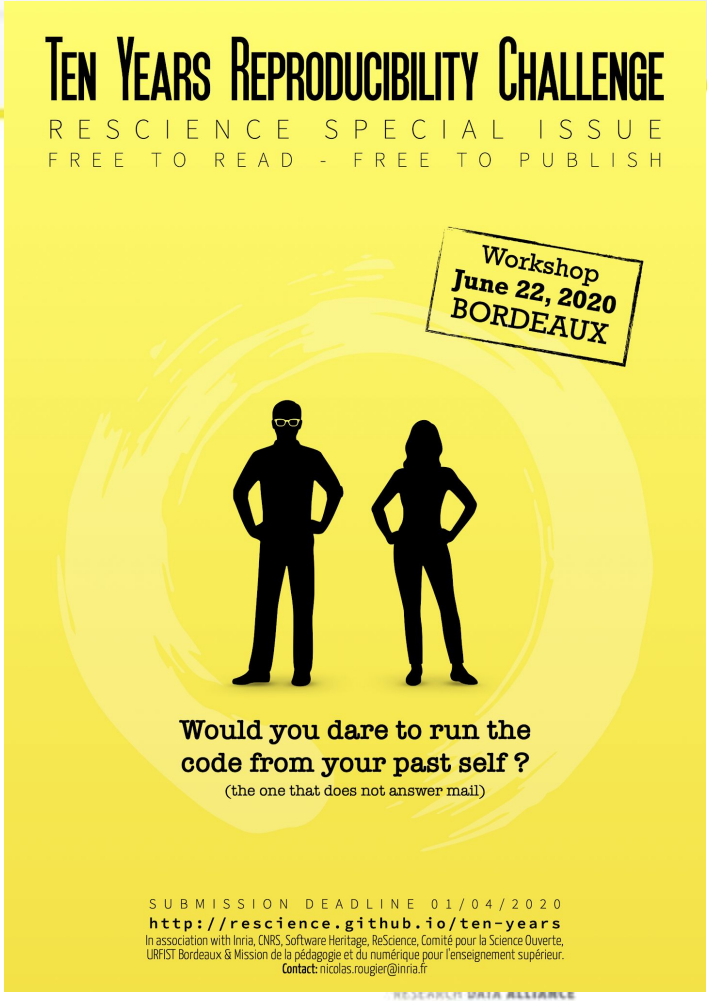
A *researcher* wants to reproduce* an experiment from an article **[Archive] [Reference]**

See the *10 years Reproducibility challenge*:

1. **find the source code**
2. make small modifications
3. **run** and **reproduce**
4. **write** (reproducible) report and share

Here is a detailed example:

Reproducing and replicating the OCamlP3l experiment

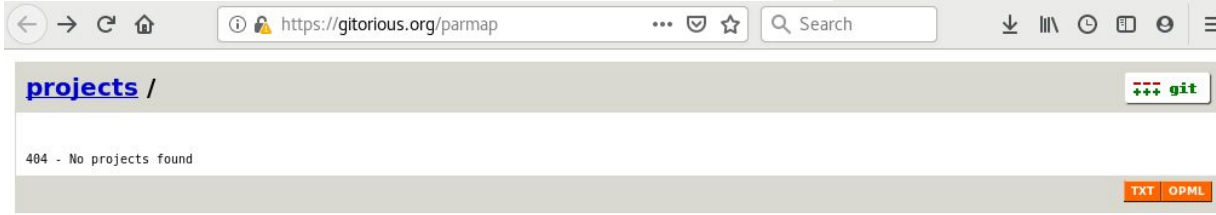


Use case: (re)use a software tool

A *researcher* wants to **access and use** SSC presented in an article, that might no longer be available on a collaborative development platform [**Archive**]

6. Conclusions

Parmap is a minimalistic library allowing to exploit multi-core architecture for OCaml programs. It has been designed with the goal of providing parallel map and reduce to OCaml programmers in a fairly natural way, such that the "minimal disruption" principle stated by Cole in his skeleton manifesto paper is enforced. In fact, in order to use Parmap, it is sufficient to substitute the calls to List functions with calls to the equivalent Parmap functions. The clean and efficient implementation of Parmap is such that nearly optimal speedups are achieved on state-of-the-art multi-core architectures when suitable grain computations are parallelized. The full source code of the Parmap library is available under the LGPL licence from http://gitorious.org/parmap, and is now also incorporated in the GODI installation system for OCaml librairies.

