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RO-Crate: A framework for packaging research products into FAIR Research Objects



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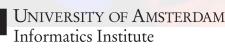
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BioExcel Centre of Excellence

The University of Amsterdam

b https://orcid.org/0000-0001-9842-9718

✓ @soilandreyes





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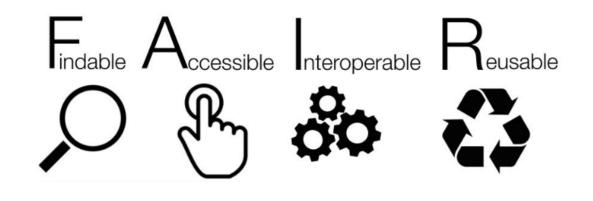


tl;dr

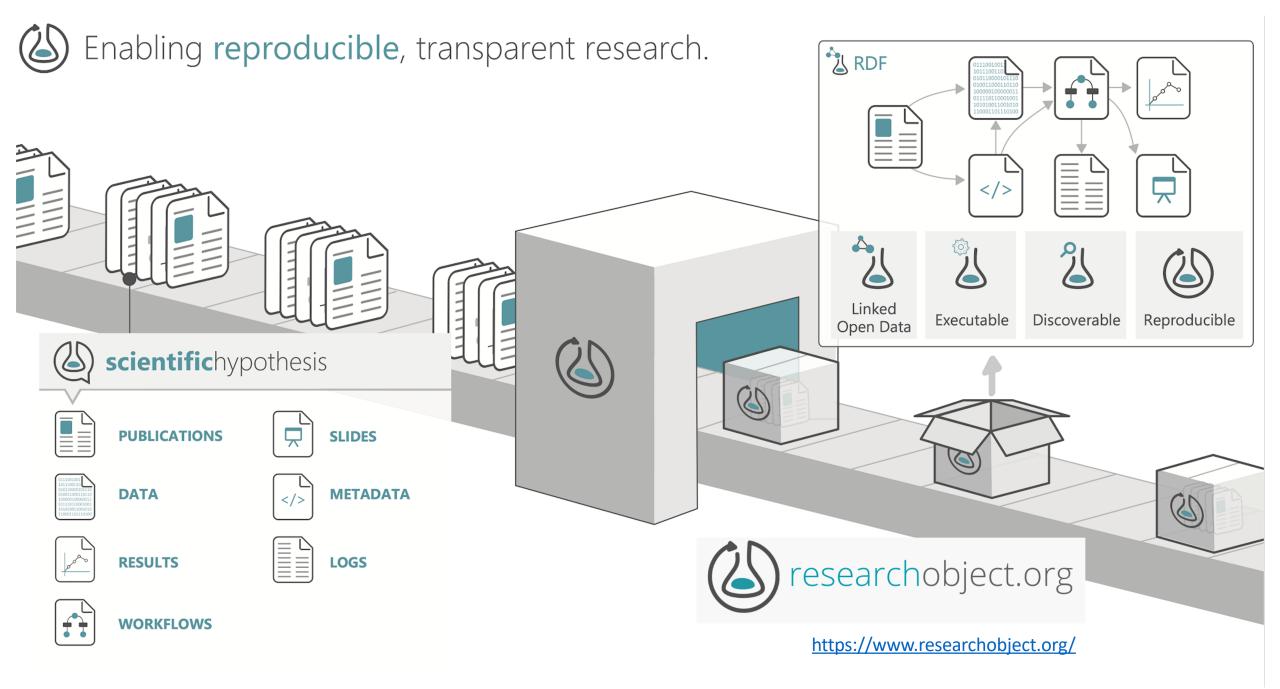
Web standards-based metadata framework for bundling resources with their context into citable reproducible packages

Machine actionable Metadata + Identifiers + Web protocols => FAIR

- What and Why
- Examples
- How and Tools
- Alignment with FDOF



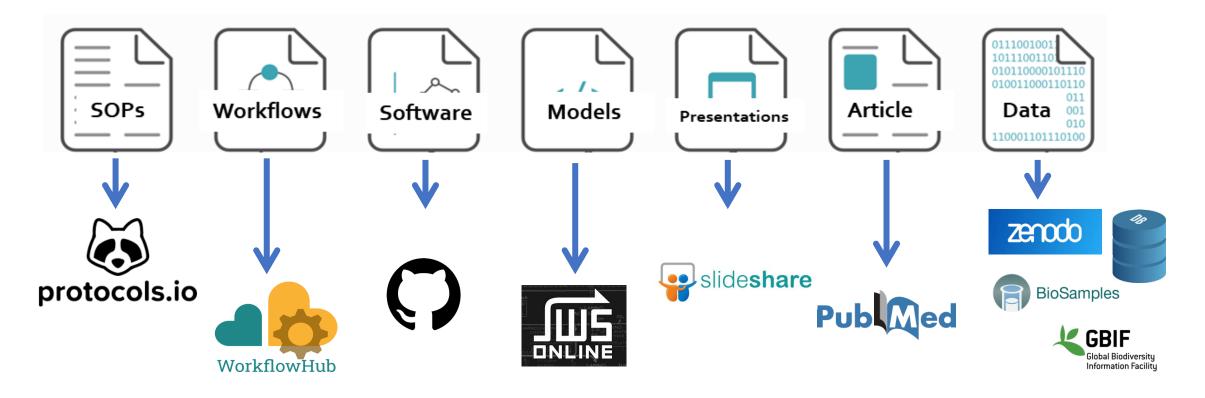
Bechhofer et al (2013) Why linked data is not enough for scientists <u>https://doi.org/10.1016/j.future.2011.08.004</u> Bechhofer et al (2010) Research Objects: Towards Exchange and Reuse of Digital Knowledge, <u>https://eprints.soton.ac.uk/268555/</u>



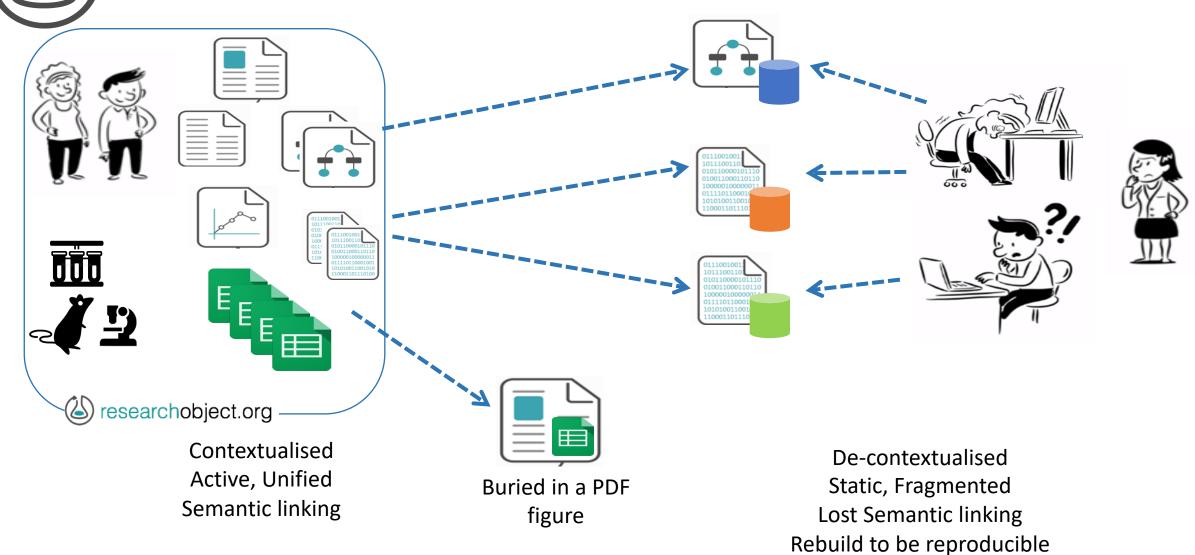
Many Objects are the Outcomes of Research

