PresQT

Demonstrating PresQT Services for FAIR Software and Data Preservation

presqt.crc.nd.edu

CNI Fall 2020 Virtual Membership Meeting

Dec 1, 2020

Rick Johnson, Natalie Meyers

These slides: doi:10.17605/OSF.IO/3GNQD, available at osf.io/3gngd



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Hi we're Natalie Meyers and Rick Johnson from the PresQT Team Here's a link to the google slides we're presenting

[SHARE IN CHAT]

https://docs.google.com/presentation/d/1YcaLB-HDb81p9GT5LrRaRCKbmU8D-ISdDRL59-7NUHw/edit?usp=sharing

Or come back anytime using this URL https://osf.io/3GNQD/

PresQT

An **implementation grant** and previous **planning grant** funded effort to address needs for preserving data and software. The goal is to **collaboratively design, develop, and connect** interoperable and repository agnostic Data and Software **Preservation Quality Tools**.



- Implementation grant: https://www.imls.gov/grants/awarded/LG-70-18-0082-18
- Planning grant: https://www.imls.gov/grants/awarded/lg-72-16-0122-16



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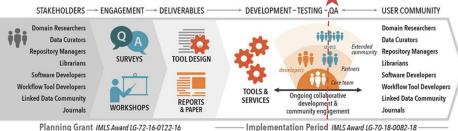


Presqt is . . . An **implementation grant** and previous **planning grant** funded effort to address needs for preserving data and software.

The goal is to **collaboratively design, develop, and connect** interoperable and repository agnostic Data and Software **Preservation Quality Tools**.

Collaborative Effort

Today - Dec 1, 2020



Planning Grant IMLS Award LG-72-16-0122-16

Concept

- Not standalone solutions
- · Partner systems and services easily integrable via standard APIs
- User-centered open design and collaborative development
- Open resources at https://osf.io/d3jx7/
- Open source software at https://github.com/ndlib/presqt



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We're now in the implementation grant's QA phase. We'll describe the services and features we've built and how you and your organization can:

- build an endpoint or nominate one,
- 2. learn to use the features that interest you,
- 3. and try our FAIR tests.

Thi is an open grant All the planning phase resources gathered during stakeholder engagement are available to inform stakeholders' future projects. Tool designs and final report will be actionable by anyone who wants to inform their planning through the priorities identified in PresQT.

Everything produced for the PresQT project is shared on github and the Open Science Framework (OSF)

- Open resources at https://osf.io/d3jx7/ [SHARE IN CHAT]
- Open source software at https://github.com/ndlib/presqt [SHARE IN CHAT]

PresQT Acknowledgements

Funded sub-awardees

- Sheridan Libraries, Johns Hopkins University
- National Data Service
- HUBzero team, Purdue University
- UC San Diego Library
- Yale University Library (EaaSI)

Collaborators and Testing Partners

- Members of Confederation of Open Access Repositories (COAR), Libraries at Amherst College, Fontbonne University, Tuskegee University
- Center for Open Science, CERN, Data Curation Network, Project Jupyter, Midwest Big Data Hub, ReproZip, RDA Groups, Science Gateways Community Institute, Software Preservation Network, URSSI (US Research Software Sustainability Institute)

Workshops:

Data Futures: Preserving Annotation with Peter Cornwell

SDSC: David Valentine and Ilya Zaslavsky Mark Wilkinson: FAIR Evaluation Services

Daniel Clarke and Avi Ma'ayan FAIRShake, Assessment Rubrics



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We'd like to acknowledge and thank PresQT Stakeholders including:

Funded sub-awardees

- Sheridan Libraries, Johns Hopkins University
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Mark Wilkinson: FAIR Evaluation Services Daniel Clarke and Avi Ma'ayan FAIRShake , Assessment Rubrics

Research Data Management Archipelago Identifying Data and Software Preservation Tool Gaps





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PresQT's Planning phase task was to identify Data and Software Preservation Tool gaps

Through Surveys and workshops we established an understanding of the concerns of

- Different Repositories, Different Cultures of data management, processes, technology/tools, etc
- We heard the Switch cost between stand alone systems is [TOO] high for researchers:
- And that, Data flow/transactions between systems can be very difficult

Our analogy for this situation is a research data management archipelago - where stand alone systems and the data in them grow in isolation from one another and there are data islands.