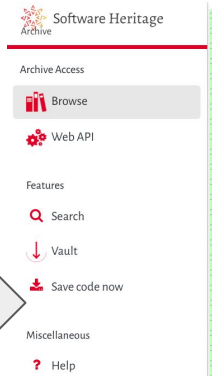


Use case: link to the *algorithm*

Researcher references in an article the exact relevant code fragment **[Reference]**

```
let simplemapper ncores compute opid al combine =
  (* init task parameters *)
  let ln = Array.length al in
  let chunksize = ln/ncores in
  (* create descriptors to mmap *)
  let fdarr=Array.init ncores (fun _ -> tempfd()) in
  (* spawn children *)
  for i = 0 to ncores-1 do
    match Unix.fork() with
      0 -> (* children code: compute on the chunk *)
           (let lo=i*chunksize in
            let hi=if i=ncores-1 then ln-1
                   else (i+1)*chunksize-1 in
            let v = compute al lo hi opid in
            marshal fdarr.(i) v;
            exit 0)
    | -1 -> failwith "Fork error"
    | pid -> ()
  done;
  (* wait for all children *)
  for i = 0 to ncores-1 do ignore(Unix.wait()) done;
  (* read in all data *)
  let res = ref [] in
  (* accumulate the results in the right order *)
  for i = 0 to ncores-1 do
      res:= ((unmarshal fdarr.((ncores-1)-i)):'d)::!res
  done;
  (* combine all results *)
  combine !res;;
```

Clickable link
(click here!)




```
let simplemapper ncores compute opid al collect =
  (* flush everything *)
  flush_all();
  (* init task parameters *)
  let ln = Array.length al in
  let chunksize = ln/ncores in
  (* create descriptors to mmap *)
  let fdarr=Array.init ncores (fun _ -> tempfd()) in
  (* call the GC before forking *)
  Gc.compact ();
  (* spawn children *)
  for i = 0 to ncores-1 do
    match Unix.fork() with
      0 ->
        begin
          let lo=i*chunksize in
          let hi=if i=ncores-1 then ln-1 else (i+1)*chunksize-1 in
          let exc_handler e j = (* handle an exception at index j *)
            info "error at index j=%d in (%d,%d), chunksize=%d of a total of %d got exception
              j lo hi chunksize (hi-lo+1) (Printexc.to_string e) i;
            exit 1
          in
          let v = compute al lo hi opid exc_handler in
          marshal fdarr.(i) v;
          exit 0
        end
    | -1 -> info "fork error: pid %d; i=%d" (Unix.getpid()) i;
    | pid -> ()
  done;
  (* wait for all children *)
  for i = 0 to ncores-1 do
    try ignore(Unix.wait())
    with Unix.Unix_error (Unix.ECHILD, _, _) -> ()
  done;
  (* read in all data *)
  let res = ref [] in
  (* iterate in reverse order, to accumulate in the right order *)
  for i = 0 to ncores-1 do
      res:= ((unmarshal fdarr.((ncores-1)-i)):'d)::!res;
  done;
  (* collect all results *)
  collect !res
;;
```

Permalink

Figure from a real research article

Corresponding code fragment

Use case: highlight software fragments

A *journalist* links to telltale fragments of the Apollo11 SSC **[Reference][Archive]**

[The code that took America to the moon was just published to GitHub, and it's like a 1960s time capsule July 9, 2016 By Keith Collins]

QUARTZ EMAILS EDITIONS B

One of the source code files, for example, is called `BURN_BABY_BURN--MASTER_IGNITION_ROUTINE`, and the opening comments explain why:

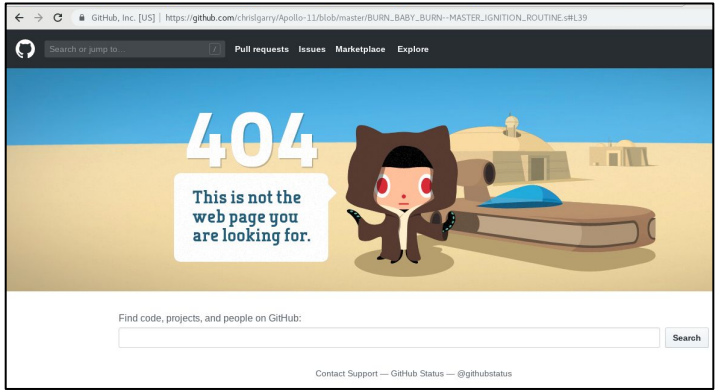
About 900 lines into that subroutine, a reader can see the playfulness of the original programming team come through, in the first and last comments in this block of code:

In the file called `LUNAR_LANDING_GUIDANCE_EQUATIONS.s`, it appears that two lines of code meant to be temporary ended up being permanent, against the hopes of one programmer:

In the same file, there's also code that appears to instruct an astronaut to "crank the silly thing around."

"That code is all about positioning the antenna for the LR (landing radar)," Burkey explained. "I presume that it's displaying a code to warn the astronaut to reposition it."

