

European Research Projects as EOSC Service Providers

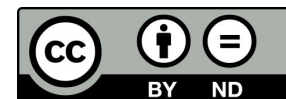
Pedro Principe (University of Minho / OpenAIRE)
Alexandre Bonvin (University of Utrecht)
Susanna Assunta Sansone (University of Oxford)



with



The EOSC Future, C-SCALE, DICE, EGI-ACE, OpenAIRE-Nexus, Reliance and ARCHIVER projects are funded by the European Union Horizon Programme calls INFRAEOSC-03-2020 and INFRAEOSC-07-2020 and H2020-ICT-2018-20





Agenda

1. 11.00-11.10- Introduction - Pedro Principe (University of Minho)
2. 11.10-11.15- HADDOCK Use Case -
Alexandre Bonvin (University of Utrecht)
3. 11.15-11.20 - FAIRsharing Use Case -
Susanna-Assunta Sansone (University of Oxford)
4. 11.20-11.45 - Q&A lead by Katrien Witpas (Arctik & EOSC Future)

Research Project as EOSC service providers (1 / 3)

What Research Projects can offer to EOSC

SERVICES

Compute Resources, Data management services, Virtual Research Environments, Data Analysis tools...

RESEARCH PRODUCTS

Publications, Datasets, Software, other research outputs...

+ Training tools (resources & materials)



Research Project as EOSC service providers (2 / 3)

Why Research projects should become an EOSC provider

- Increase **visibility** of research resources, content and services.
- Improve **discoverability** of the project research outcomes.
- Sharing resources **beyond community** boundaries.
- Reporting **scientific production** to funders (e.g. EC) and scholarly communication services.
- Direct **access to Data and services**
- Contribute & access **training** materials, **helpdesk** service and **OS metrics**.



Research Project as EOSC service providers (3 / 3)

For onboarding of the research project resource (service/tool...)

- ★ Provider (of the service as outcome of a project) fulfilling necessary info in the **Provider Profile**.
- ★ Service (offered by a Provider) available to customers in Europe with sufficient **maturity** (\geq TRL8)
- ★ Service targeted to **EOSC communities** and to build on/leverage EOSC capability
- ★ Service with a **completed profile** with basic info of the **resource & policies**, not forgetting the **helpdesk** function and the **training** materials.



Tip: do not forget to integrate the onboarding features into the research project exploitation or sustainability plan.

European Research Projects as EOSC Service Providers

HADDOCK/WeNMR Use Case

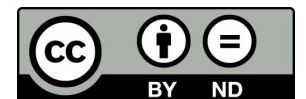
Alexandre Bonvin (University of Utrecht)



with

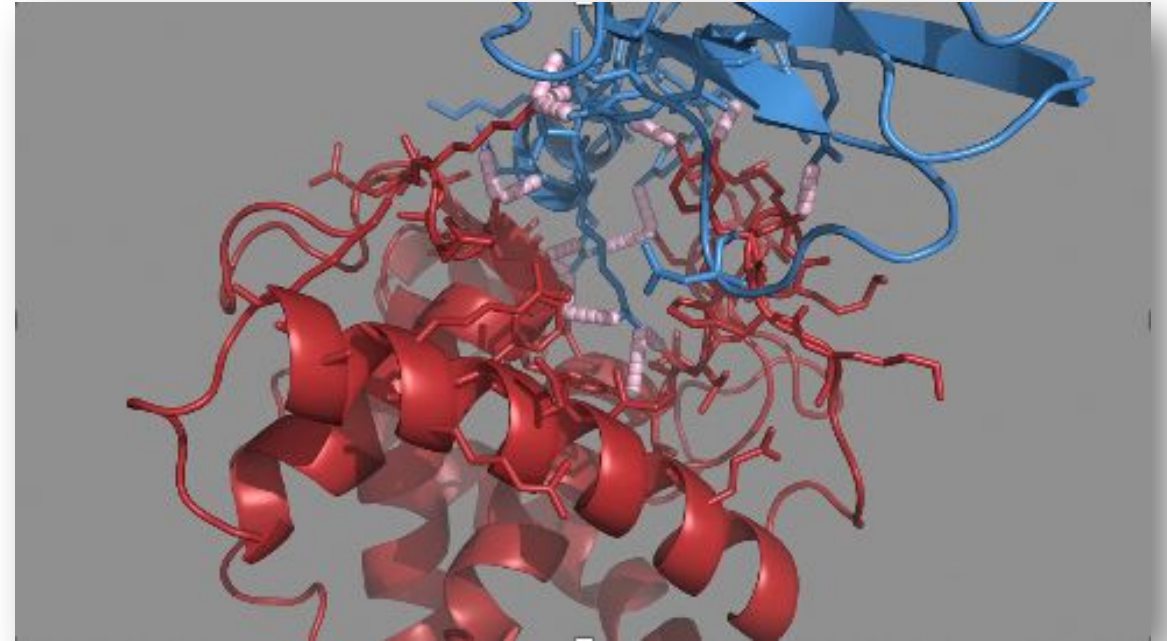
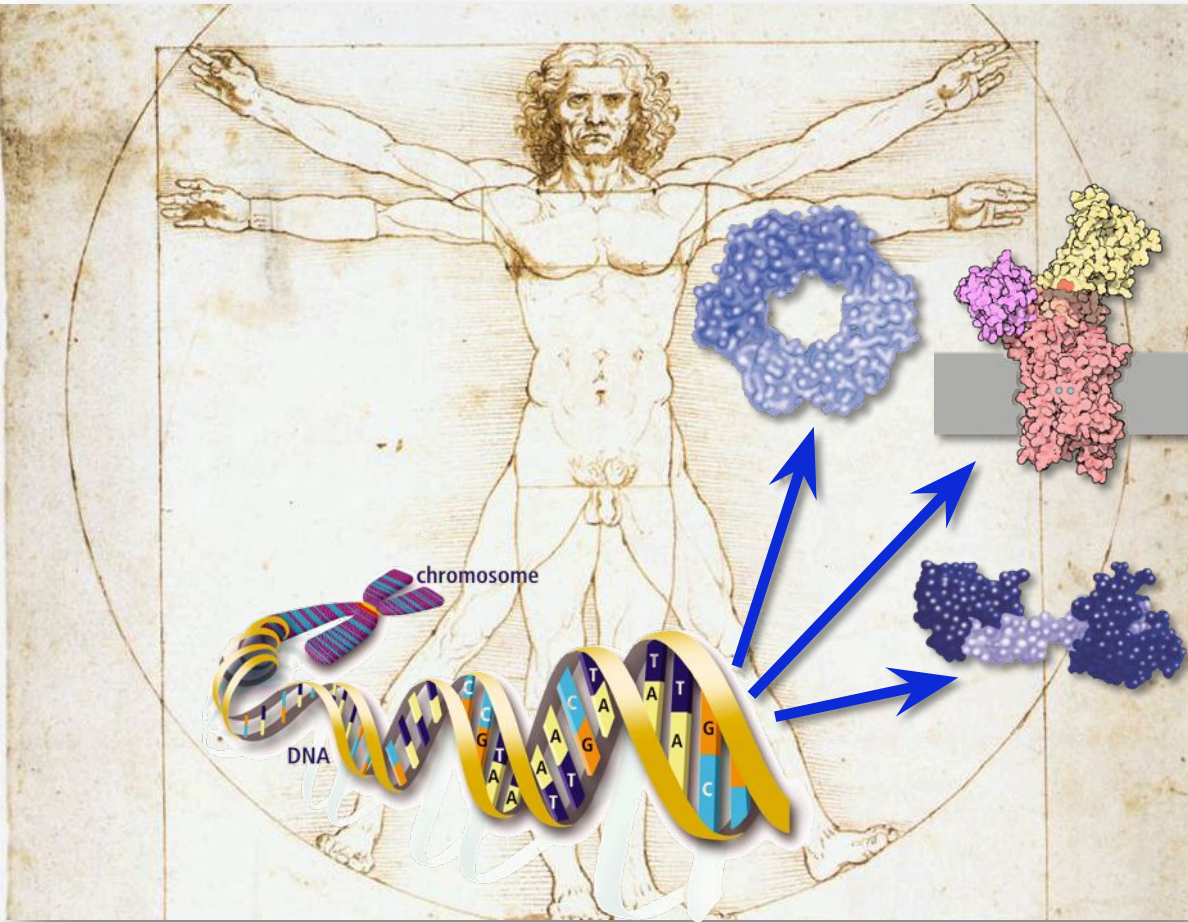