All are first class citizens and are required to make research FAIR+R

Each object has its own metadata and repositories



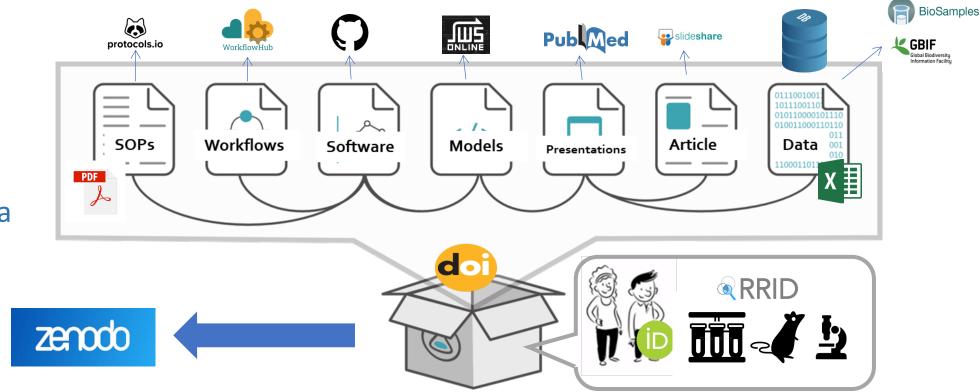
Scattered Reporting and Reading





Encapsulated content and references to external resources

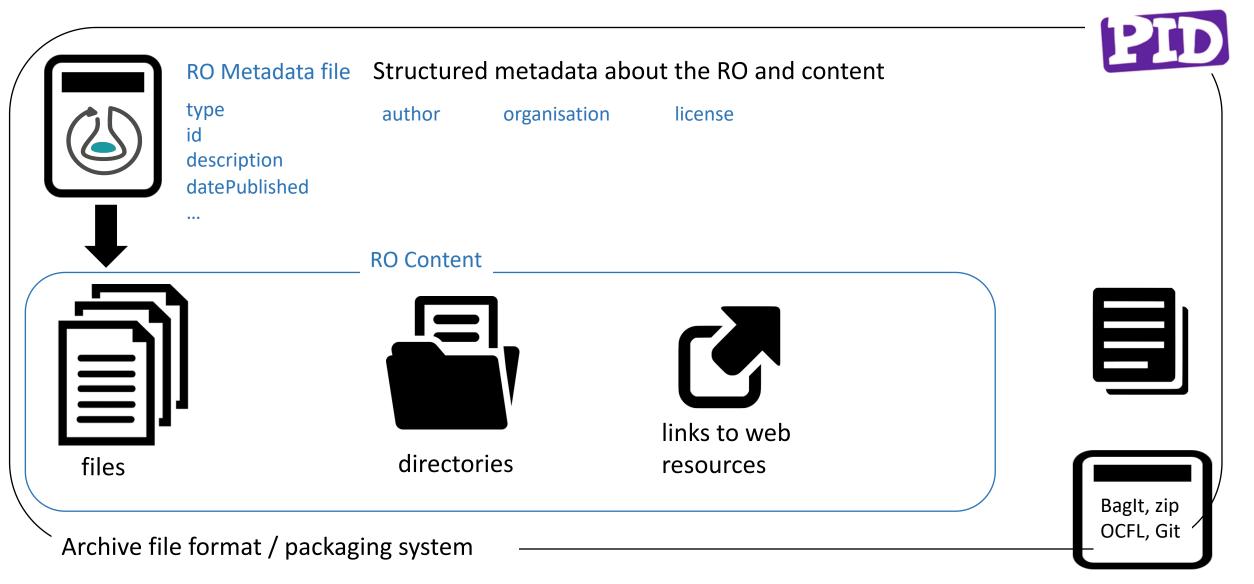
integrated view over fragmented resources using PIDs and metadata



The RO package has its own metadata, can be registered and deposited in its own right, unpackaged and accessed, activated and reproduced if appropriate

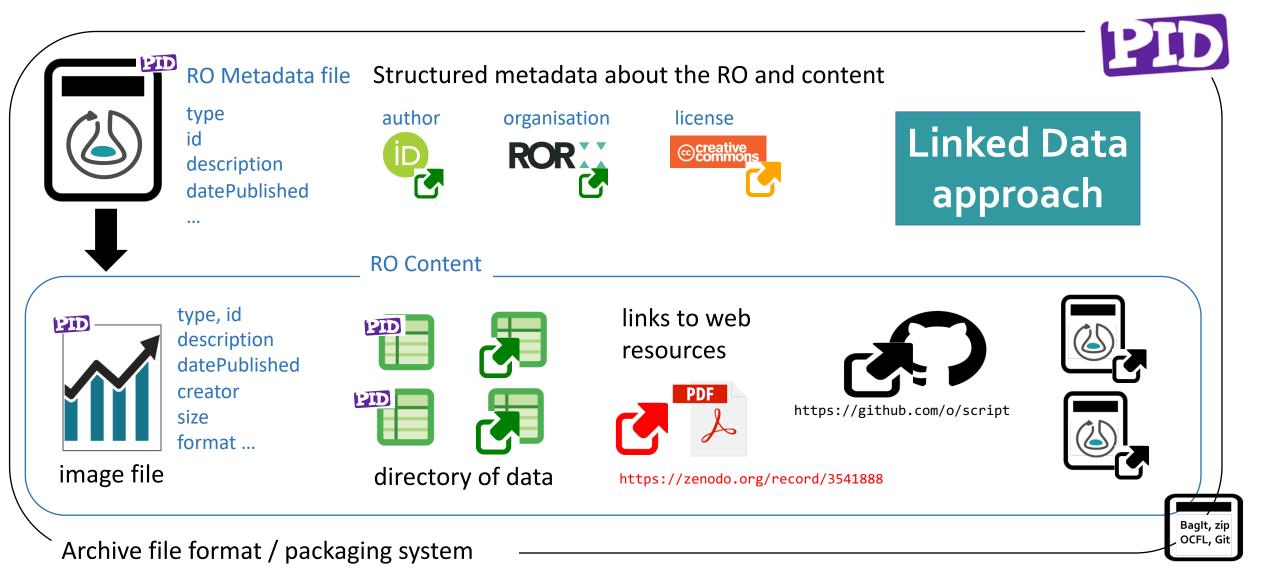


self-describing, chiefly metadata, objects





self-describing, chiefly metadata, objects





Self-describing, chiefly **metadata**, objects Strict Structure, Open ended content

http://www.researchobject.org/ro-crate/

How do we describe the metadata?

- PIDs + JSON-LD + Schema.org descriptors
- Opinionated profile of <u>schema.org</u>
- Linked Data by Stealth: JSON with gradual path to extensibility with LD e.g. ad-hoc terms
- Example-driven documentation

How can I add additional metadata?

• Schema.org, domain ontologies

How do I define a checklist of what is expected to be in a type of RO?

RO-Crate Profiles

Adding new or ad hoc vocabulary terms $\,\mathscr{S}\,$



Context terms must ultimately map to HTTP(s) URIs which poses challenges for crate-authors wishing to use their own vocabularies.

