Open research: Why it's important, how to make research more open and how to drive change

Iryna Kuchma, Open Access Programme Manager

eifl KNOWLEDGE WITHOUT BOUNDARIES

https://eifl.net/where-we-work

https://www.amicalnet.org/members

Note: some institutions overlap each other on the map, so they are not visible.

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POLICY 09 FEB 2023

Immediate open access 'should be EU default', says presidency

By Andrew Silver

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POLICY 03 FEB 2023

EU R&D ministers to debate infrastructures and publishing

https://www.researchprofessionalnews.com/rr-news-europe-infrastructure-2023-2-immediate-open-access-should-be-eu-default-says-presidency/

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Press release

8 February 2023 | 15:53

Research ministers discussed research infrastructures and open science

Implementing FAIR (Findable, Accessible, Interoperable and Reusable) principles in all research outputs and across disciplines is a significant undertaking for Europe, and requires changes in research culture and infrastructure. These changes must also align with international partners in like-minded regions and countries, and the ministers exchanged views on whether the EU should take action to accelerate this work.

> "There is room for improvement when it comes to the share of research data that can be accessed and reused, so we can accelerate scientific progress and increase societal impact."
>
> Mats Persson. Swedish Minister for Education

https://swedish-presidency.consilium.europa.eu/en/news/research-ministers-discussed-research-infrastructures-and-open-science/

https://swedish-presidency.consilium.europa.eu/en/news/research-ministers-discussed-research-infrastructures-and-open-science/

FEBRUARY 13, 2023

African researchers are ready to share more work openly—now policy must make it possible

by Lara Skelly and Ellsha Chiware, The Conversation

https://phys.org/news/2023-02-african-ready-openlynow-policy.html

Policy readiness

Our second study, a systematic review, found there was no shortage of examples of open science policies, nor was there a lack of implementation frameworks that could guide African open science stakeholders to develop their own policies, that would set out the open science intent and delineate the roles and responsibilities of stakeholders and researchers.

Some African countries are already doing well in open science. Botswana is one; stakeholders are working on a national policy to support open data activities. Botswana shows that all stakeholders must be included in policy development. Another is South Africa. The country's National Research Foundation is working towards an African open science platform. This is a collaboration of several national and international entities.

However, the lack of policy synergies appears to be holding back the African open science environment. Other researchers have put it like this: "African science systems largely operate independently of each other, creating silos of incompatible

https://phys.org/news/2023-02-african-ready-openlynow-policy.html

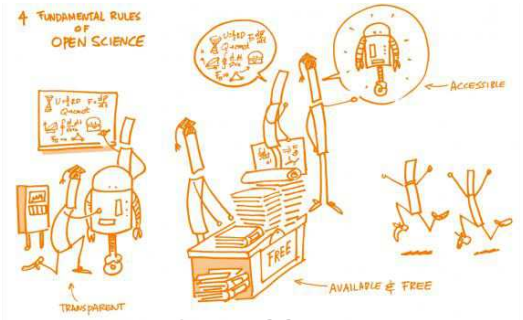
https://www.unesco.org/en/open-science

Definition of Open Science

Open Science:

- makes multilingual scientific knowledge openly available, accessible and reusable for everyone,
- increases scientific collaborations and sharing of information for the benefits of science and society,
- opens the processes of scientific knowledge creation, evaluation and communication to societal actors beyond the traditional scientific community.

Talking points



- Why open science is an issue that researchers can't afford to ignore
- How to go about making research more open
- What funders/institutions expect to see about open access, data sharing and open science when applying for new grants
- How to progress research career through practicing open science
- What reproducibility and replication is and how to practice them; improvement science initiatives on statistics, measurement, teaching, data sharing, code sharing, pre-registration, replication
- Questionable research practices and suggested improvements, good practice advice to early career researchers

PLOS

Iryna, three small actions that could give your next paper an extra boost

At PLOS we want your next research paper to maximize its reach, find its audience, and make a difference within its field and to wider society.