-MASTER_IGNITION_ROUTINE.s#L39



[Software Heritage blog post with all archived references]

Important remark: *relevant SSC may not be author archived!*

RDA RESEARCH DATA ALLIANCE

Use case(s): career and activity reports

- **Researcher**: curriculum vitae, promotion, activity report, grant applications
- **Lab/team**: track software production and contributions
- **University/Research institution**: tech transfer, metrics, scientific policy

Granularities can be ***coarser*** than a release:

“Inria created OCaml and Scikit-learn”

Contributions can be more fine grained than just “author/contributor”:

Architecture, Management, Development, Documentation, Testing, ...

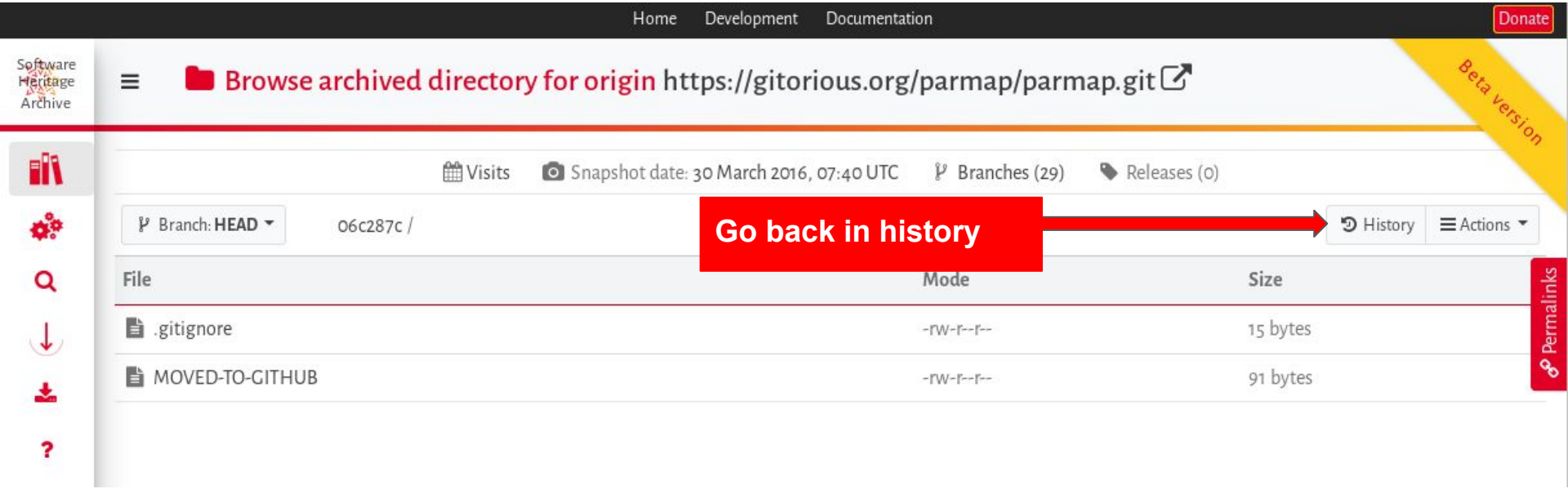
More use cases

https://tinyurl.com/qpg7n7m

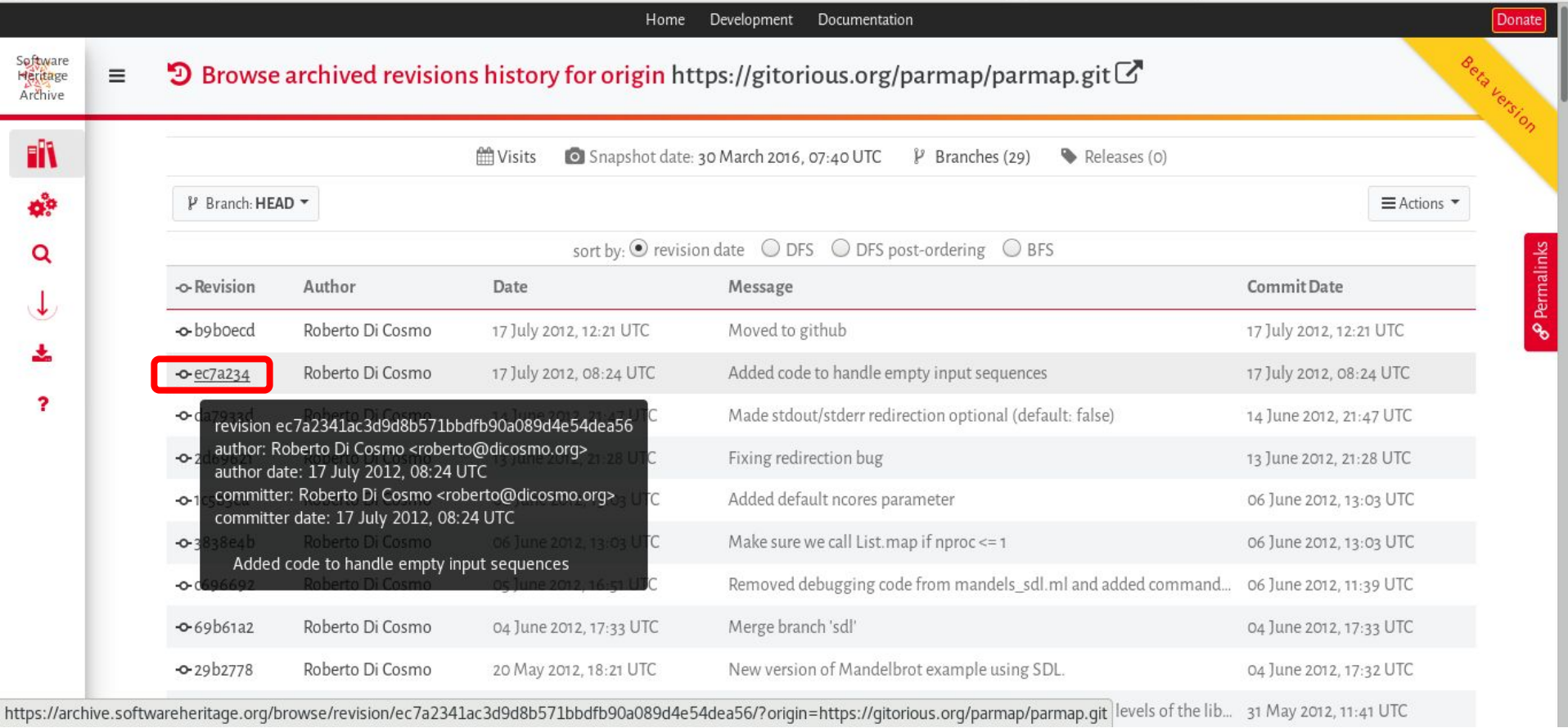
- software engineer :
  - **contribute** and improve existing SSC **[Contribute]**