RO-Crate provides some strategies to add a new term (a Class or Property) that is not in Schema.org or another published vocabulary, so that there is a stable URI that can be added to the @context.

Choosing URLs for ad hoc terms

For projects that have their own web-presence, URLs MAY be defined there and SHOULD resolve to useful content. For example for a project with web page https://criminalcharacters.com/ the property education could have a URL: https://criminalcharacters.com/vocab#education which resolves to an HTML page that explains the term using HTML anchors:

<div id="education">

<hl>Property: education</hl>
<hl>Prisoner. Prison authorities would record the prisoner's statement as to whether they could

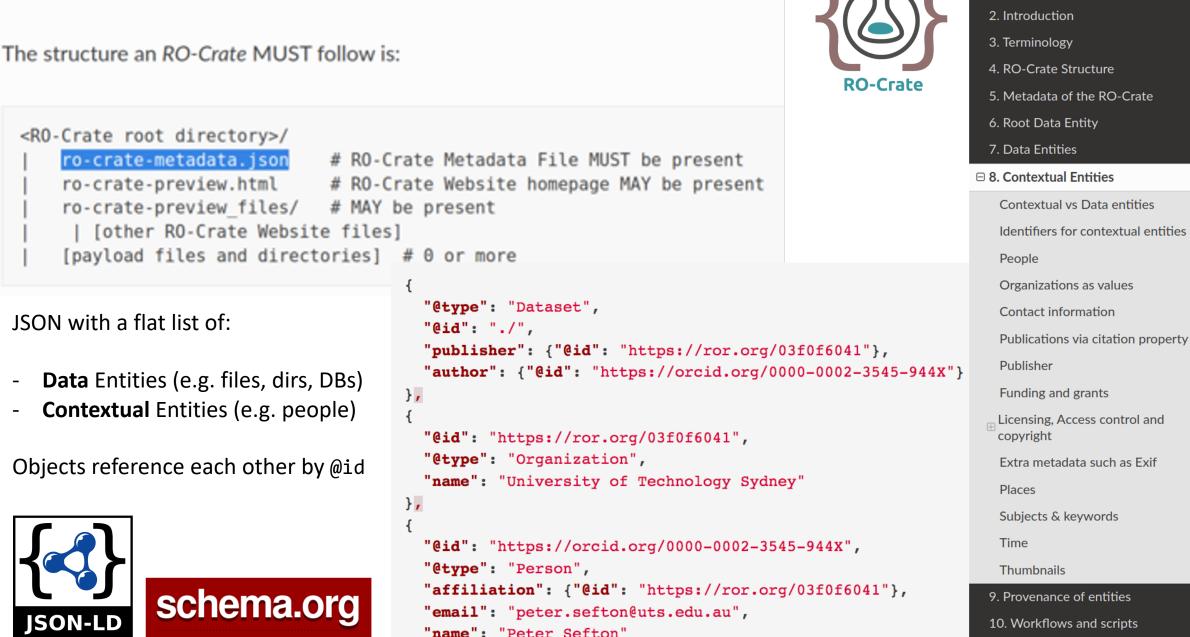
🕒 Tip

Ensure you have a consistent use of http or https (preferring https) as well as consistent path /vocab vs /vocab/ vs /vocab/index.html (preferring the shortest that is also visible in browser).

For ad hoc terms where the crate author does not have the resources to create and maintain an HTML page, authors may use the RO-Crate public namespace (https://w3id.org/ro/terms/) to reserve their terms. For example, an ad-hoc URL MAY be used in the form https://w3id.org/ro/terms/) to reserve their terms. For example, an ad-hoc URL MAY be used in the form https://w3id.org/ro/terms/) to reserve their terms. For example, an ad-hoc URL MAY be used in the form https://w3id.org/ro/terms/criminalcharacters#education where criminalcharacters#education where criminalcharacters#education where criminalcharacters#education where criminalcharacters#education Ad-hoc namespaces under https://w3id.org/ro/terms/ are available on first-come-first-serve basis; to avoid clashes, namespaces SHOULD be registered by submitting terms and definitions to the RO-Crate terms project.

RO-Crate Structure

https://w3id.org/ro/crate/1.1



Appendix

RO-CRATE 1.1

1. About this document



Summary: RO-Crate in a nutshell

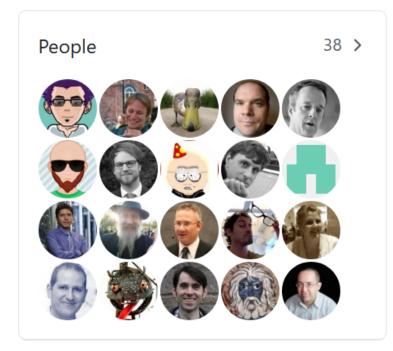
Practical lightweight approach to packaging research data entities (any object) with metadata

Aggregate **files** and/or **any URI-addressable content**, with contextual information to aid decisions about re-use: Who What When Where Why How.

Web Native Machine readable. Human readable. Search engine friendly. Familiar.

Extensible and Incremental: add additional metadata; nested and typed by their profile.

Open Community effort



http://www.researchobject.org/ro-crate/



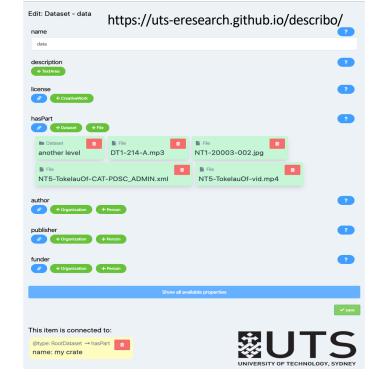
<u>Describo</u> interactive desktop application to create, update and export RO-Crates for different profiles. (~ beta)

- <u>CalcyteJS</u> is a **command-line** tool to help create RO-Crates and HTMLreadable rendering (~ *beta*)
- <u>ro-crate</u> JavaScript/NodeJS library for RO-Crate rendering as HTML. (~ beta)
- <u>ro-crate-js</u> utility to render HTML from RO-Crate (~ *alpha*)
- <u>ro-crate-ruby</u> Ruby library to consume/produce RO-Crates (~ *alpha*)
- <u>ro-crate-py</u> Python library to consume/produce RO-Crates (~ *planning*)

These applications use or expose RO-Crates:

- <u>Workflow Hub</u> imports and exports <u>Workflow RO-Crates</u>
- <u>OCFL-indexer</u> NodeJS application that walks the <u>Oxford Common File Layout</u> on the file system, validate RO-Crate Metadata Files and parse into objects registered in Elasticsearch. (~ *alpha*)
- ONI indexer
- <u>ocfl-tools</u>
- <u>ocfl-viewer</u>
- <u>Research Object Composer</u> is a REST API for gradually building and depositing Research Objects according to a pre-defined profile. (RO-Crate support *alpha*)

User facing



Infrastructure facing

Software libraries



https://www.npmjs.com/package/ro-crate https://github.com/ResearchObject/ro-crate-ruby https://pypi.org/project/rocrate/

https://www.researchobject.org/ro-crate/implementations.html



SCALEABLE

SUSTAINABLE

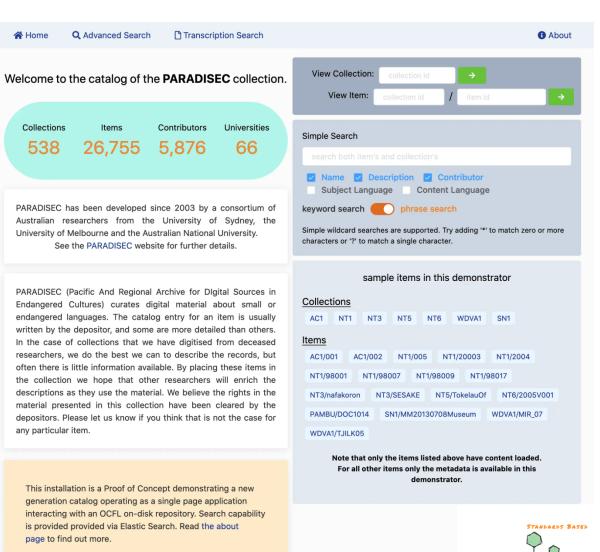
Pacific and Regional Archive for Digital Sources in Endangered Cultures

A race against time to digitise analog records of materials from endangered cultures from all over the world.