PresQT Inter-Repository File Transfer

Building Bridges Between Systems





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PresQT's charge coming developing out of the planning phase was developing tools for connecting communities of practice and bringing preservation features together without moving files up and down to the desktop

This way, Users and repository managers can move projects between systems and enhance their assets with fixity information, FAIR testing and better keywording along the way

Data islands become connected by PresQT's services.

Accessing PresQT Services

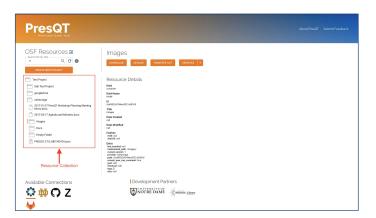
Web GUI:

https://presqt-prod.crc.nd.edu/ui/

API

https://presqt.readthedocs.io/en/latest/api_endpoints.html

Feel free to stand up your own PresQT Services from the PresQT open source distribution: https://github.com/ndlib/presqt





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You can visit the Web GUI at presqt-prod.crc.nd.edu/ui/ [SHARE IN CHAT]

and try the services described in today's talk

It's a stateless auth token based utility service proptotype we built for enabling wide audiences to engage in testing the PresQT services

Or, You can access the PresQT endpoints directly through the API [SHARE IN CHAT] https://presqt.readthedocs.io/en/latest/api endpoints.html

Or, You can stand up the PresQT service using the open source distribution on github https://github.com/ndlib/presqt [SHARE IN CHAT]

PresQT Service Features

PresQT design: pluggable, configurable architecture easily extendable for diverse systems under consideration of diverse structures

Set of services:

- Configure additional partner systems via JSON and Python functions
- Transfer in BagIt format
- Metadata in JSON
- Fixity checks
- Keyword enhancement
- EaaSI Emulation
- FAIR tests

https://presqt.readthedocs.io/en/latest/



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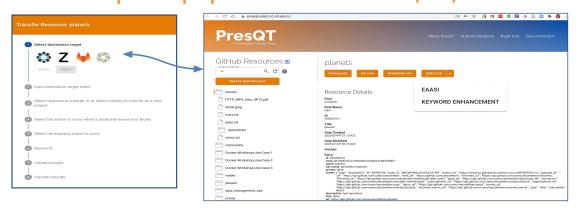


PresQT (Preservation Quality Tool) is an open-source toolsuite with RESTful services to improve Preservation and Re-use of Research Data and Software

At (and between) each endpoint you can use PresQT for a variety of services

The PresQT services are documented at https://presqt.readthedocs.io/en/latest/ [SHARE IN CHAT]

Transfer between Repositories presqt-prod.crc.nd.edu/ui/



And More: Establish and Check Fixity information, Enhance Keywords w/SciGraph, Do FAIR testing, Connect to Emulation services



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You can use the GUI or API to

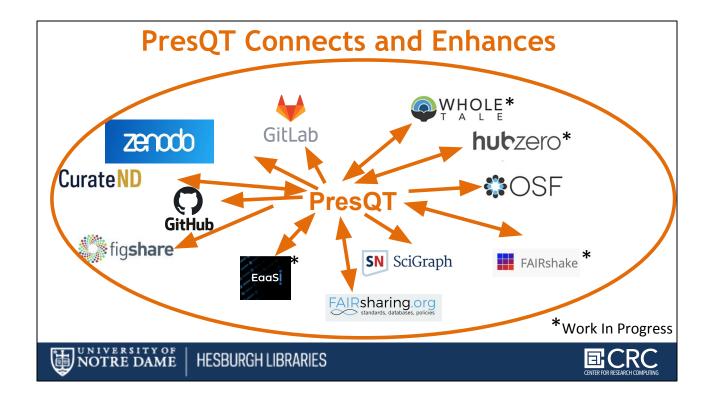
- transfer files between repositories,
- establish and check fixity information
- enhance keywords
- connect to emulation services
- or do FAIR testing.