- digital archivist :
  - **browse** the development history of legacy SSC (Apollo11 example) **[Archive]**
- funder :
  - **identify and evaluate** the impact of the funded software projects **[Describe][Credit]**
- registry :
  - **identify** and **curate** the software entries I hold **[Archive] [Reference] [Describe] [Cite]**
- Audience may suggest additional use cases here

Access Parmap example (archived copy)

[Software Heritage guidelines for research software]



Access and identify a point in history



Ice-breaker: propose your use case

https://tinyurl.com/qpg7n7m

Identifiers schemas

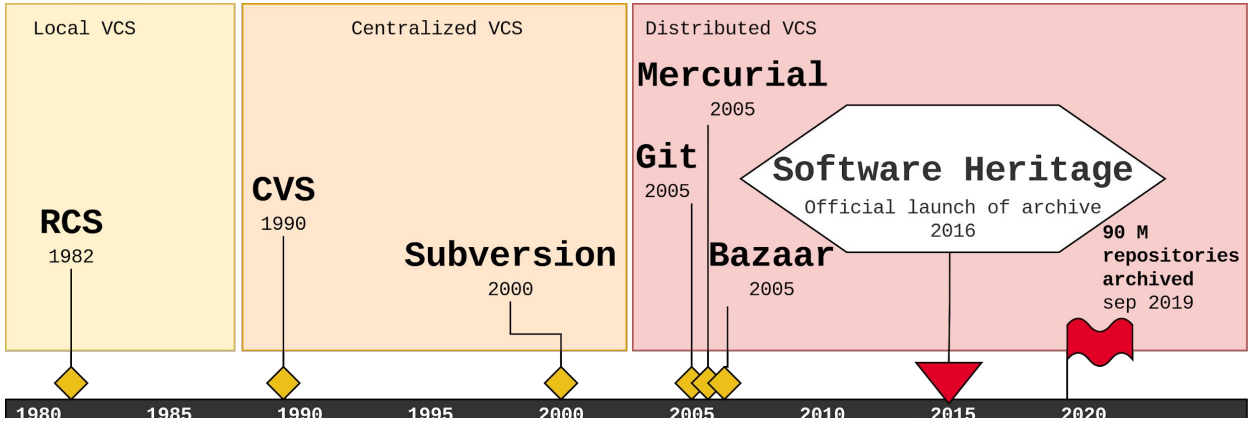
Cryptographic Hashes in VCS

Version control system (VCS)

- records changes made to a (set of) source code file (s)
- allows to operate on versions: diff/merge/fork/recover etc.
- essential tool for software development