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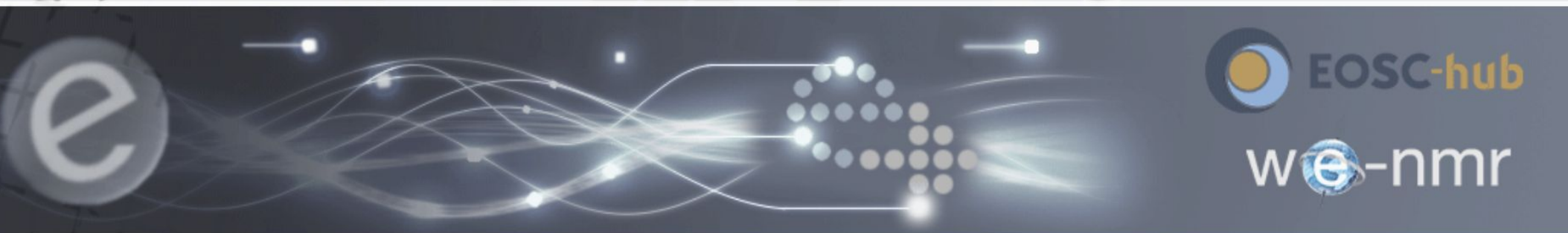
Domain: life sciences / structural biology

Understand life at a molecular level



Main use cases:

- Disease-causing mutations
- Engineer better molecules for material, health or food applications
- Obtain a starting point for drug design to combat disease



*WeNMR is a
worldwide e-
Infrastructure for
NMR and structural
biology*

- ✉ Email
- Facebook
- LinkedIn
- GitHub
- YouTube

WeNMR is a Virtual Research Community supported by EGI. WeNMR aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for data analysis and modelling.

This is a new re-design of the WeNMR entry. At the moment, WeNMR is operating as a thematic service in the [EOSC-hub](#) project.


The old registration system has been discontinued, but we are working to provide a new one soon.

[Home](#) > [My Providers](#)

Show: ☒ Approved ☐ Pending ☐ Rejected ☐ Incomplete

Approved

Approved




A Worldwide e-Infrastructure for Structural Biology

Provider Status: Approved
First Resource Status: Approved

[Update Provider](#) [More](#)

Approved



Bijvoet Centre - Utrecht University

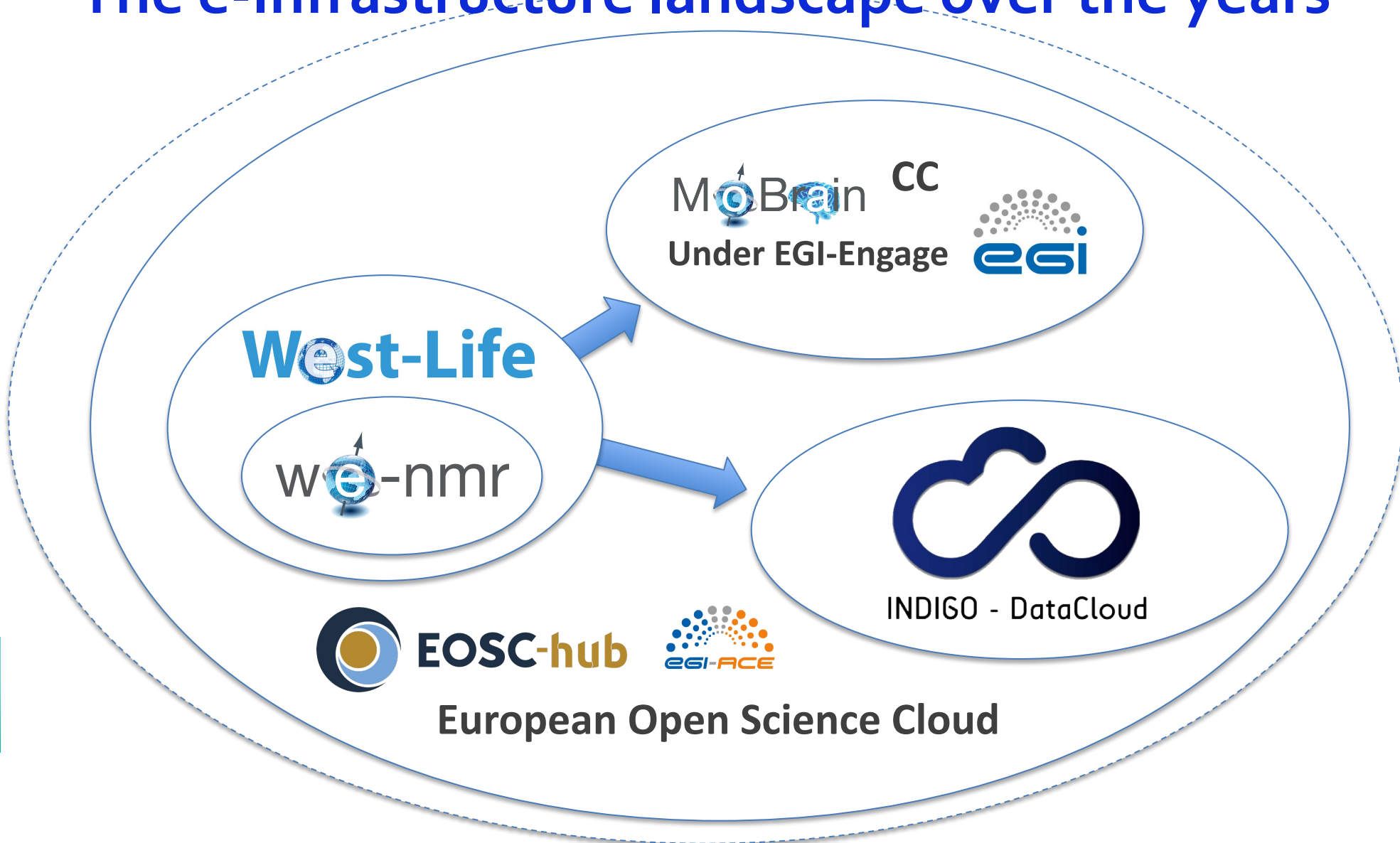
Provider Status: Approved
First Resource Status: Approved

[Update Provider](#) [More](#)

<https://providers.eosc-portal.eu/dashboard/wenmr>

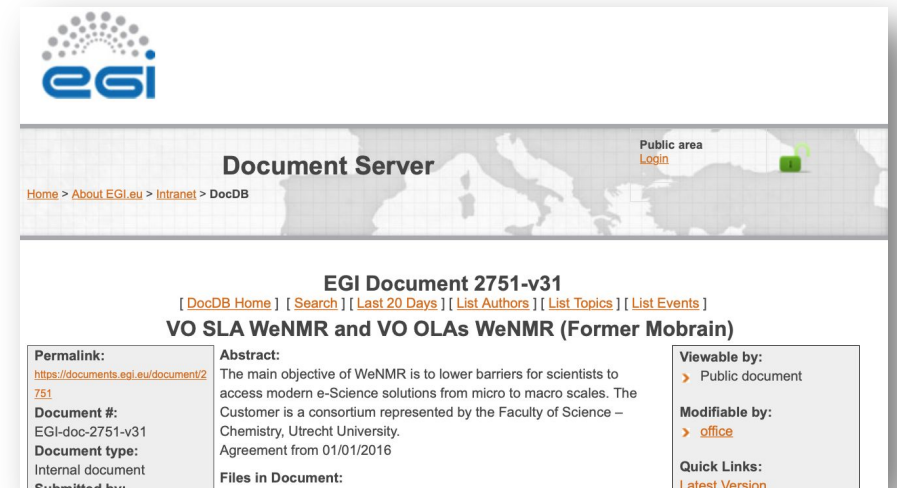
How did we get there?