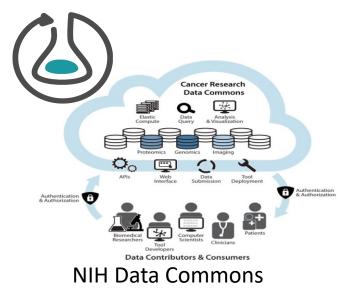


Cultural Heritage: A data curation service for endangered languages: 500,000 files in 28,624 items and 574 collections

long term preservation and accessibility of research data objects

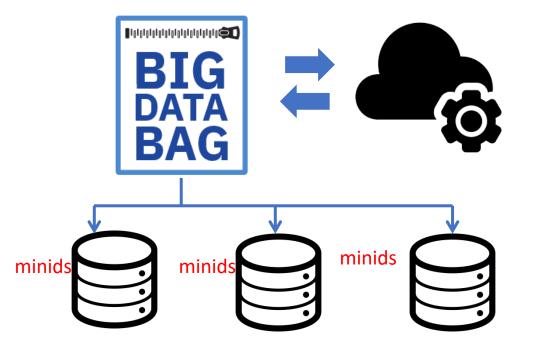


https://arkisto-platform.github.io/



Processing big genomic & clinical data distributed over multiple locations

Scalable verified collections of references

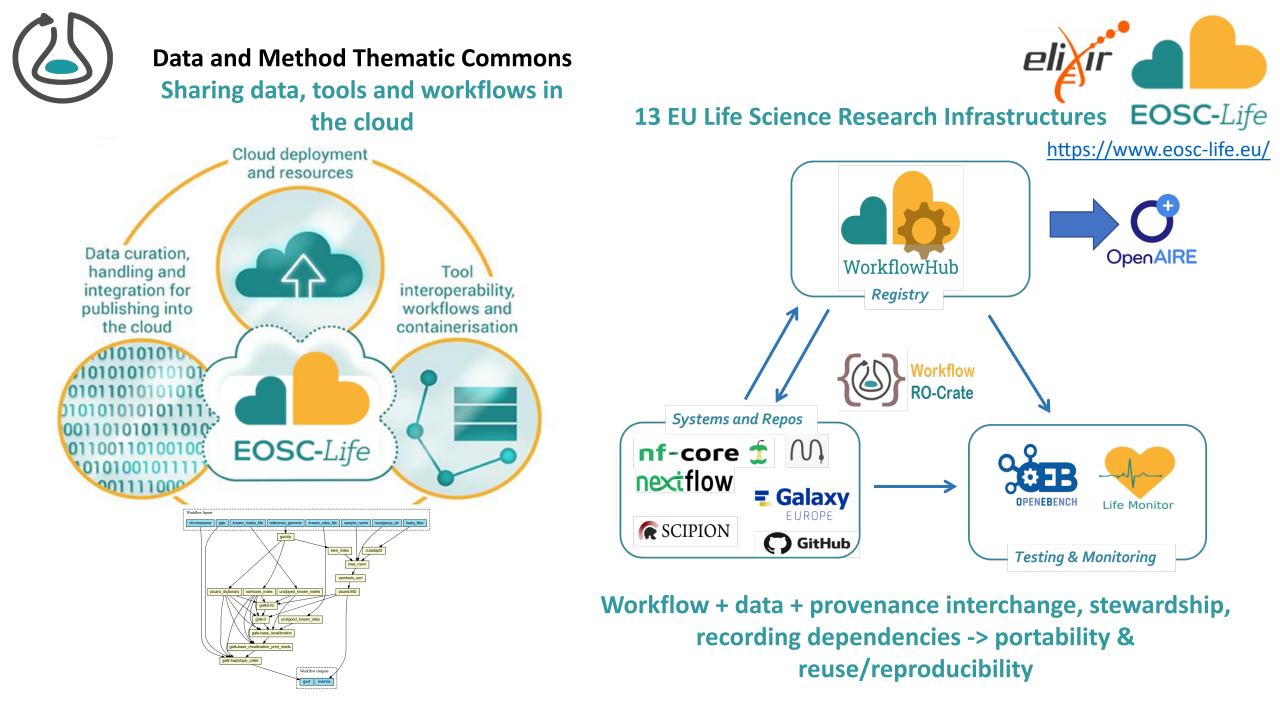


Retain and archive processed datasets Reference and transfer large data on demand Controlled access to sensitive data

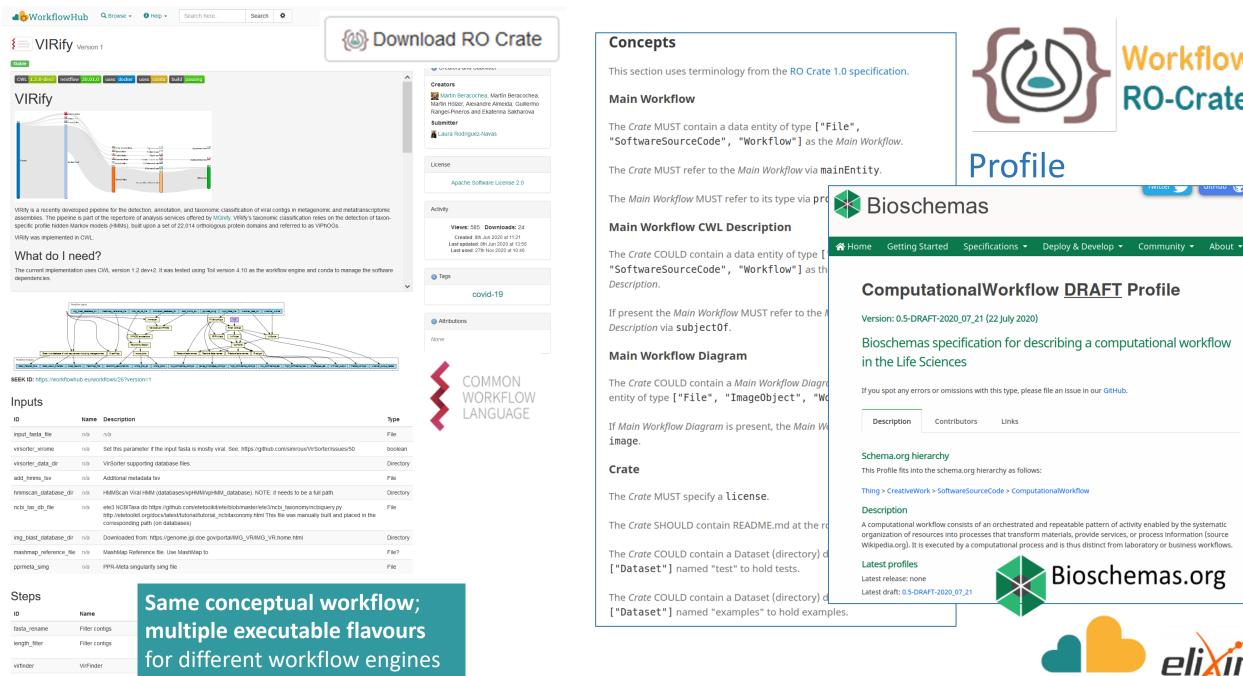
[Kesselman, Foster]