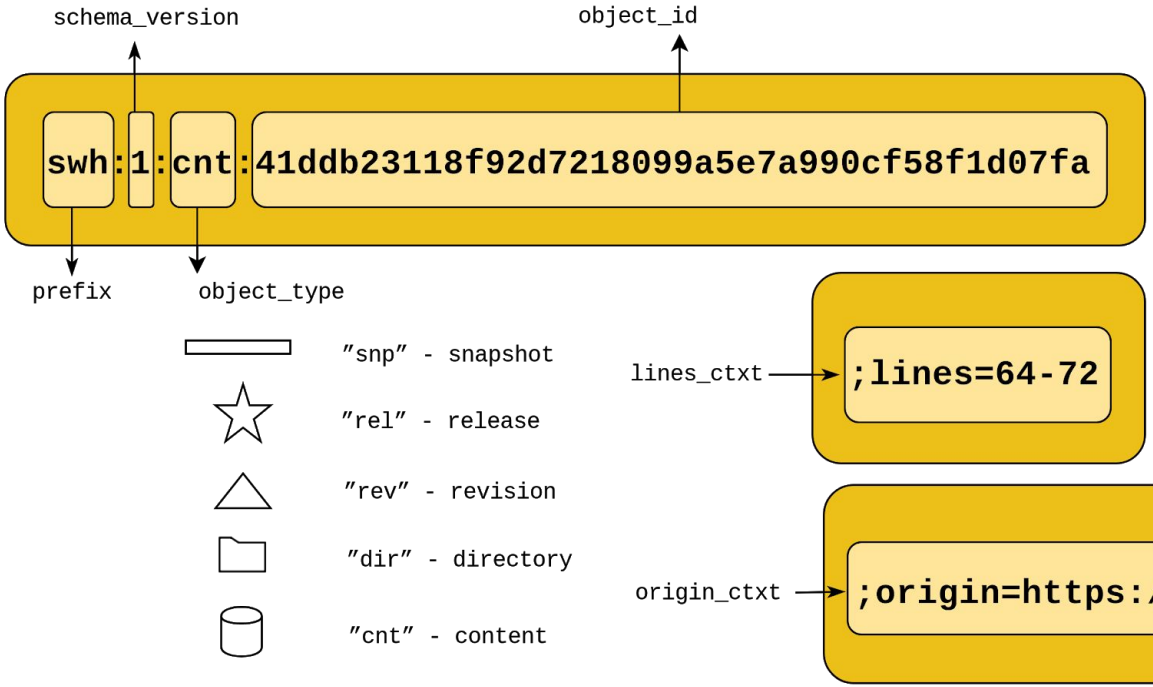
Guarantees:

- Unique identification
- Artifact integrity
- Work for tree structure



Software Heritage ID (more info here)

[Archive][Reference]