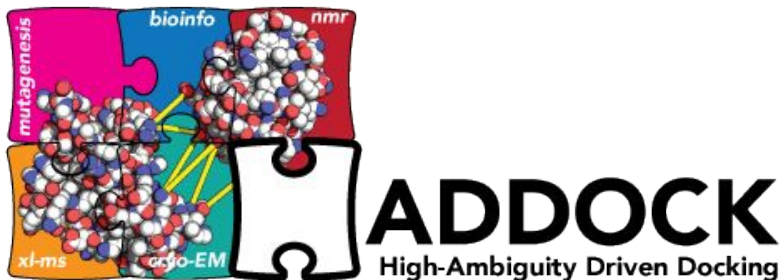
The e-Infrastructure landscape over the years



Why registering in EOSC?

- The WeNMR services have been in production since >10 years under various projects (eNMR, WeNMR, West-Life, EOSC-Hub, EGI-ACE)
- Thematic services under EOSC
- Access to resources formalized via EGI through a SLA agreement valid until 06/2023
 - **50+ million CPU hours (opportunistic access)**
 - 500+ cloud CPU cores
 - ~60 TB storage





- > 28000 registered users
- > 425000 served runs since June 2008
- > 55% on EOSC/EGI HTC resources

De Vries *et al.* Nature Prot. 2010

Van Zundert *et al.* J.Mol.Biol. 2016

HADDOCK 2.4
@Bonvinlab

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

Welcome! **HADDOCK** (High Ambiguity Driven protein-protein **DOCK**ing) is an information-driven flexible docking approach for the modeling of biomolecular complexes.

HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. It also allows to define specific unambiguous distance restraints (e.g. from MS cross-links) and supports a variety of other experimental data including NMR residual dipolar couplings, pseudo contact shifts and cryo-EM maps.

HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes, including multi-bodies (N>2) assemblies.

HADDOCK is one of the **flagship software** in the EU H2020 **BioExcel** Center of Excellence for Biomolecular Research.

New to HADDOCK? To use the HADDOCK docking server you must have registered for an account.

Register

Our server is **easier than ever** to use.
Try our new submission interface!

Submit a new job

HADDOCK is used for **excellent science** and so far it has been cited more than **5000 times!**

See our tutorials

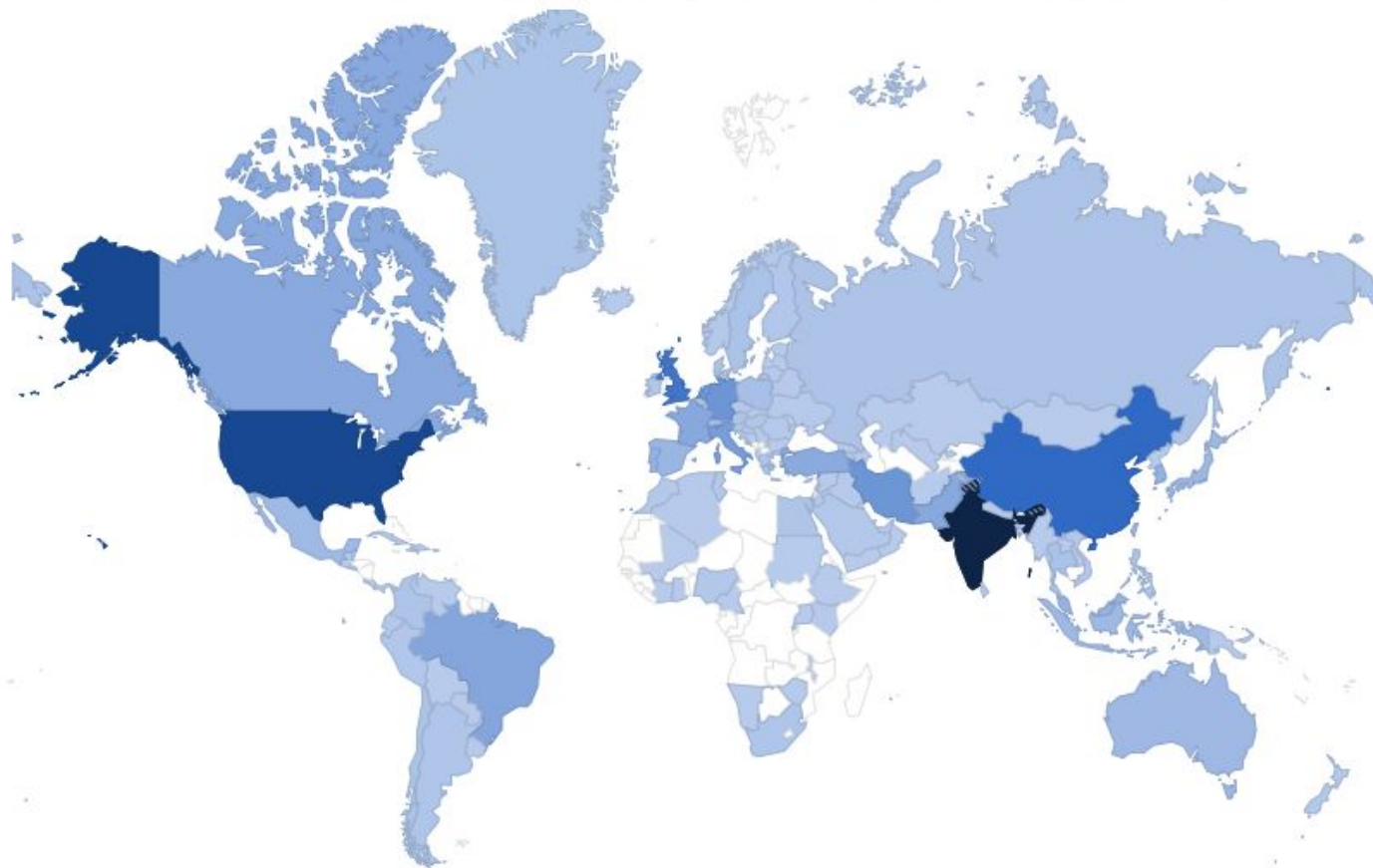
Looking for support or **questions about HADDOCK's usage?** Check our BioExcel forum!

Get Help

<https://wenmr.science.uu.nl>

Worldwide User Map

The HADDOCK web portal is being used by **29221 users** accross **135 countries!**