[Chard, et al 2016]

https://doi.org/10.1109/BigData.2016.7840618



RO-Crate as interchang	e format (Download RO Crate
Example of setting up a simulation System Version 2 -	t Solutions -	graph.svg md_list.cwl
Work-In-progress	() Creators and Submitter	o ro-crate-metadata.json
	Creators Not specified Submitter	ro-crate-preview.html "license": "Apache-2.0",
	License Apache Software License 2.0	<pre>"identifier": "https://workflowhub.eu/workflows/98?version=2" "url": "https://workflowhub.eu/workflows/98/ro_crate?version= "isBasedOn": "https://github.com/douglowe/biobb_hpc_cwl_md_li "sdPublisher": {</pre>
	Activity Views: 40 Downloads: 0 Created: 29th Jan 2021 at 16:37 Last updated: 29th Jan 2021 at 16:56 Last used: 4th Feb 2021 at 08:12	<pre>"@id": "https://orcid.org/0000-0002-1248-3594" }, "sdDatePublished": "2021-02-04 11:33:41 +0000", "creativeWorkStatus": "Work-in-progress" }, { "@id": "md_list.cwl",</pre>
	Tags This item has not yet been tagged.	<pre>"@type": ["File", "SoftwareSourceCode", "ComputationalWorkflow"</pre>
Wapper of the GROMACS gromp module repL.gs_table repL.gs_table revenue, Sees revenue, Sees	Solution Add your tags -	<pre>], "programmingLanguage": { "@id": "#cwl" }, """"""""""""""""""""""""""""""""""</pre>
In the lew workflow workput I Workflow Cospus	() Attributions	<pre>"url": "https://github.com/douglowe/biobb_hpc_cwl_md_list/blo "image": {</pre>
SEEK ID: https://workflowhub.eu/workflows/98?version=2 https://workflowhub.eu/workflowhub.eu/	None	<pre>"@id": "graph.svg" }, "contentSize": 10444</pre>



https://workflowhub.eu/

EOSC-Life

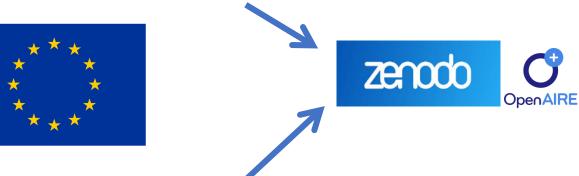
and specific use-cases

Embedding into Infrastructures & Standards

EGI-ACE data spaces for Earth Science researchers



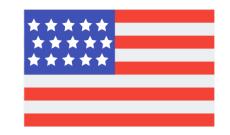
Earth Science Communities and Copernicus users in EOSC





Seven Bridges

exchange between genomics platform and repository.





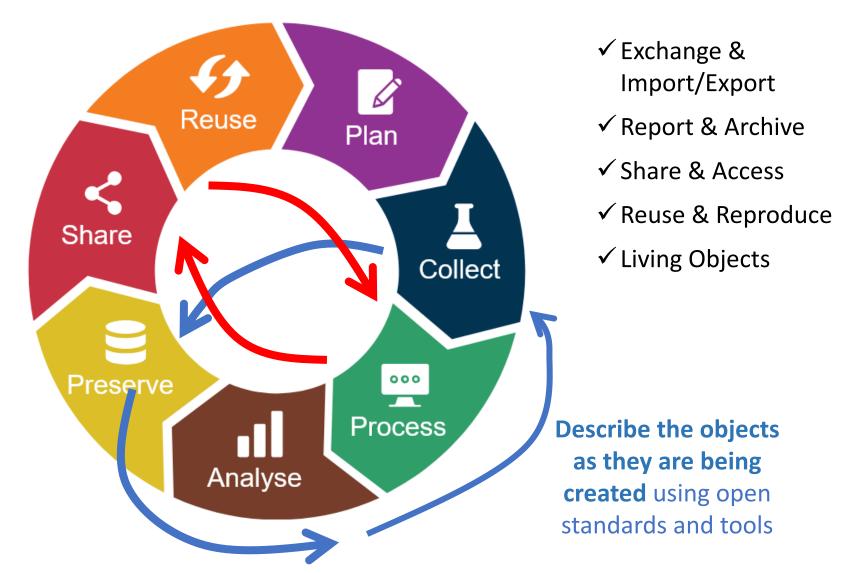
standardise and share analyses generated from genome sequencing. IEEE 2791-2020



FAIR and GDPR compliant data storage and sharing fabric <u>Science</u> <u>Mesh</u> using Cloud Services for Synchronization and Sharing



Supporting the Research Life Cycle



Release the objects as they are created, updated and used

Figure: RDMKit, https://rdmkit.elixir-europe.org/

Science 2.0 Repositories: Time for a Change in Scholarly Communication Assante, Candela, Castelli, Manghi, Pagano, D-Lib 2015

Machine-processable

Standards E X A M P L E S

LOW TECH Incremental

MULTI-PLATFORM

Graceful degradation

Commodity tooling

Technology Independent

Keep it simple Developer friendliness Just enough complexity / standards

 sufficient extra benefits from what already exists...without compromising developer entry-level experience so they do their own thing

Just Enough Linked Data Just In Time

• simplifications instead of generalizations

Retain Linked Data benefits

- querying, graph stores, vocabularies, clickable URIs) Plus the developer needs
- documentation, examples, libraries, tools, community ...

Limited flexibility frees up developers Familiarity is important for uptake





From FAIR data to FAIR Digital Objects





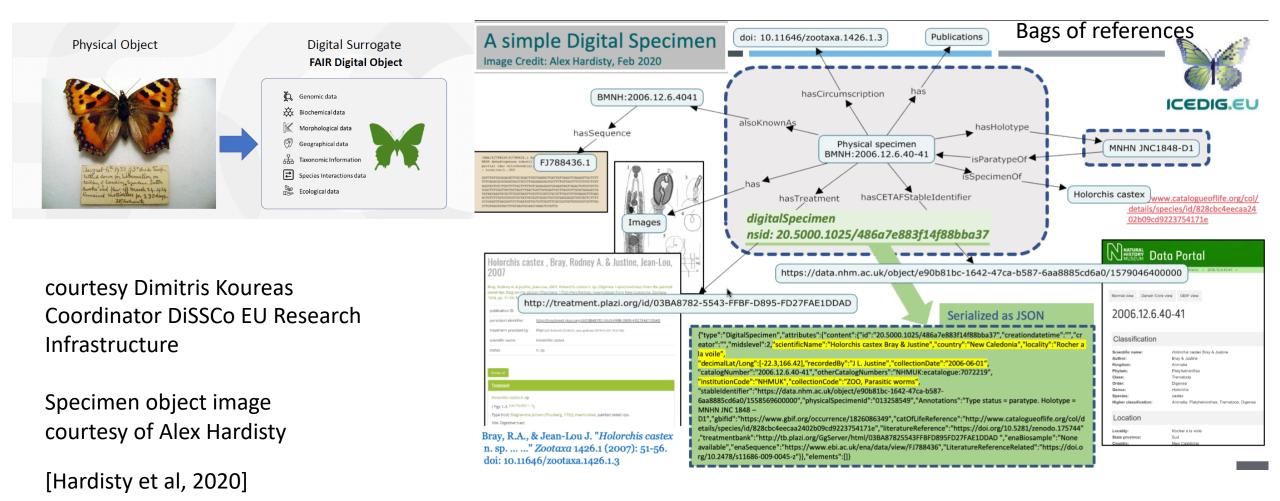
FAIR Digital Objects for Science: From Data Pieces to Actionable Knowledge Units: https://doi.org/10.3390/publications8020021

https://op.europa.eu/en/publication-detail/-/publication/d787ea54-6a87-11eb-aeb5-01aa75ed71a1/language-en/format-PDF/source-190308283