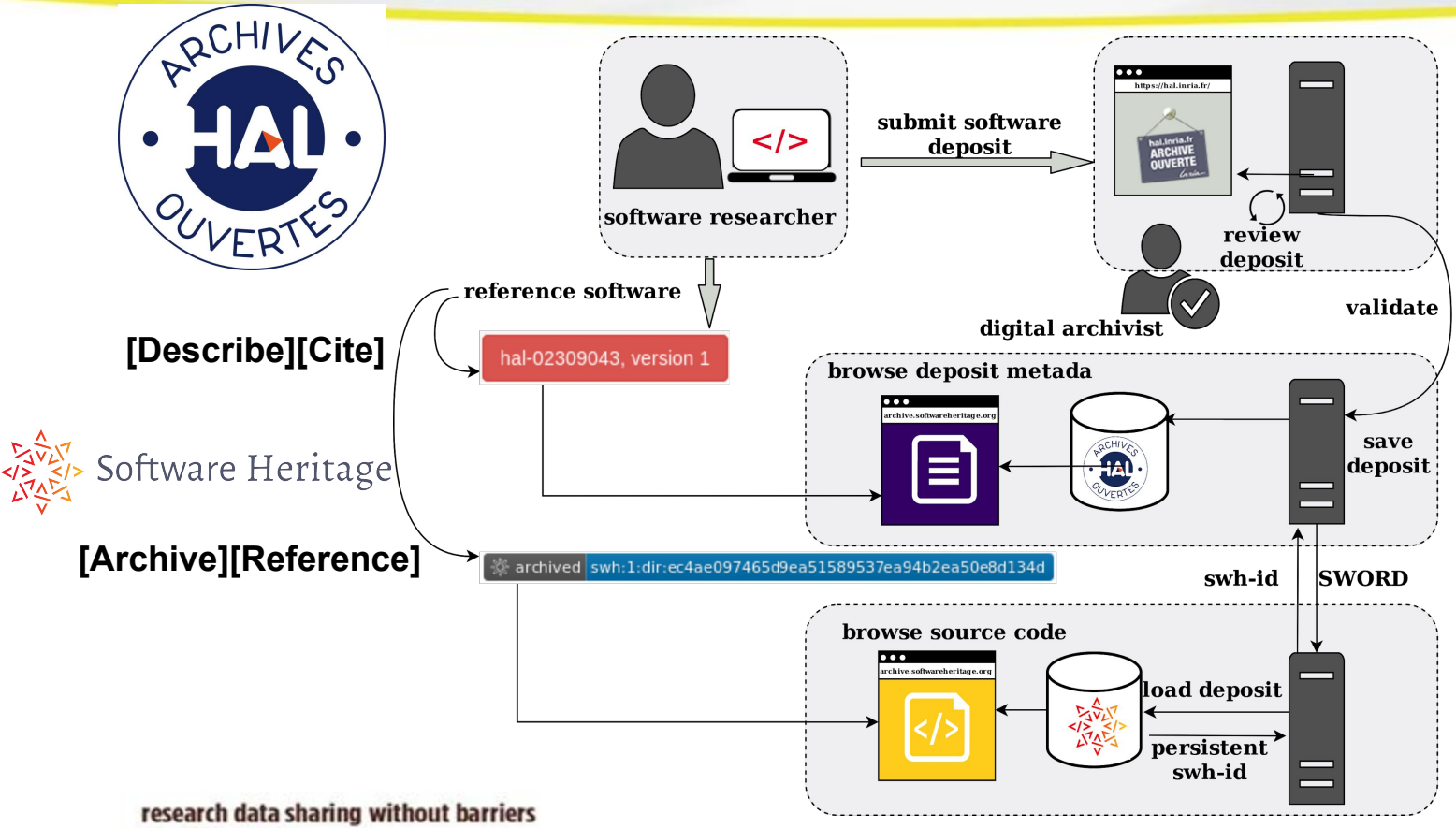
- An intrinsic software fingerprint
- A cryptographic hash
- Git compatible
- Resolvable on :
  - archive.softwareheritage.org
  - n2t.net
  - Identifiers.org
- Linkable with :
  - HAL
  - swMATH
  - Wikidata

Deposit software on the french national archive **HAL**

[Deposit guide]

[Describe][Cite]

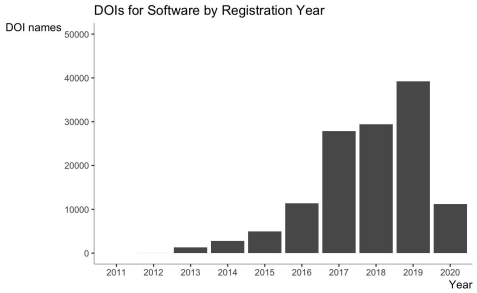
[Archive][Reference]



Software Heritage

DOI (Digital Object Identifier)

Persistent identifier supporting standard citation metadata, and linking to other PIDs. DataCite has registered 128,276 DOIs (84% in Zenodo) for software as of March 26,2020.



Cited, e.g. in bioRxiv preprint https://doi.org/10.1101/534834:

[14] A. Gitter, "Single-cell RNA-seq pseudotime estimation algorithms," *doi:10.5281/zenodo.1297422*, Jun 2018.

Included in ORCID record, e.g. http://orcid.org/0000-0002-9247-0530:

bcbi/ModelSanitizer.jl: v0.3.0
Zenodo
2019-08-06 | other
DOI: 10.5281/zenodo.3361519

Source: DataCite ★ Preferred source (of 4)

ARK (Archival Resource Key)

With no fees, 3.2 billion ARKs have been assigned by 580 institutions to things digital, physical, & abstract; resolution is decentralized or, via n2t.net, centralized

Assigners choose (e.g., legacy commit ids) or generate (e.g., opaque ids such as UUID or Noid) name strings, which are registered with redirection target URLs

Example: **`ark:/12345/b67c89d/part3.cvs`**, where **`12345`** is the institution, **`b67c89d`** the thing, **`/part3`** optional subthing, and **`.cvs`**, optional variant qualifier

Cite in actionable form, eg, **`n2t.net/ark:/12345/f98g76`**; ARKs appear in the Data Citation Index, Wikipedia, Wikidata, ORCID profiles, and Internet Archive

Registries identifiers: ASCL-ID

Astrophysics Source Code Library: Registry and repository for source code in astrophysics

Items registered by authors (or sometimes journal editors or users) or added by ASCL editors based on their appearing in the astrophysics literature

Identifiers are **`ascl:`*`yymm.xxx`***, where *yy* & *mm* are year & month of addition to ASCL, and *xxx* indicates that software was the xxx'th ASCL entry in the month