Try it yourself at presqt-prod.crc.nd.edu/ui/

[SHARE IN CHAT]

The presqt system runs on token based authentication so you'll need to get access tokens from the service endpoints you are interested in

Don't worry if you've never done this before, the documentation explains what tokens are and how to get them for the service endpoints you are interested in.



We connect to the services you see above

The services denoted with an asterisk are integrations in progress.

If you want to plug in one of your own services you can work with us to connect via APIs

(lirrent	Integrations
Carrent	incegracions

Target	Collection	Search	Detail	Download	Upload	Transfer In [Targets]	Transfer Out [Targets]	Hash	Keyword Get	Keyword Upload	FAIR testing
OSF	V	V	V	V	V	√ [Github, CurateND, Zenodo, GitLab, FigShare]	√ [Github, Zenodo, GitLab, FigShare]	[sha256, md5]	V	V	V
curateND (Fedora)	V	V	V	V	ТВА	ТВА	√ [OSF, Github, Zenodo, GitLab, FigShare]	[md5]	V	ТВА	V
Github	V	V	V	V	V	√[OSF, CurateND, Zenodo, GitLab, FigShare]	√ [OSF, Zenodo, GitLab, FigShare]	[]	V	V	V
Zenodo	V	V	V	V	V	√[OSF, Github, CurateND, GitLab, FigShare]	√ [OSF, Github, GitLab, FigShare]	[md5]	V	V	V
GitLab	V	V	V	V	V	✓[OSF, Github, CurateND, Zenodo, FigShare]	√ [OSF, GitHub, Zenodo, FigShare]	[sha256]	V	V	V
FigShare	V	V	V	V	V	V [OSF, Github, CurateND, Zenodo, Gitlab]	√ [OSF, Github, Gitlab, Zenodo]	[md5]	V	V	V



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• Here's more detail about service features for each PresQT endpoint

Fixity During the resource upload process, fixity is checked in two locations: When files are saved to the disk from the request. After files are uploaded to the target. POST Disk Upload to OSF OSF Save files to disk -Update process fileprocess_info.json Request Check Fixity Check Fixity UNIVERSITY OF NOTRE DAME

Let's look at Fixity:

First Fixity Check

Resources are delivered in the POST request in BagIt format as a zip file. After unzipping the file and saving it to the server we validate the bag using BagIt's built in validator. If any files saved don't match the manifest originally given then the fixity has failed and the server will return an error.

Generate New Hashes If Necessary

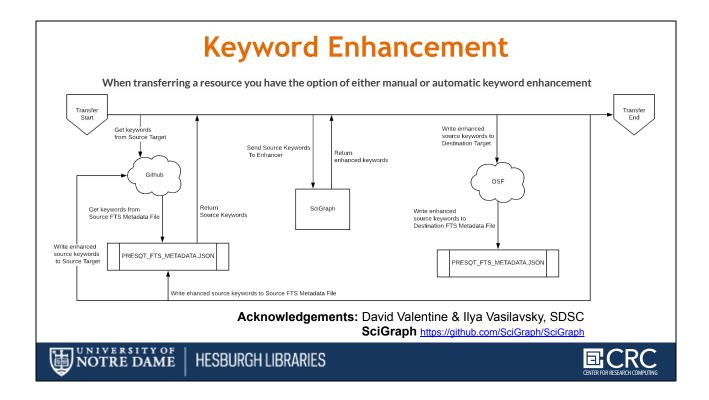
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We now know that the currently saved files are the same as what the user sent forward. Before uploading resources to the target we will make sure that there is a dictionary of hashes available generated by a hash algorithm supported by the target. If the target supports a hash algorithm provided by the resource's 'bag' then we will simply use those. If not, then we need to generate new hashes based on a target supported hash algorithm.