FAIR Digital Objects Actionable knowledge unit

Digital butterfly – digital twins



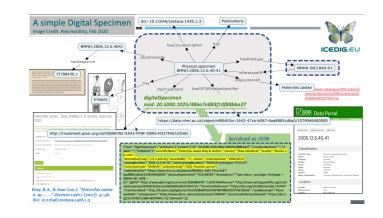


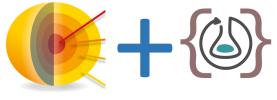
Specimen Data Refinery

Workflows to Digitise Natural History Specimens FAIR Digital Objects -> Packaged + Actionable



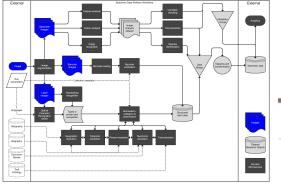
FAIR Digital Object Framework Open Digital Specimen







Workflow Infrastructure RO-Crate

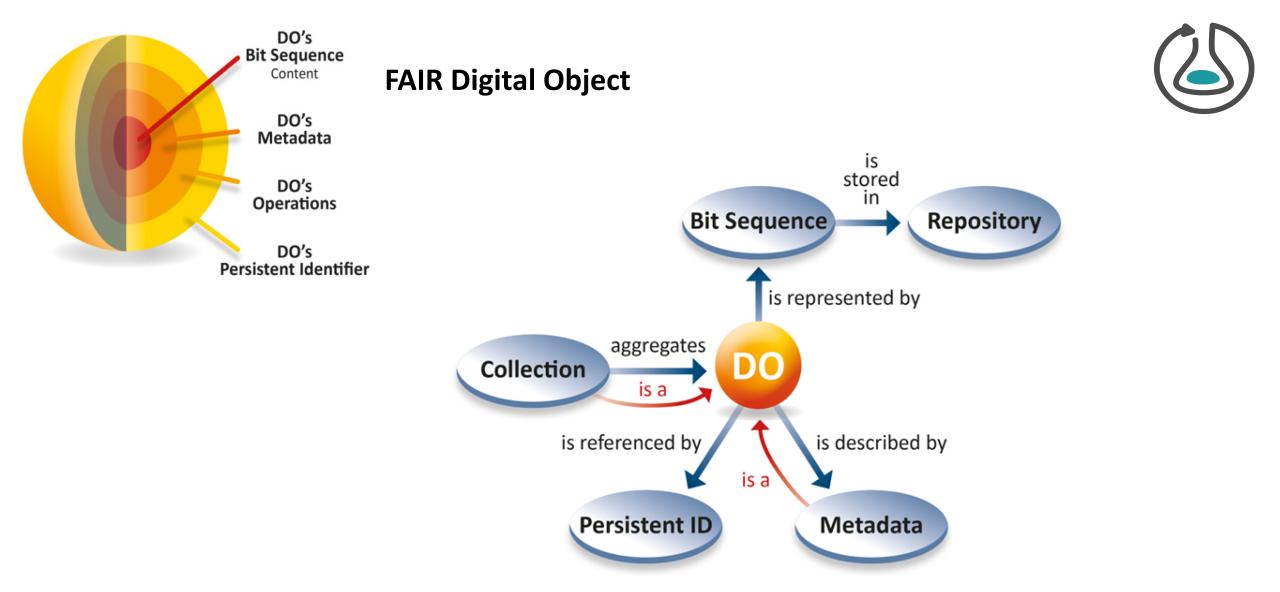


Same conceptual workflow; multiple executable flavours

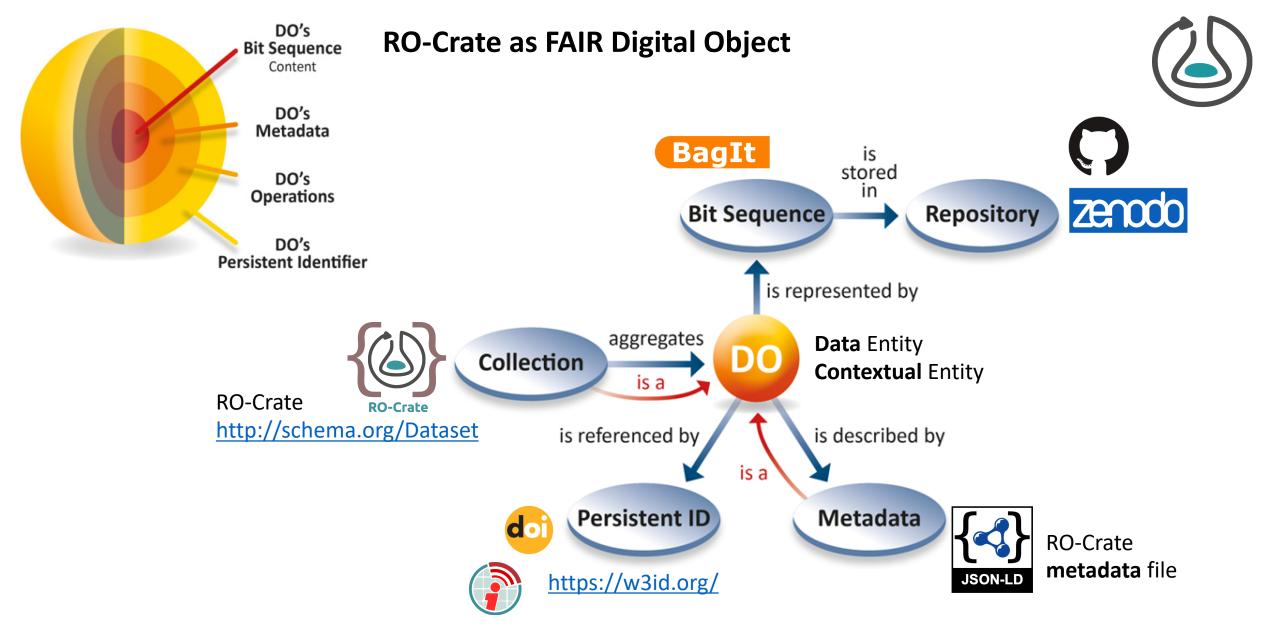




researchobject



Adapted from <u>https://doi.org/10.3390/publications8020021</u>

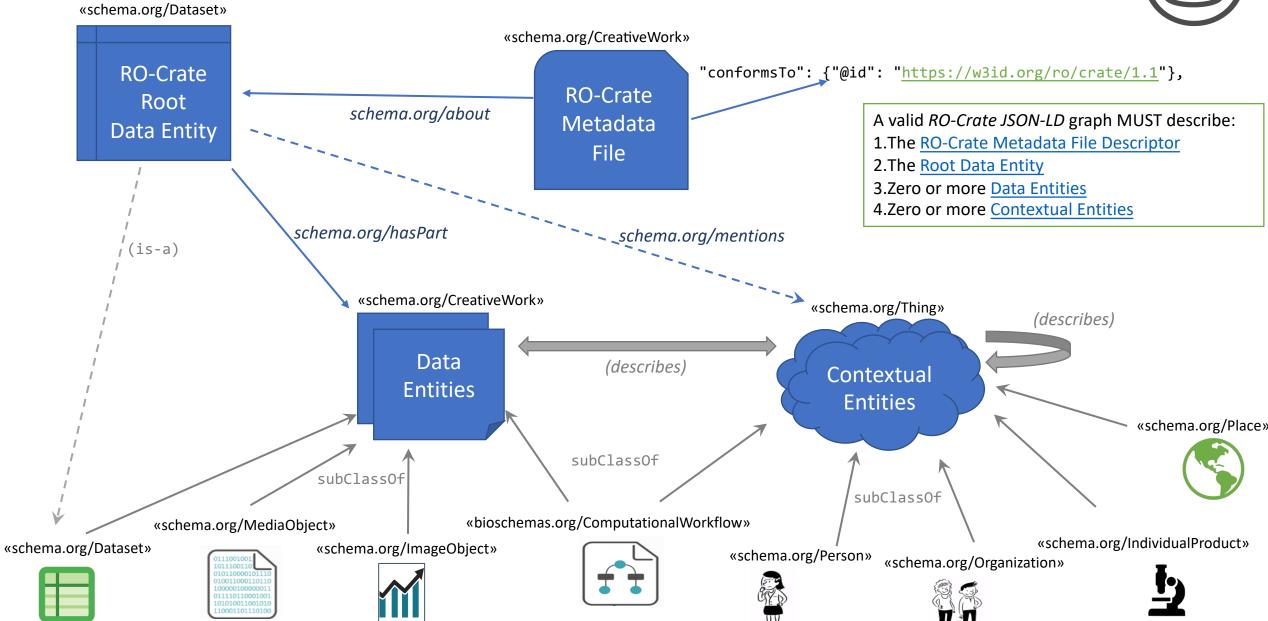


Adapted from https://doi.org/10.3390/publications8020021

RO-Crate model as UML

https://www.researchobject.org/ro-crate/1.1/structure.html





<pre>{ "@context": "https://w3id.org/ro/crate/1.1/context",</pre>	JSON-LD preamble
<pre>{ "@type": "CreativeWork", "@id": "ro-crate-metadata.json", "conformsTo": {"@id": "https://w3id.org/ro/crate/1.1"}, "about": { "@id": "./" }</pre>	RO-Crate metadata file descriptor
<pre>} { "@id": "./", "identifier": "https://doi.org/10.5281/zenodo.1009240", "@type": "Dataset",</pre>	RO-Crate root dataset
<pre>"hasPart": [{ "@id": "cp7glop.ai" }, { "@id": "lots_of_little_files/" }, { "@id": "communities-2018.csv" }, { "@id": "https://doi.org/10.4225/59/59672c09f4a4b" }, { "@id": "SciDataCon-Presentations/AAA_Pilot_Abstract.html"}],</pre>	aggregates Data entities
<pre>"author": { "@id": "https://orcid.org/0000-0002-8367-6908" }, "publisher": { "@id": "https://ror.org/03f0f6041" }, "citation": { "@id": "https://doi.org/10.1109/TCYB.2014.2386282"}, "name": "Presentation of user survey 2018" },</pre>	described w/ contextual entities
{ "@id": "cp7glop.ai",	Flat list of metadata per entity

"@type": "File", "name": "Diagram showing trend to increase",

••• },

Flat list of metadata per entity

"@id": "figure.png",
"@type": ["File", "ImageObject"],
"name": "XXL-CT-scan of an XXL Tyrannosaurus rex skull",
"identifier": "https://doi.org/10.5281/zenodo.3479743",
"author": {"@id": "https://orcid.org/0000-0002-8367-6908"},
"encodingFormat": "image/png"

Metadata



Data and **Contextual** entities described *within* RO-Crate Metadata File

Base vocabulary & types: schema.org