ASCL is indexed by the SAO/NASA Astrophysics Data System (ADS) and Web of Science; entries can be cited using their unique ASCL identifier

Registries identifiers: RRID

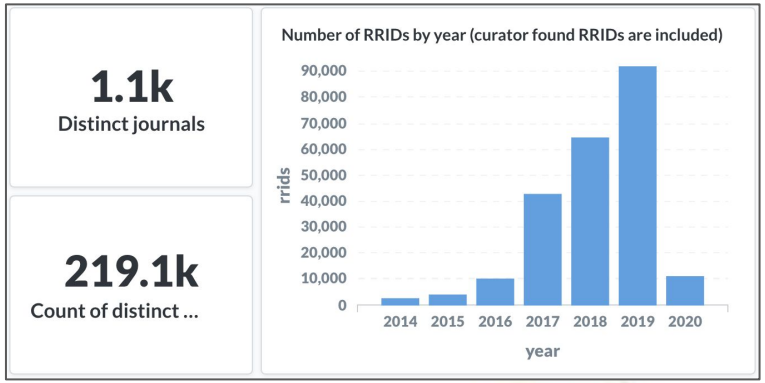
Research Resource Identifiers are used mostly in biomedicine, registered via SciCrunch: a system that aggregates ~25 RRID registries or repositories, such as the antibody registry, or Addgene repository

The SciCrunch registry is a listing of software projects (e.g., SPSS, ImageJ), services (e.g., core facilities), and data projects (e.g., NeuroMorpoho.org) that may need to be cited as **aggregate entities** in the scientific literature, but authors may not wish to cite a specific bit of source code

RRID format: **`RRID:SCR_12345`** (*SCR* = repository code, *12345* = local identifier in that repository)

Why register? Journals ask authors to do so.

Where are they? Methods sections (table of reagents) ->

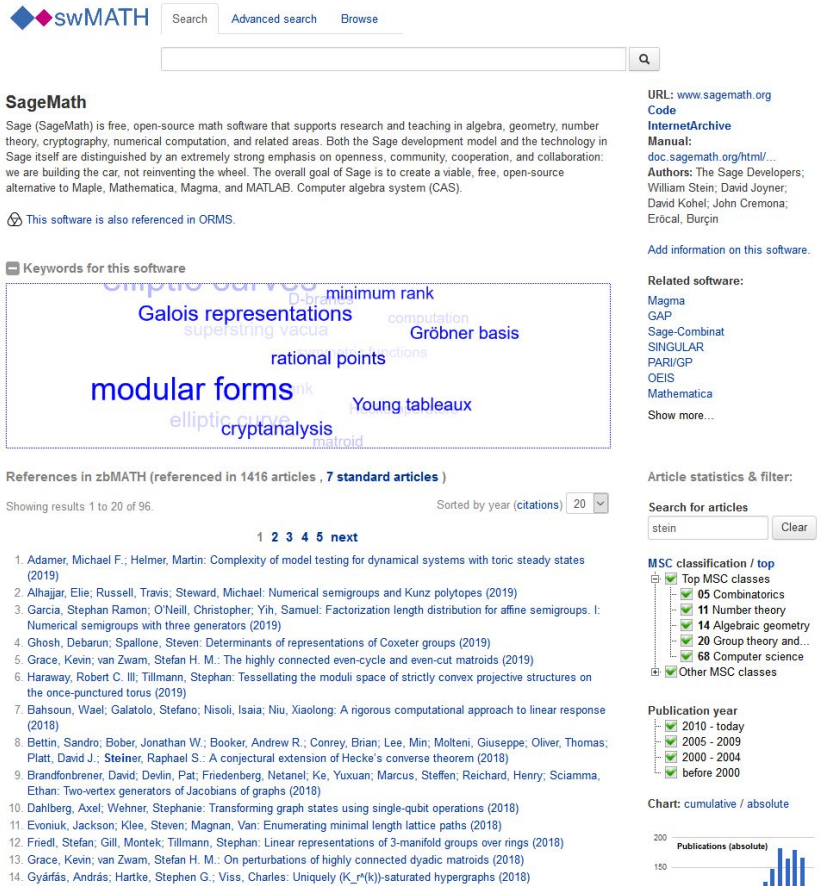


FORCE11
The Future of Research Communications and e-Scholarship

RDA
RESEARCH DATA ALLIANCE

Registries identifiers: swMATH-ID

- swMATH provides information on software referenced in mathematical publications
- Software is identified with a numeric Identifier, e.g., 825=SageMath
- In addition it provides informations on
  - Authors
  - Classification of the software
  - Information on citations in mathematical Publications
- The dataset is manually curated
- Back and forth linking efforts with
  - Wikidata
  - Software Heritage