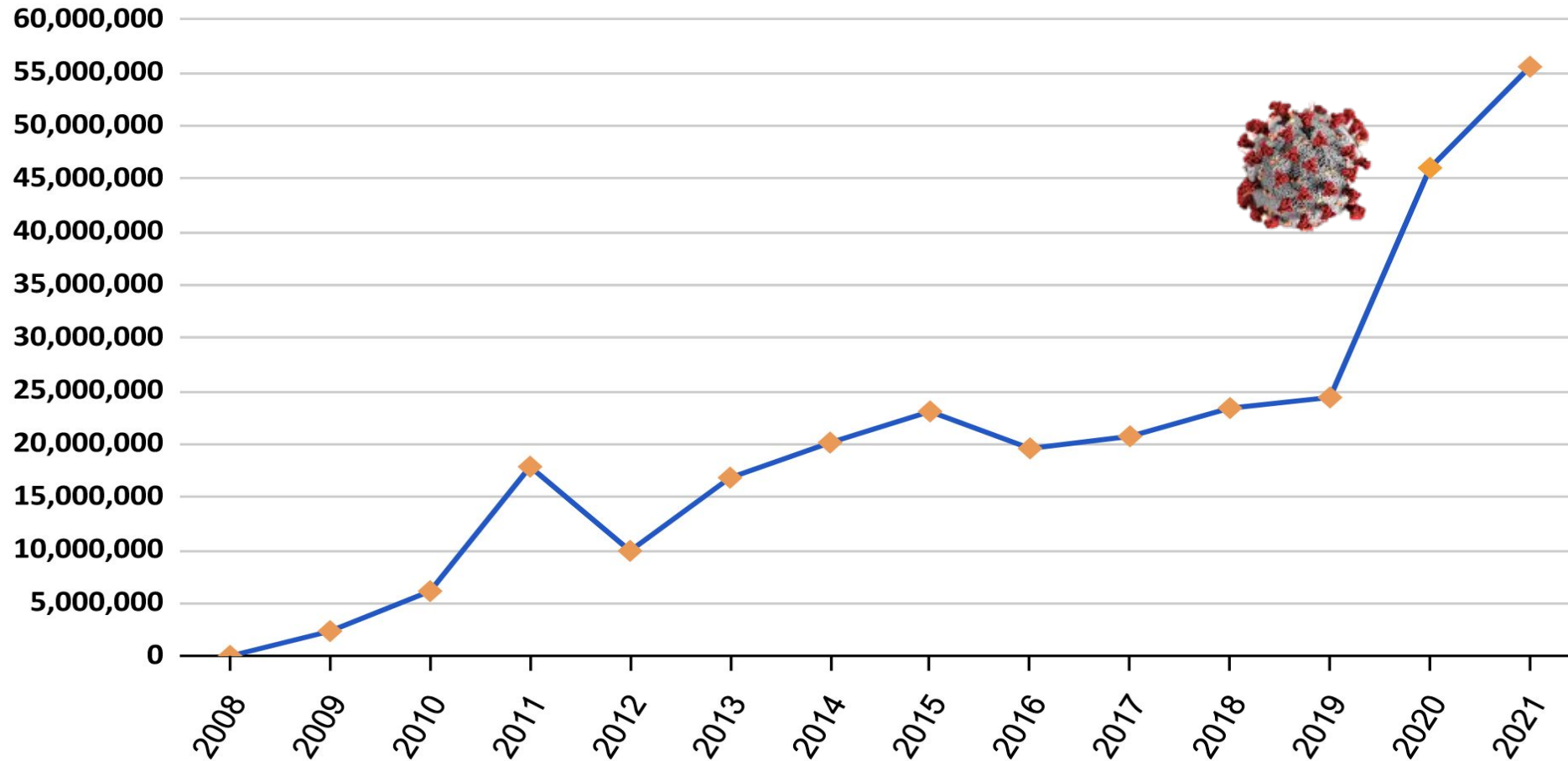
Show entries

Search:

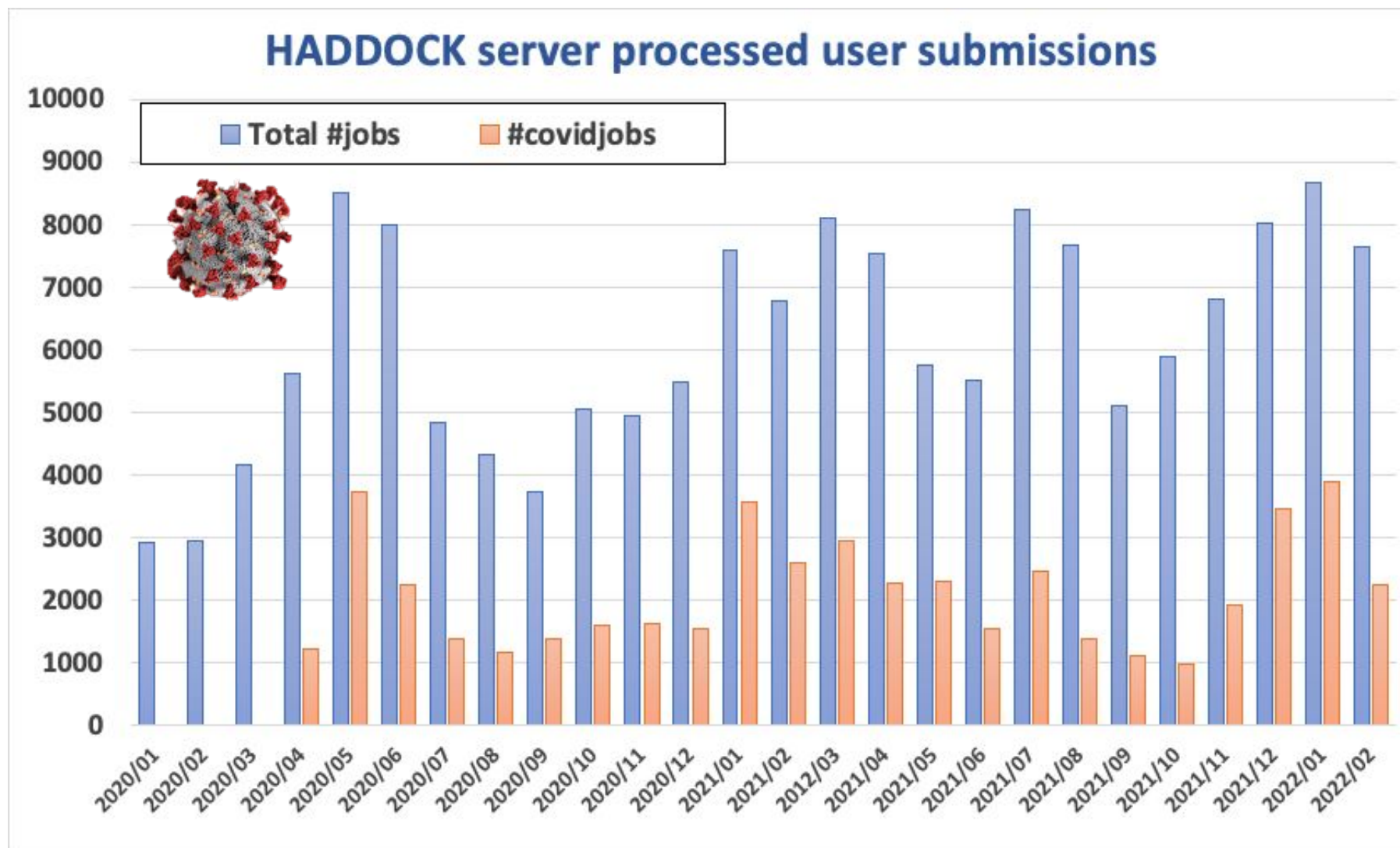
Country	Total	HADDOCK	DisVis	PowerFit	SpotON
Worldwide	29221	28274	4641	3779	4300
Europe	5984	5717	908	633	732
India	5888	5739	952	851	954
United States	4013	3878	610	447	546
China	2053	2020	361	323	358