Cross-references to further contextual entities

RO-Crate **principle**: **Reuse** existing PIDs and URLs

..but always **describe entities** which lack a human-readable resolution

"@id": "https://ror.org/03f0f6041", "@type": "Organization", "name": "University of Technology Sydney", "url": "https://www.uts.edu.au/"

"@id": "https://orcid.org/0000-0002-8367-6908",

"affiliation": { "@id": "https://ror.org/03f0f6041" },

"@type": "Person",

"name": "J. Xuan"

Persistent IDs Gradual ascent towards FAIR

Base line: **Relative paths** from *RO-Crate Metadata File*

Use cases: Describing dataset on **desktop** Ad-hoc **web-hosting** (e.g. GitHub pages) Institutional **archives** (e.g. Oxford Common File Layout)

Reuse existing PIDs and URLs

Use cases: Large data, not a file (e.g. database), reference datasets

Cite/reference existing resources (e.g. via identifiers.org)

Distinguish and crosslink contextual entities

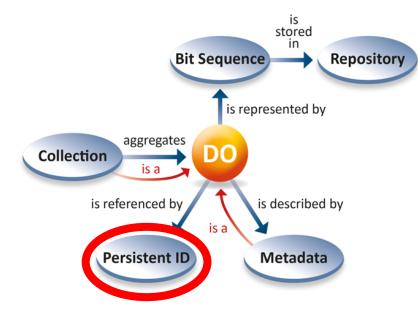
Make paths absolute, using **location-independent PIDs**

(UUIDs, Naming Things with Hashes, ARCP)

Use cases: Found RO-Crate "in the wild", ZIP archives, workflow outputs

Assign PIDs to RO-Crate (and its entities)

Use cases: Long-term availability, citations, permalinks





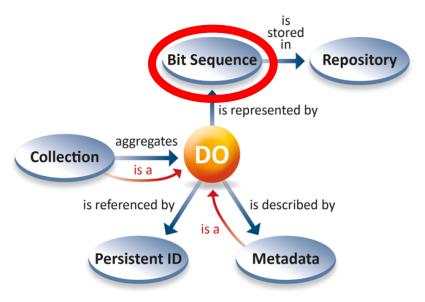
Bit Sequences

Base line: Files on disk within **RO-Crate Root** folder + **URLs**

Downloadable **Web resources** listed w/ content size and access time.

Packaging/archiving RO-Crate Root folder:

- BagIt (<u>RFC8493</u>): Manifest of all (local) files and their checksums Use case: Ensure all files are transferred/archived
- <u>BDBag</u>: Include external files by ARK/MinID PIDs
 Use case: "thin" RO-Crate, **Big Data**, shared immutable files
- OCFL: Archival storage with revision tracking, infrequent changes
- <u>Git LFS</u>: Tracked **frequent changes**, collaborative editing



Repository

Base line: zip/tar download

• e.g. "supplementary data", GitHub release

Export from web platforms

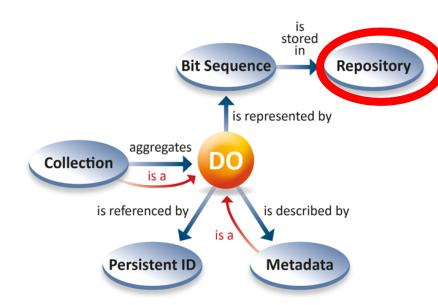
e.g. workflowhub.eu, Galaxy workflow system

Deposit in **general/institutional repositories**

• e.g. Zenodo, Mendeley Data

Deposit in **domain-specific** repositories

• e.g. GBIF



Deposit individual files

• e.g. ARK, S3, B2SHARE

Deposit metadata

• e.g. WikiData, nanopubs

What can FDO learn from RO-Crate?