Second (Post transfer Fixity Check)

After resources are uploaded to the target, we compare the resources' hashes

brought back from the target to the hashes we captured before. If any hashes don't match then fixity fails. Since the resources have already been uploaded we simply capture which resources' fixity fails and pass that along the response payload along with the message, 'Upload successful but fixity failed'.



Keyword Assignment During Transfer

You and your organization can use PresQT services to auto-enhance Keywords via Sci Graph thanks to workshop help from David Valentine and Ilya Zaslavsky at SDSC.

You can get more information at https://github.com/SciGraph/SciGraph [SHARE IN CHAT]

When transferring a resource you have the option of either manual or automatic keyword enhancement.

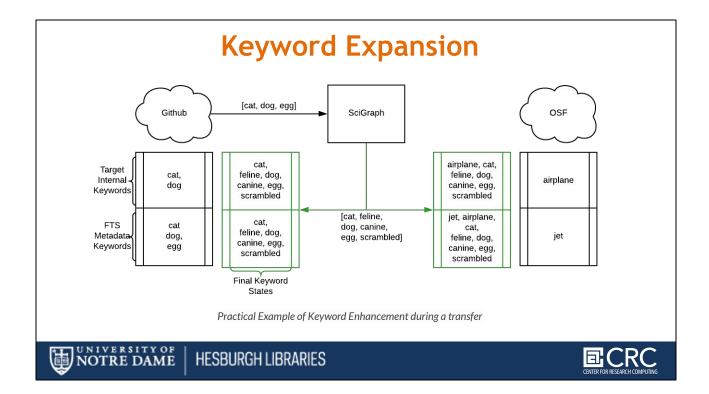
- Manual enhancement will only add source keywords and the keywords provided in the request body.
- Automatic will add all enhancements including any provided in the request body.
 - These can be set by setting presqt-keyword-action in the headers to
 either manual Or automatic

If presqt-keyword-action is manual then PresQT will only add keywords found in the source target and keywords given in the body of the request. This means you need to get the possible enhancements before initiating a transfer.

Automatic Keywords

If presqt-keyword-action is automatic then PresQT will add keywords found in the source, keywords given in the request body, and any keyword enhancements found during the transfer process. The following steps occur during the transfer in this case:

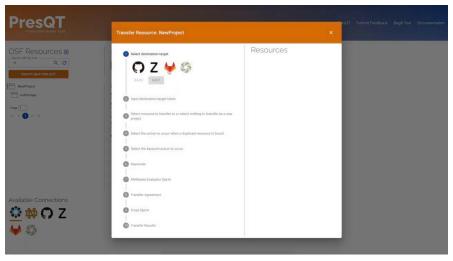
- 1. Fetch all source keywords both in the target and in the FTS metadata file for the transferred resource.
- Get enhancements with the given enhancer (Defaults to SciGraph for now).
- Upload keyword enhancements to the Source Target and Destination
 Target.
- 4. Add the keyword enhancements to the FTS Metadata file that gets written to the Destination Target during the transfer.
- 5. Add the keyword enhancements to the FTS Metadata file that gets written to the source Target during the transfer.



Practical Example/Demo of using PresQT for Keyword expansion

Keyword Enhancement w/ Transfer

Utilizing github.com/SciGraph/SciGraph

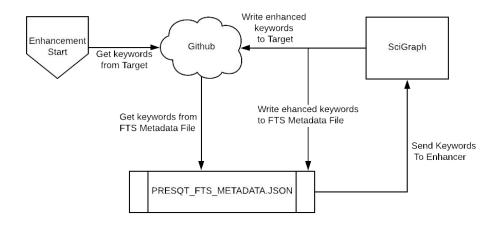






Or try the service on PresQT web GUI against your own endpoints

Keyword Enhancement w/o Transfer





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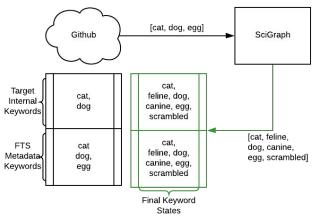


Keyword Enhancement can also be done without transferring.