Impact: Resources usage

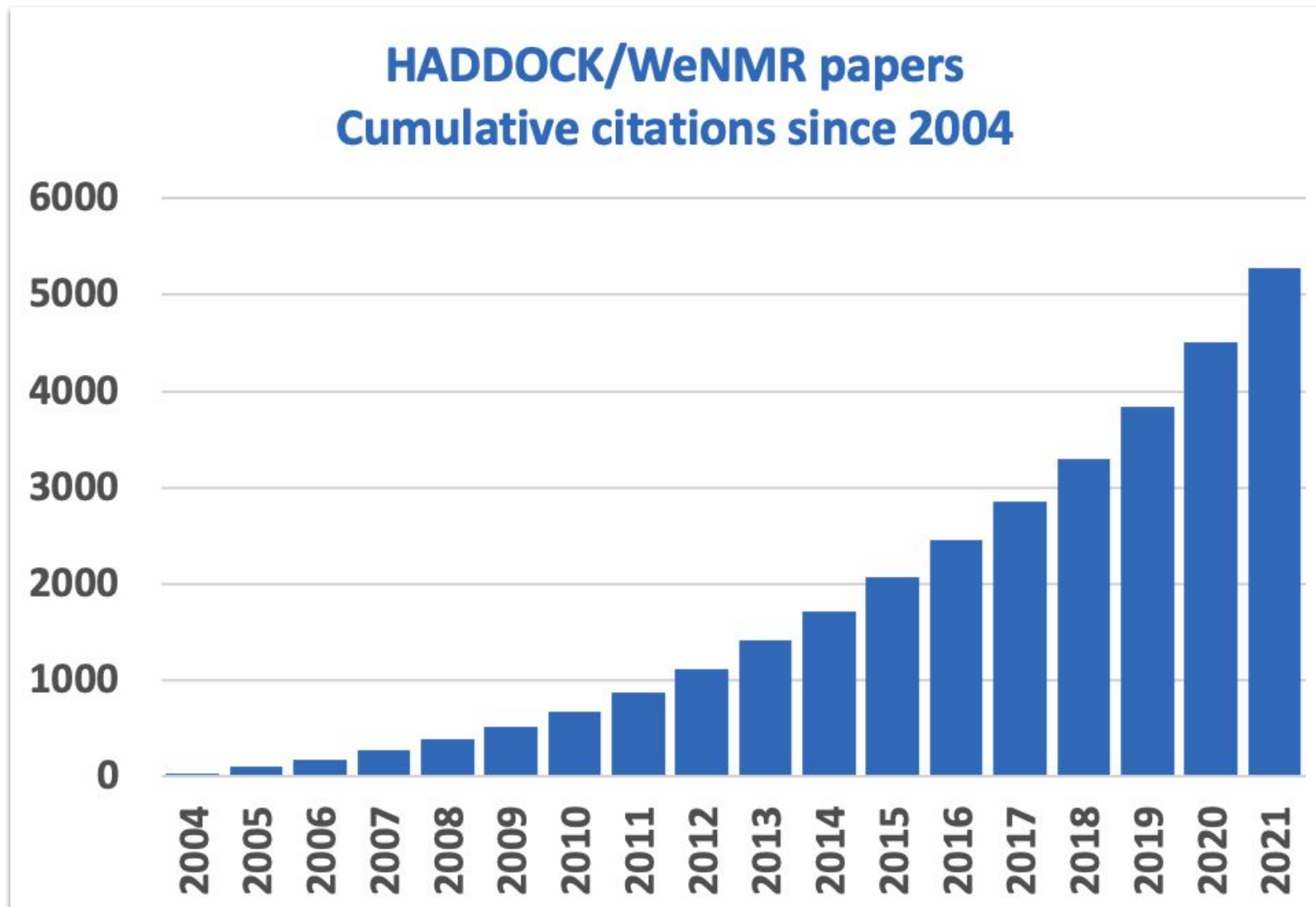
enmr.eu VO normalized CPU hours/year



Impact: User submissions



Impact: Citations of resources





In summary

- A long history of providing services to a worldwide user community
- A long history of using EU e-Infrastructure (HTC)
- WeNMR well-established thematic service provider
- Natural transition into EOSC
- Main benefits:
 - Ensuring access to computational resources
 - Strong network that helps sustainability (e.g. via EU projects)

European Research Projects as EOSC Service Providers

FAIRsharing Use Case

Susanna-Assunta Sansone (University of Oxford)

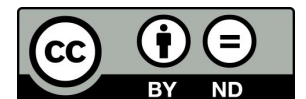
FAIRsharing.org




with



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FAIRsharing in the EOSC Marketplace


**EUROPEAN OPEN
SCIENCE CLOUD**

Find resource...

All resources

Resources > Sharing & Discovery > Scholarly Communication > Discovery > FAIRsharing



**FAIRsharing**
FAIRsharing: making standards, databases and policy count
Organisation: **Oxford e-Research Centre, University of Oxford, UK**
Provided by: **ELIXIR United Kingdom**

☆☆☆☆☆ (0.0 / 5) 0 reviews ☐ Add to comparison ☐ Add to favourites

Access the resource

OPEN ACCESS

[Webpage](#) [Helpdesk e-mail](#) [Manual](#) [Training information](#)

Provide feedback

SCIENTIFIC CATEGORISATION



Generic

- Generic
 - Generic

CATEGORISATION

- Scholarly Communication
 - Discovery
- Education & Training
 - Other
- Data Management
 - Interlinking
- Aggregators & Integrators
 - Services

Classification

- Target Users:
Funders, Resource Managers, Resource Provider Managers, Researchers, Policy Makers, Research Communities, Providers
- Access Types:
Virtual
- Access Modes:
Free
- Tags:
standards databases repositories policies formats
models schema metadata reporting guidelines
terminologies vocabularies ontologies fair
fair training fair education rdm data management

Availability

- Geographical Availabilities:
[World](#)
- Languages:
English

Marketing

- [Use case 1](#)
- [Use case 2](#)

Public Contacts

- contact@fairsharing.org

Maturity Information

- Trl:
TRL-9
- Life Cycle Status:
Production
- Certifications:
RDA endorsed output (<https://www.rd-alliance.org/group/fairsharing-registry-connecting-data-policies-standards-databases-wg/outcomes/fairsharing>), ELIXIR Recommended Interoperability Resource (<https://elixir-europe.org/platforms/interoperability/rirs>)
- Standards:
schema.org, JSON, DOI

Management

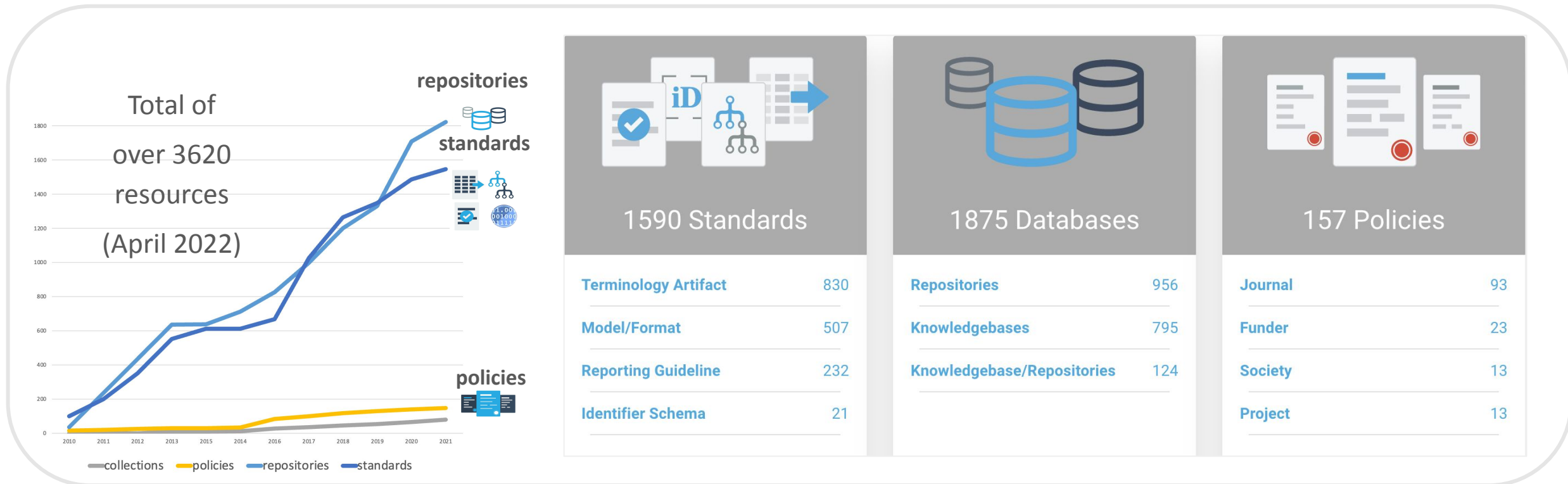
- [Manual](#)
- [Terms of use](#)
- [Privacy policy](#)
- [Access policies](#)
- [Training information](#)

<https://fairsharing.org/communities>

URL: <https://marketplace.eosc-portal.eu/services/fairsharing-c5d1ca3e-ef5a-4a98-845e-46e72ffb3419>