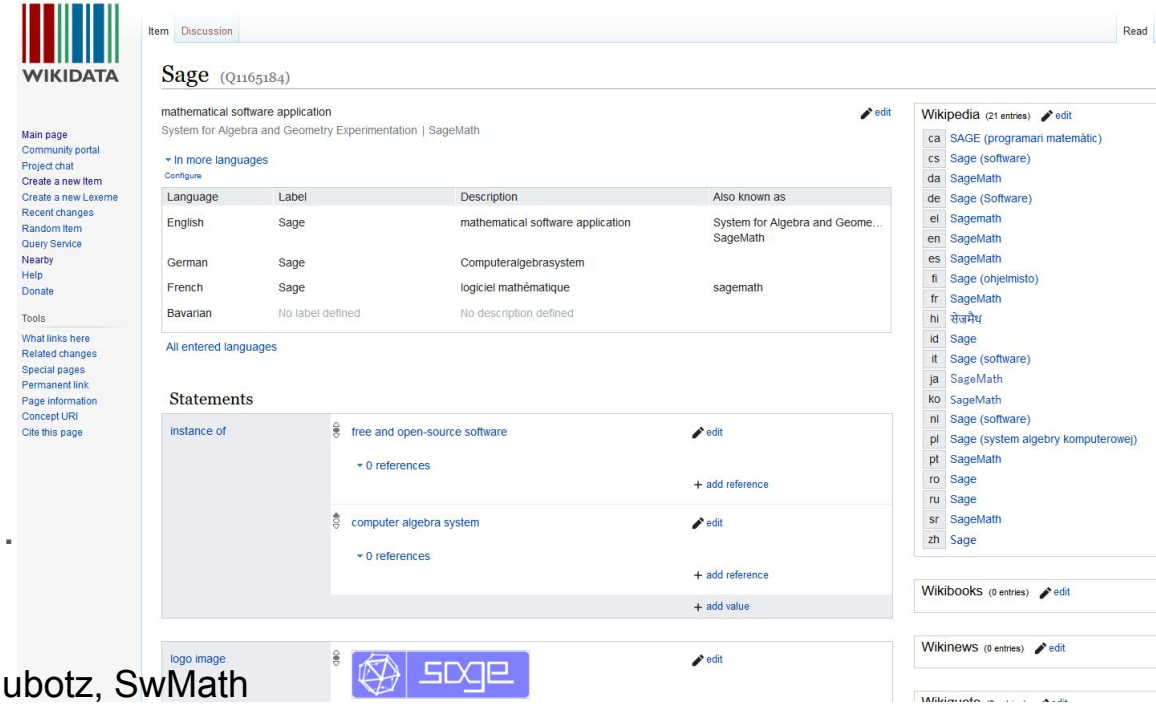


research data sharing without barriers
rd-alliance.org

Slide credit: Moritz Schubotz, SwMath

Wikidata entities

- Numeric identifiers prefixed with Q, e.g, Q1165184=SageMath
- Version information is maintained with the property software version identifier P348
- Identifier can be merged to remove duplicates
- Open editing
- Multilingual
- All kinds of “external” Identifiers, e.g, zbMATH Work ID, P6830, Twitter username, P2002, …



research data sharing without barriers
rd-alliance.org

Slide credit: Moritz Schubotz, SwMath

Identification target - what do we want to identify?

Taken from: Identifiers and targets crosswalk

Software artifact

- Executable (download link)
- Software source code
  - Dynamic artifact - current development code (on collaborative development platform)
  - Archived copy
    - Release / Package
    - Commit / a specific point in development history
    - Directory
    - File / algorithm

Software concept / project / collection

- Description in registry
- Homepage

Software context

- Complementary artifacts
- Data
- Articles
- Documentation

Ice-breaker v2: propose the identification target for a use case (as a comment)

https://tinyurl.com/qpg7n7m

Discussion in small groups

https://tinyurl.com/qpg7n7m

1. Introduce yourself to your neighbours (name, affiliation, a software identification use case that interest you)
2. Choose group use case
   - You can choose a use case from the list in the use cases directory or propose a new use case
3. Document use case
   - Make a copy of use case template in use cases directory
4. Analyse use case
   - Pros for each identifier schema
   - Cons for each identifier schema
5. Discuss which identifiers are most relevant for the particular use-case

Use case: Title

Use case summary	
Actor/s	**Step by step scenario** • •
Goal **Use case extensions**	**Examples** • •
Target for identifier Metadata record / software source code artifact / software executable (with/without container) / other:_____	**Granularity level (bold selection)** project / collection / repository / branch / release / commit / directory / file / lines of code
Identifiers schemas and examples	

ASCL	ARK	DOI	HAL	Hash	RRID	SWH	SwMath	Wikidata	Other:

Thanks