- Use the Keyword Enhancement GET endpoint to fetch the keywords from the resource.
- 2. Pass the keywords you want to enhance to the Keyword Enhancement POST endpoint.
- 3. Enhanced keywords will get uploaded to the target and a new action will get written to the FTS metadata file.

•

Keyword Enhancement w/o Transfer



Practical Example of Keyword Enhancement without a transfer



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Practical Example of how keyword enhancement without transferring.

- Use the Keyword Enhancement GET endpoint to fetch the keywords from the resource.
- Pass the keywords you want to enhance to the Keyword Enhancement POST endpoint.
- Enhanced keywords will get uploaded to the target and a new action will get written to the FTS metadata file.



Findable: Metadata and data should be easy to find for both humans and computers.



Accessible: The exact conditions under which the data is accessible should be provided in such a way that humans and machines can understand them.



Interoperable: The (meta)data should be based on standardized vocabularies, ontologies, thesauri etc. so that it integrates with existing applications or workflows.



Reusable: Metadata and data should be well-described so that they can be replicated and/or combined in different research settings.



Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* **The FAIR Guiding Principles for scientific data management and stewardship.** *Sci Data* 3, 160018 (2016). doi.org/10.1038/sdata.2016.18

Mons, Barend et al. 'Cloudy, Increasingly FAIR; Revisiting the FAIR Data Guiding Principles for the European Open Science Cloud'. 1 Jan. 2017: 49 – 56. DOI: 10.3233/ISU-170824



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The FAIR principles were introduced in 2016. You can see them on the left. The guiding principles allow many different approaches to rendering data and services Findable, Accessible, Interoperable, to serve the ultimate goal: the reuse of valuable research objects.

What FAIR is...

FAIR refers to a set of principles for humans or machines/software.

The FAIR principles emphasize that re-useful data (Data which actually can be reused) will be become as valuable as is possible.

From Cloudy, Increasingly FAIR written by FAIR's originators and stakeholders emphasizes that the principles

deliberately do not specify technical requirements, but are a set of guiding principles that provide for a continuum of increasing reusability, via many different implementations.

The principles describe characteristics and aspirations for systems and services to

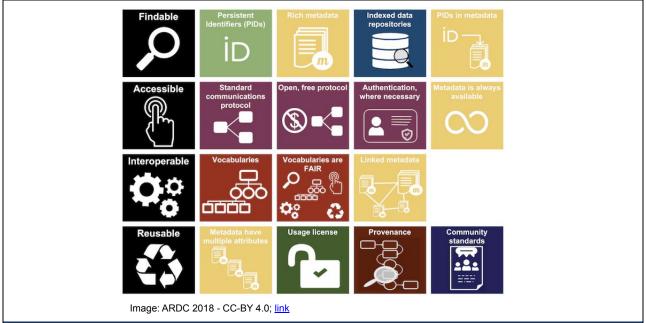
....and what FAIR is not

FAIR is not a standard: The FAIR guiding principles are sometimes incorrectly referred to as a 'standard', even though the original 2016 publication explicitly states they are not [25].

FAIR simply describes the qualities or behaviours required of data resources to achieve – possibly incrementally – their optimal discovery and scholarly reuse.

Standards are prescriptive, while guidelines are permissive.

FAIR originators and stakeholders suggest that a variety of follow-on valuable standards can and should be developed atop the FAIR principles, each of which can be guided by the FAIR Principles.







Here's a example of that incremental approach. Here you see an infographic from ARDC Australian Research Data Commons that communicates essential elements of FAIRness in easy to understand chunks aligned with the principles