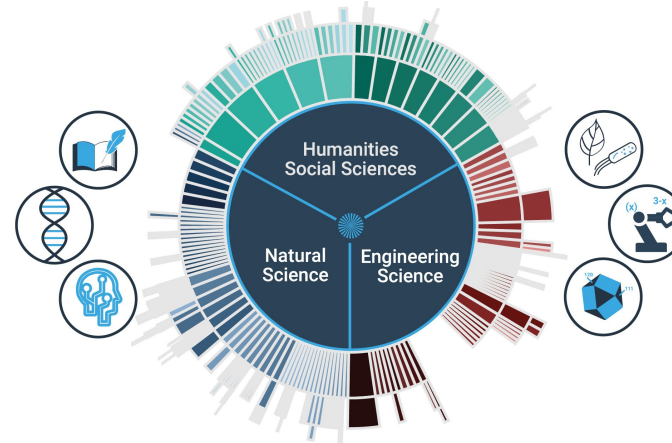
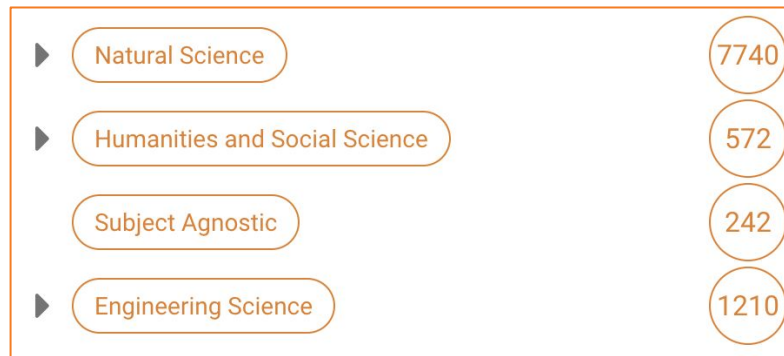


Promoting databases, standards, policies

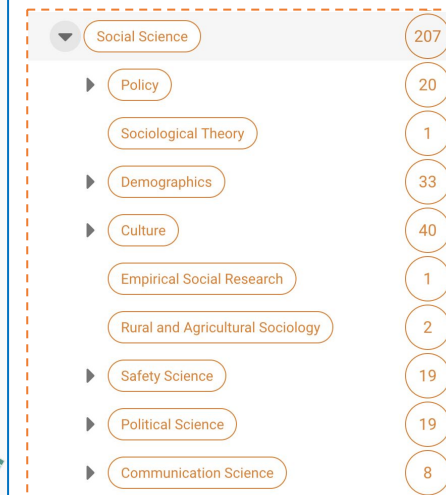
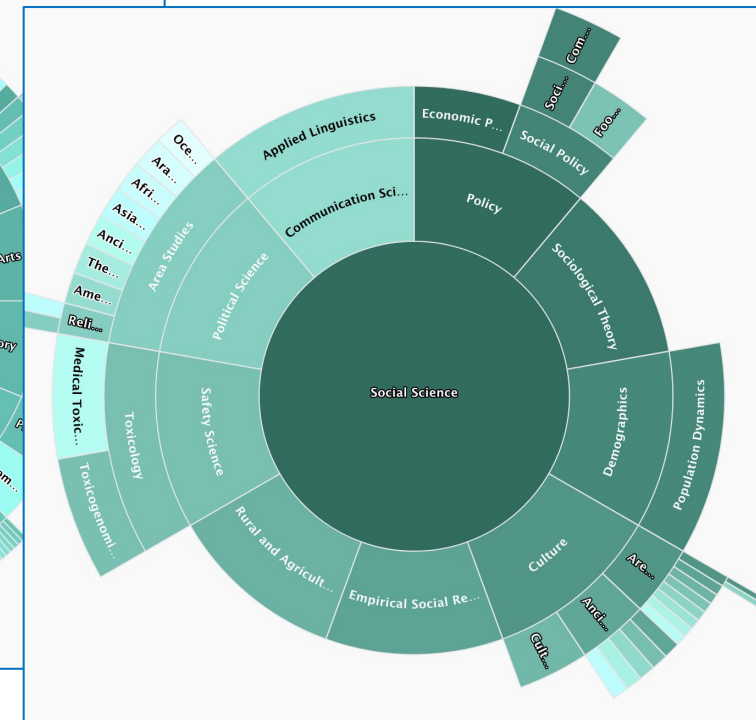
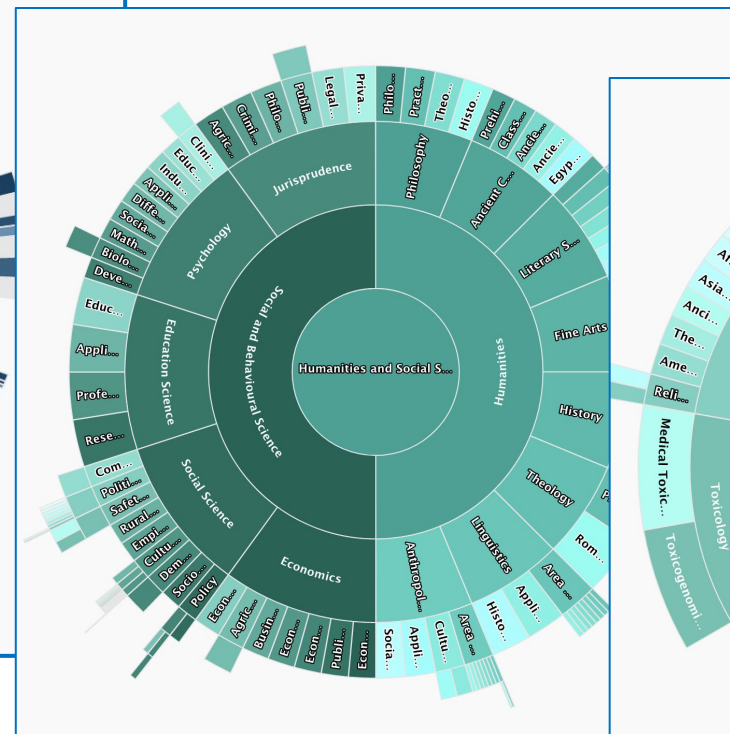
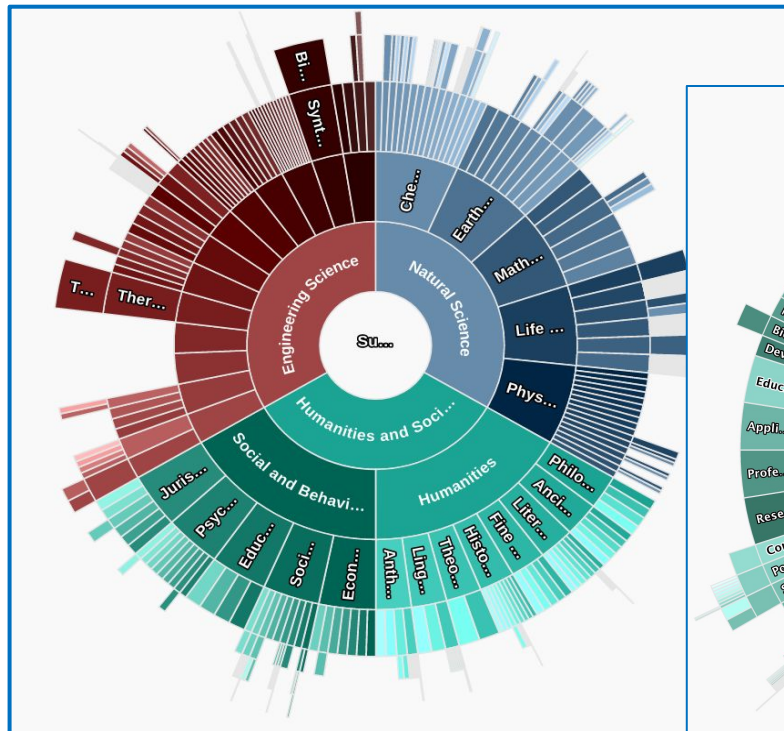