Data and **Contextual** entities are equally important

Use wheels already invented

- Fit into researchers' existing working practices and familiar technologies.
 - Aim for gradual improvements.
- Reuse existing technology
 - .. But only when not too complex
- Reuse existing PID infrastructure, including URLs
 - Human consumers recognize and click hyperlinks
- Build on existing metadata standards
 - Which is both simple and extendable

Remember people ... especially Developers

- Keep human consumption in focus
 - Ensure metadata is easily rendered and edited
- Provide Best Practice guidance
 - Firm, but not too restrictive
- Developer producer and consumer friendly
 - Rather than academically elegant

Not everything is known before hand

- Existing PID metadata not always relevant
 - Allow contextualized metadata
- Types not always known in advance
 - Allow "casting" or reinterpretation
- Operations not always known in advance
 - Allow *open-ended* generation and use

What can RO-Crate learn from FDO?



Provide stronger guidance on **PID** and availability

- Recommend deposit infrastructure for end-users and framework developers
- Tools to assist e.g. generate Zenodo Datacite metadata from RO-Crate

Provide stronger typing of RO-Crates and its content

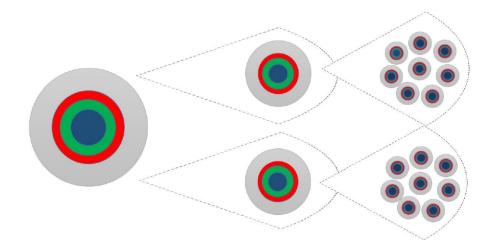
Profiles as first approach

Expose potential **operations** on an RO-Crate

Build general RO-Crate services, e.g. index

Turtles all the way down!

- Document better how RO-Crates can/should be nested
- How to choose granularity of RO-Crates?
- Tools to liberate/reuse an entity from a single RO-Crate



RO-Crate as part of the FDO ecosystem

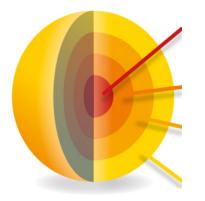




A bag of references + metadata

A metadata framework for FDO Developer friendly practical and web-native implementations Community Infrastructure applications





A bag of references + metadata Framework for actionable objects

RO-Crates enable active operations for FDOs FDO offers additional infrastructure and practice SYNTHESYS+ Synthesis of Systematic Resources a DISSCo project

Synthesys+ Project gives a concrete

use case for practically join the two up.

RO-Crate Community

https://www.researchobject.org/

RO-Crate

Team

The RO-Crate team is:

ro-crate/

- Peter Sefton https://orcid.org/0000-0002-3545-944X (co-chair)
- Stian Soiland-Reyes https://orcid.org/0000-0001-9842-9718 (co-chair)
- Eoghan Ó Carragáin https://orcid.org/0000-0001-8131-2150 (emeritus ch
- Oscar Corcho https://orcid.org/0000-0002-9260-0753
- Daniel Garijo https://orcid.org/0000-0003-0454-7145
- Raul Palma https://orcid.org/0000-0003-4289-4922
- Frederik Coppens https://orcid.org/0000-0001-6565-5145
- Carole Goble https://orcid.org/0000-0003-1219-2137
- José María Fernández https://orcid.org/0000-0002-4806-5140
- Kyle Chard https://orcid.org/0000-0002-7370-4805
- Jose Manuel Gomez-Perez https://orcid.org/0000-0002-5491-6431
- Michael R Crusoe https://orcid.org/0000-0002-2961-9670
- Ignacio Eguinoa https://orcid.org/0000-0002-6190-122X
- Nick Juty https://orcid.org/0000-0002-2036-8350
- Kristi Holmes https://orcid.org/0000-0001-8420-5254
- Jason A. Clark https://orcid.org/0000-0002-3588-6257
- Salvador Capella-Gutierrez https://orcid.org/0000-0002-0309-604X
- Alasdair J. G. Gray https://orcid.org/0000-0002-5711-4872
- Stuart Owen https://orcid.org/0000-0003-2130-0865
- Alan R Williams https://orcid.org/0000-0003-3156-2105
- Giacomo Tartari https://orcid.org/0000-0003-1130-2154
- Finn Bacall https://orcid.org/0000-0002-0048-3300
- Thomas Thelen https://orcid.org/0000-0002-1756-2128
- Hervé Ménager https://orcid.org/0000-0002-7552-1009
- Laura Rodríguez Navas https://orcid.org/0000-0003-4929-1219
- Paul Walk https://orcid.org/0000-0003-1541-5631
- brandon whitehead https://orcid.org/0000-0002-0337-8610
- Mark Wilkinson https://orcid.org/0000-0001-6960-357X
- Paul Groth https://orcid.org/0000-0003-0183-6910
- Erich Bremer https://orcid.org/0000-0003-0223-1059
- LJ Garcia Castro https://orcid.org/0000-0003-3986-0510
- Karl Sebby https://orcid.org/0000-0001-6022-9825
- Alexander Kanitz https://orcid.org/0000-0002-3468-0652
- Ana Trisovic https://orcid.org/0000-0003-1991-0533
- Gavin Kennedy https://orcid.org/0000-0003-3910-0474 Bi-weekly calls &
- Mark Graves https://orcid.org/0000-0003-3486-8193
- GitHub Jasper Koehorst https://orcid.org/0000-0001-8172-8981
- Simone Leo https://orcid.org/0000-0001-8271-5429

WorkflowHub Club

The weekly WorkflowHub Club is chaired by Frederik Coppens.

Participants include:

- Alan R Williams (The University of Manchester)
- Alexander Vasilenko (VKM IBPM RAS, MIRRI)
- Alexander Kanitz
- Alban Gaignard
- Ambarish Kumar (Jawaharlal Nehru University, New Delhi, India)
- Antonio Rosato
- Bert Droesbeke (ELIXIR-BE, VIB-UGent Center for Plant Systems Biology)
- Björn Grüning (University of Freiburg, ELIXIR-DE, Galaxy Project)
- Carole Goble (The University of Manchester, ELIXIR-UK)
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Bi-weekly calls & Slack

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FAIR all the way down Unbounded FAIR Distributed FAIR Living FAIR

Analogous to FAIR Software

FAIR RO-Crate is a practical start

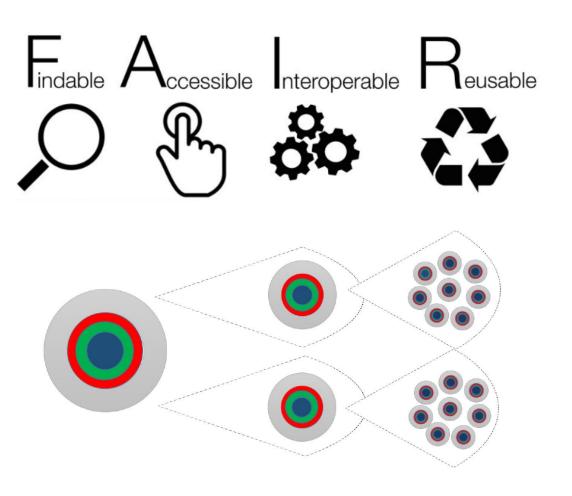


Fig from EOSC Interoperability Framework