FAIR Assessment FAIR Principles Compliance Resource and its metadata are easy to find by both, humans and computer systems. Basic machine readable descriptive metadata allows the discovery of interesting data sets and Accessibility Resource and metadata are stored for the long term such that they can be easily accessed and downloaded or locally used by humans and ideally also machine readable. A2. Publications and data repostories have contingency plans to assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible even when the resource assure that metadata remains accessible for download or manipulation by humans and is ideally also machine readable. assure that metadata remain accessible, even when the resource or the repository are no longer available. Interoperability Metadata should be ready to be exchanged, interpreted and combined in a (semi)automated way with other data sets by humans as well as computer systems. 1. Resource is uploaded to a repository that is interoperable with other platforms. 2. Repository meta-data schema maps to or implements the CG fore metadata schema CG Core metadata schema. I3. Metadata use standard vocabularies and/or ontologies. Reusability Data and metadata are sufficiently well-described to allow data to be reused in future research, allowing for integration with other compatible data sources. Proper citation must be facilitated, and the conditions under which the data ran the used should be clear to machines data can be used should be clear to machines UNIVERSITY OF NOTRE DAME **HESBURGH LIBRARIES**

Once funders like ARDC began to request FAIR data of their funded projects, the stakeholder community began pairing compliance aspects with the principles.

In turn, the growing maturity in FAIR digital objects and repositories began to create an information ecosystem where FAIRness could be tested

But what should FAIR testing aim for?

This is tricky to implement because remember FAIR is for people and machines!

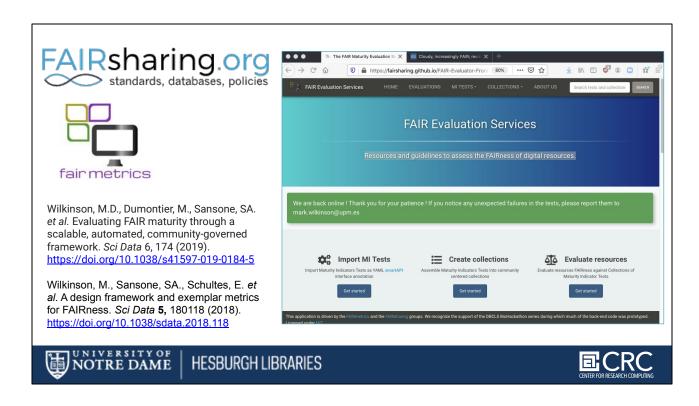
Early tests relied on surveys people would fill out answering questions about their data

While FAIR testing today is increasingly automated and focused more on whether data is FAIR for "machines" / software.

To learn more about automating FAIR assessment, PresQT did workshops with Mark Wilkinson, Daniel Clarke and Avi Ma'ayan to learn their approaches to FAIR assessment

Then we stood up FAIR testing using Mark's evaluator service for

PresQT endpoints, let's take a look:



The FAIR Maturity Indicator Authoring Group wanted to provide an objective, automated way of testing (meta)data resources against the FAIR Maturity Indicators

They defined maturity indicators and tests aligned with the FAIR principles, aligned with the metric they test for

You can browse them online. I'll share them in the chat so you can have a look at:

https://fairsharing.github.io/FAIR-Evaluator-FrontEnd/#!/metrics

[SHARE IN CHAT]

You can read more about the indicators in the papers on the left

Mark Wilkinson and the group also created the FAIR Evaluator which runs as a demonstration service. You can see a screenshot of it on the right. I'll share the URL in the chat:

https://fairsharing.github.io/FAIR-Evaluator-FrontEnd/#!/

[SHARE IN CHAT]

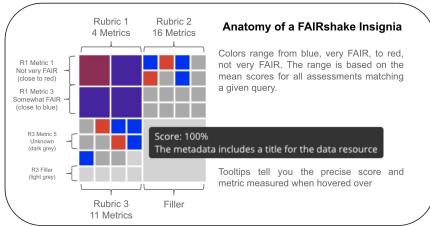
The Evaluator provides a registry and execution functions for:

- Maturity Indicator Tests
- Community-defined Collections of Maturity Indicator Tests
- Quantitative FAIRness evaluations of a Resource based on these Collections

FAIR Assessments - FAIRSharing **Control Board | **Control Board

Demo runs

FAIR Assessments - FAIRShake (In progress)



fairshake.cloud

Clarke DJB, Wang L, Jones A, Wojciechowicz ML, Torre D, Jagodnik KM, Jenkins SL, McQuilton P, Flamholz Z et al. [...] Ma'ayan A. **FAIRshake: Toolkit to evaluate the FAIRness of research digital resources.** *Cell Systems* 9(5):417-421 (2019) PMID: 31677972



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FAIRshake is another web-based software toolkit that enables the assessment of compliance of biomedical digital research objects with the FAIR guiding principles.