Guides **consumers** to *discover, select* and *use* these resources with confidence

Helps **producers** to make their resources more *visible*, more widely *adopted* and *cited*



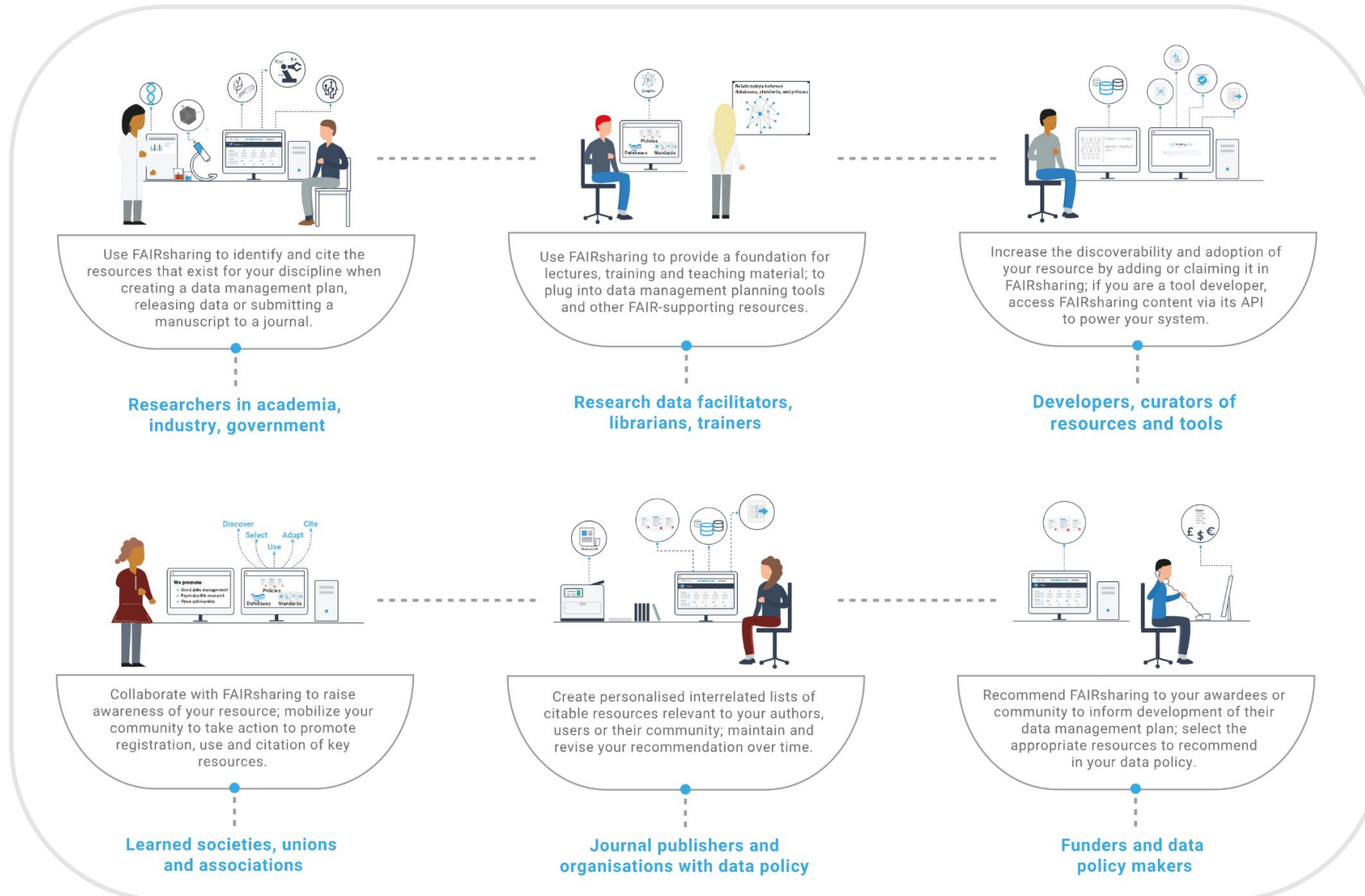
EOSC category: generic, all disciplines



Classification of standards, repositories and policies is powered by our open **Subject Ontology** of 436 terms

<https://fairsharing.org/browse/subject>
<https://github.com/FAIRsharing/subject-ontology>

Target users: all stakeholders



Why registering in EOSC?

A natural step, because FAIRsharing is already an element of the EOSC ecosystem

Users, adopters and collaborators include:

Users from all stakeholder groups



Researchers

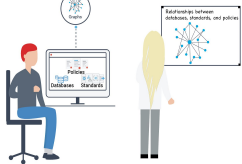


Developers and curators

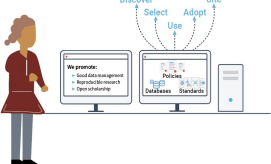


Journal publishers

Librarians and Trainers



Societies and Alliances



Funders



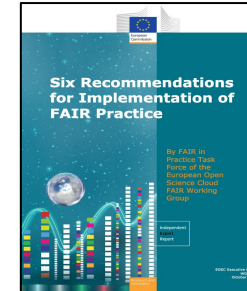
An endorsed output of the
FAIRsharing WG (since 2015):



A recommended resource in EOSC reports



A WG (since 2015) in:



WILEY
SPRINGER
NATURE



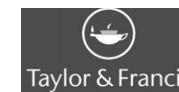
F1000
FACULTY of 1000



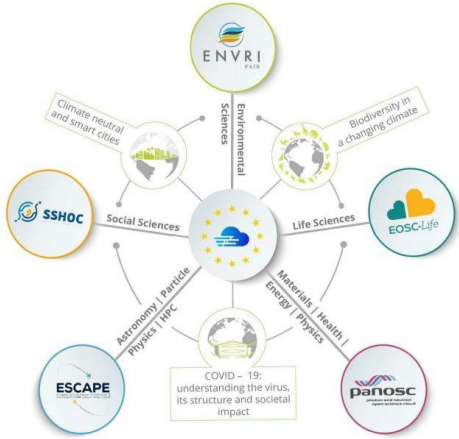
(GIGA) SCIENCE

OXFORD
UNIVERSITY PRESS

THE
ROYAL
SOCIETY
PUBLISHING

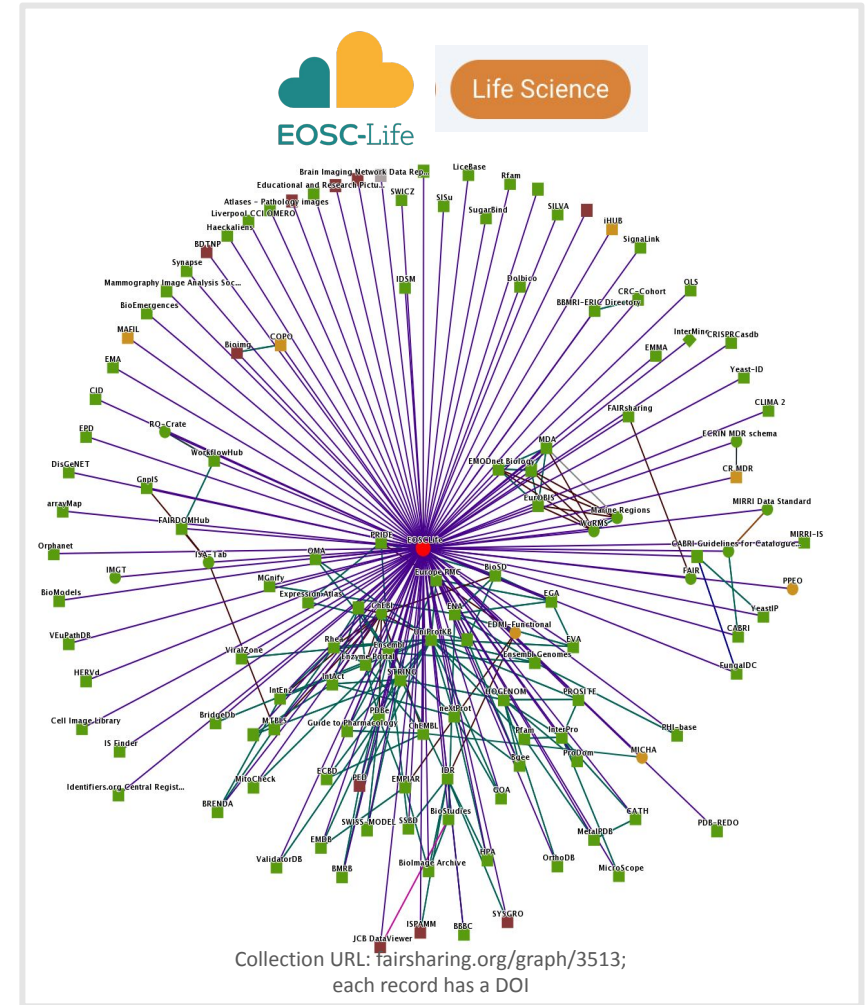
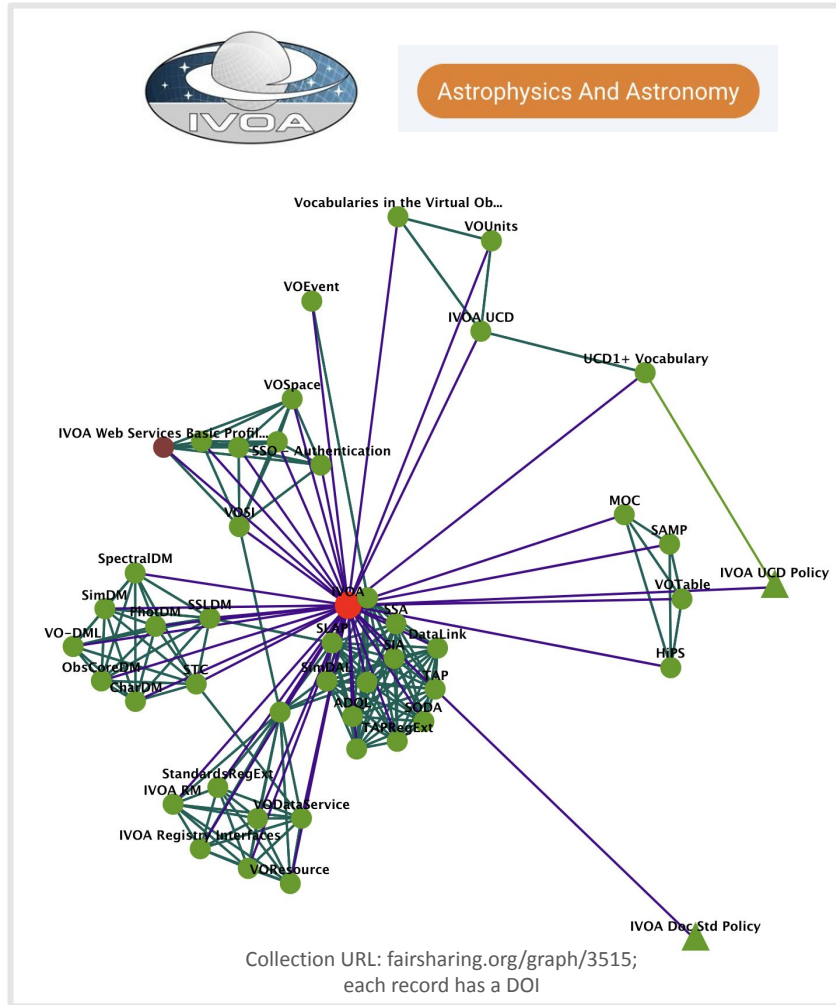


Contributing to EOSC and its knowledge graphs



Working with EOSC clusters to **curate** the **descriptions** and **visualize** the **relations** of their **databases** and the data/metadata **standards** they implement (as well as **cross-walks**)

=> "FAIR profiles"



Following EOSC's FAIRness & FAIR enablement

Findability



Sitemap.xml, JSON



Markup with Schema.org for search indexes

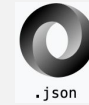


DOI unique persistent identifiers for each record



ORCID for author credit and authentication

Interoperability



JSON markup



Standardized semantics



Cross-links to or import from records in other registries



ROR for organizations (*ongoing*)



FundRef for funders (*ongoing*)

Accessibility



read/write REST API



read OAI-PMH

Reusability



CC BY 4.0 license



JSON export

In summary

- Launched in 2011, FAIRsharing has also matured under EOSC, working with and for many communities
 - it is part of EOSC projects, working with the clusters, and it is *de facto* element of its ecosystem
- The FAIRsharing onboarding process in the EOSC Portal:
 - first discussion Nov 2018; the process was evolving; first release in Dec 2019; updates made in 2021
- For FAIRsharing being in the EOSC Portal is
 - a natural step: a resource can never be visible and discoverable enough!
 - a way to identify how our content (standards, databases, policies) can contribute to building the Portal
 - EOSC Research Product Catalog, via our existing collaboration with OpenAIRE
 - EOSC Interoperability Registry, via EOSC Future
- Prospective benefits:
 - More users for FAIRsharing
 - More and new use of its content by other services
 - More collaborative activities

Current Operational Team

- **Allyson Lister**, Content and Community Lead
- **Milo Thurston**, Technical Lead
- **Ramon Granell**, Data Enrichment & Quality Manager
- **Delphine Dauga**, Data Curator Manager
- **Hiring in progress**, Web Developer
- **Dominique Batista**, Research Software Engineer
- **Philippe Rocca-Serra**, Co-Founder
- **Susanna-Assunta Sansone**, PI and Founder
- *and many collaborators and contributors!*

Executive Advisors

- **Varsha Khodiyar**, HDRUK
- **David Carr**, Independent expert
- **Chris Graf**, Springer Nature
- **Marta Teperek**, Data Stewardship Coordinator, TUDelft
- **Robert Hanisch**, Director, NIST Office of Data & Informatics
- **Peter McQuilton**, FAIRsharing Founding Member, GSK

Early Adopter Community Curators

- | | |
|--|----------------------------------|
| • Kyle Copas , GBIF | • Lindsey Anderson , PNNL |
| • Annie Elkjær Ørum-Kristensen , GBIF | • Joe Miller , GBIF |

Stakeholder Advisors

- **Amye Kenall**, VP of Publishing and Product, Research Square
- **Adam Leary**, Oxford University Press
- **Catriona MacCallum**, Hindawi
- **Dagmar Meyer**, European Research Council, Executive Agency
- **Dominic Fripp**, JISC, UK
- **Emma Ganley**, Protocols.io
- **Geraldine Clement-Stoneham**, Medical Research Council
- **Helena Cousijn**, DataCite
- **Iain Hrynaskiewicz**, PLoS
- **Imma Subirats**, FAO of the United Nations
- **Kiera McNiece**, Cambridge University Press
- **Luiz Olavo Bonino**, GO-FAIR
- **Marina Soares E Silva and Sarah Callaghan**, Elsevier
- **Michael Ball**, Biotechnology and Biological Sciences Research Council
- **Mike Huerta**, NIH National Library of Medicine
- **Molly Cranston and Guillaume Wright**, F1000Research
- **Nick Everitt and Matthew Cannon**, Taylor and Francis
- **Scott Edmunds**, GigaScience, Oxford University Press
- **Simon Hodson**, CODATA
- **Theo Bloom**, British Medical Journal
- **Thomas Lemberger**, EMBO Press
- **Wei-Mun Chan**, eLife
- **Sowmya Swaminathan**, Springer Nature



Q&A

1. What will I obtain by registering? Triggers & benefits to onboard
2. What type of resource can be onboarded?
3. How can we onboard end-users to our services via the EOSC Portal?
4. How can we measure impact?