I'll paste a link to FAIRshake into the chat: https://fairshake.cloud/ [SHARE IN CHAT]

FAIRshake also functions as a repository to store and serve FAIR assessments.

It provides FAIRness assessments of three types of digital objects:

- 1. Datasets
- 2. Tools,
- and repositories/databases,

are based on answers to a set of questions

It has a concept of a test rubric that lets you group the tests you need together.

We'd like to thank the <u>FAIRshake</u> project for workshopping with PresQT particularly Daniel Clarke and Avi Ma'ayan, PhD Mount Sinai Center for Bioinformatics Icahn School of Medicine

We are working on integrating FAIRshake into PresQT testing.

Now let's take a look at what else is in progress:

In Progress . . . Future

Expanded services connecting:

- FAIRshake (FAIR testing with rubrics)
- EaaSI (Emulation Nomination)
- HUBzero (Repository Connection)
- WholeTale (Repository Connection)







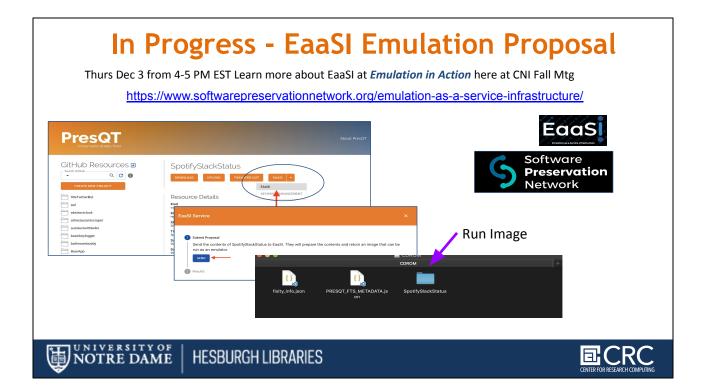




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- In addition to the FAIRshake work
- We created an demonstration integration with EaaSI. We'll show an example on the next slide.
- In 2021 Software Preservation Network Members have the opportunity to use a SPN hosted version of EaaSI - we anticipate another round of testing the PresQT prototype Emulation proposal launcher then to see how it can perform in the hosted environment
- We also have Integration testing with WholeTale and Hubzero underway



Let's take a look at EaaSI:

- With the PresQT service now we can connect to the Emulation as Service aka EaaSI decentralized node network's Universal Virtual interactor
- For that We'd like to thank
 - o Klaus Rechert, and the OpenSLX team in Freiburg
 - the EaaSI team at Yale especially Ethan Gates, Seth Anderson and Euan Cochrane
 - And Jessica Meyerson at SPN

Software Preservation Network

https://www.softwarepreservationnetwork.org/get-involved/







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Like we mentioned, in 2021 SPN is partnering with <u>EaaSI</u> to offer scaled, high-quality emulation services to members beginning in January 2021 and run until December 2021.

Here's a link to more information about the pilot that outlines the goals and structure for this exclusive, one year testing pilot of the EaaSI beta hosted service for participants in SPN member organizations.

https://www.softwarepreservationnetwork.org/hosted-emulation-services-pilot-summary/

[SHARE IN CHAT]

During this pilot, SPN would act as the first point of contact for EaaSI Hosted Emulation Services for its members, standardizing and overseeing EaaSI onboarding, and synthesizing feedback/data from members in order to inform the EaaSI development roadmap and service design.

SPN will standardize access to hosted emulation services by acting as a single "customer" and thereby streamlining invoicing, evaluation, onboarding, and documentation activities for SPN members.

Find out more at:

All this means here's never been a better time to join SPN:

Membership is 5k, and joining is easy!

Just Download, complete, and return the <u>SPN Membership Agreement</u> to Jess Farrell

PresQT QA Opportunities to Connect

- Sign up for our mail list at presqt.crc.nd.edu by Dec 4th, 2020
- Attend the PresQT community call 1 PM EST Dec 7th, 2020
- Contact us at <u>presqt-contact-list@nd.edu</u>
- Visit QA onboarding at https://presqt.readthedocs.io/en/latest/qa.html
 - Try the File Transfer QA Tests between systems you use like github & zenodo or figshare
 - Try the Keyword Enhancement QA Tests
 - Try the FAIR testing out on an object of your own at a PresQT endpoint





How else can you get involved with Data and Software Preservation?

- Join the PresQT mail list before December 4th and you'll get an invitation to participate in QA
- You can join using form at presqt.crc.nd.edu [SHARE IN CHAT]
- Then to onboard to PresQT's QA please encourage interested parties from your Organization to attend PresQT community call 1PM on Monday Dec 7th (afterward the calls will be offered twice monthly starting up again in 2021)
- On your own:
 - Try the File Transfer QA Tests between systems you use like github & zenodo or figshare
 - Try the Keyword Enhancement QA Tests
 - Try the FAIR testing out on an object of your own at a PresQT endpoint
- Contact us and give feedback about the service or endpoints you want to add

Upcoming Talks



Mon Dec 7 @11am EST

Trusted CI Webinar: Trustworthy Data A panel discussion on tools, standards, community practices for trustworthy scientific data sharing among Jim Basney: Deputy Director, Trusted CI, **Sandra Gesing:** Assoc Professor University of Notre Dame, PresQT, Bob Hanisch: Director of Office of Data & Informatics, NIST and Rebecca Koskela: Executive Director, Research Data Alliance - US (RDA-US).





Wednesday, 9 December 7:08AM EST

Sandra Gesing Improving the Publication and Re-Use of Data via PresQT Tools and Services (IN013-03) pre-recorded video & synchronous presentation at "Best Practices and Realities of Research Data Repositories: Which One Should I Choose to Publish My Data?" session of the 2020 American Geophysical Union Fall Meeting.



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We also have some upcoming talks where you can learn more about PresQT:

You can find PresQT's co-PI & Tech lead Sandra Gesing from Notre Dame's Center for Research Computing this coming Monday at the Trusted CI Webinar Here's a link to the webinar

https://blog.trustedci.org/2020/11/trustworthy-data-panel.html

[SHARE IN CHAT]

At Trusted CI you can learn more about the efforts of the NSF's Cybersecurity Center of Excellence and its Trustworthy Data Working Group (TDWG) in the broader context of related work by PresQT, NIST, and RDA-US.

And then a week from Wednesday Sandra will participating in the American Geophysical Union's Session on "Best Practices and Realities of Research Data Repositories: Which One Should I Choose to Publish My Data?"

As you can imagine, the PresQT File Transfer service makes these decisions less about end-of-the road one-size fits all solutions which we hope will interest you!

Thank You from the PresQT Team

Justin Branco, Brett Fox, Sandra Gesing, Rick Johnson, Natalie Meyers, Noel Recla, Miranda VanNevel, and John Wang

presqt.crc.nd.edu

These slides: osf.io/3gnqd doi:10.17605/OSF.IO/3GNQD

Right now you and your organization can: Add an Endpoint, Enhance your Keywords, Do FAIR testing!

Together we are: Collaboratively designing, developing, and connecting interoperable and repository agnostic Data and Software Preservation Quality Tools



An **implementation grant** (<u>LG-70-18-0082-18</u>) & previous **planning grant** (<u>LG-72-16-0122-16</u>) funded this effort to address needs for preserving data and software.



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Thank you from all of us on the PresQT Team Justin Branco, Brett Fox, Sandra Gesing, Rick Johnson, Natalie Meyers, Noel Recla, Miranda VanNevel, and John Wang

Please Test, Use, Nominate an Endpoint, Deploy, Develop Go to prestq.crc.nd.edu and join our mailing list