Read on to discover the relatively small additions you can build into your publishing process that could have big benefits for your research, the wider scientific community, and society as a whole.

PLOS

https://view.c.plos.org/?qs=807b1d67991196099ac463ecf2dfb48b3bea5f70d23cdcdb7fe648d551a2d47e0b9fd291

90%

Deposit your research data in a repository

Depositing your data in a repository is a great way to make your research more discoverable, reusable, and easier to cite. Research shows it can boost your papers citation rate by up to 25% compared with articles which do not utilize a data repository*.

Learn More

Post a preprint

A preprint is a version of a scientific manuscript posted on a public server prior to formal peer review. Posting a preprint gets your research into the public domain early, opening your work up at a time when it would otherwise be inaccessible, making it available for your peers to use, reference and build upon.

Learn More

Publish your methods

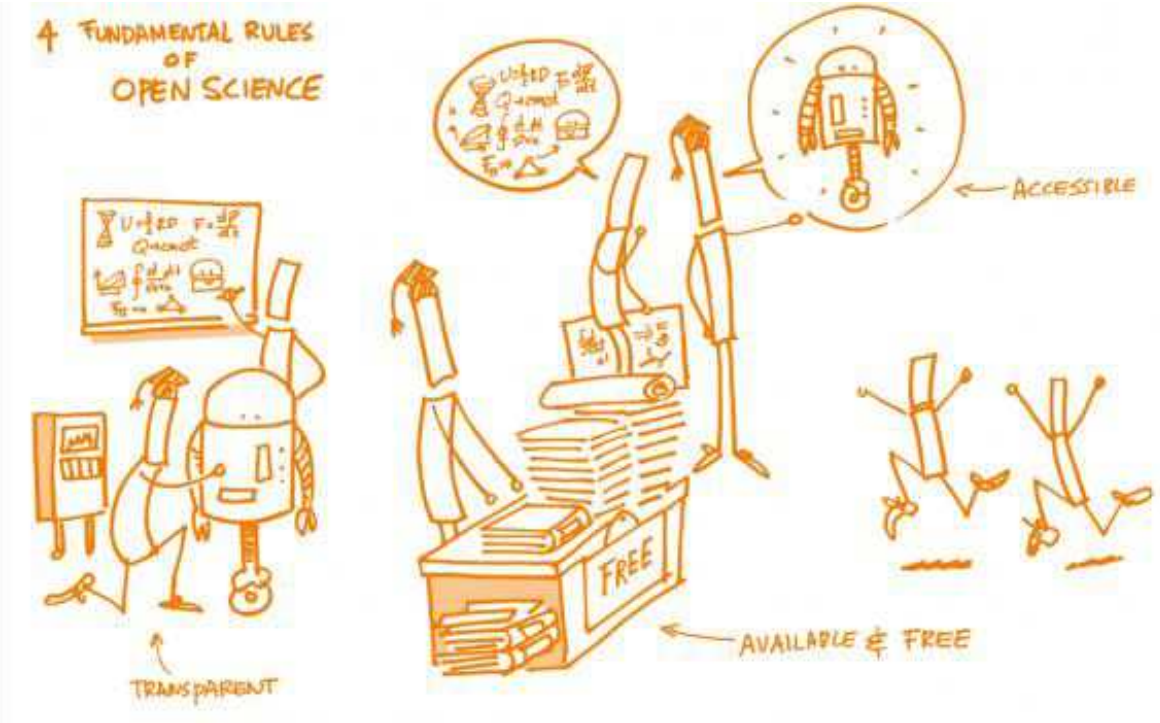
Methods help readers gain an increased respect for the integrity of your work, and have broad reuse potential,

Worries about doing Open Science

“How do I sell this to my advisor?”

“Won’t it make it harder to publish my research?”

"What if I get it wrong?“



Kathawalla, U.K., Silverstein, P. and Syed, M., 2021. Easing into open science: A guide for graduate students and their advisors. *Collabra: Psychology*, *7*(1). https://doi.org/10.1525/collabra.18684

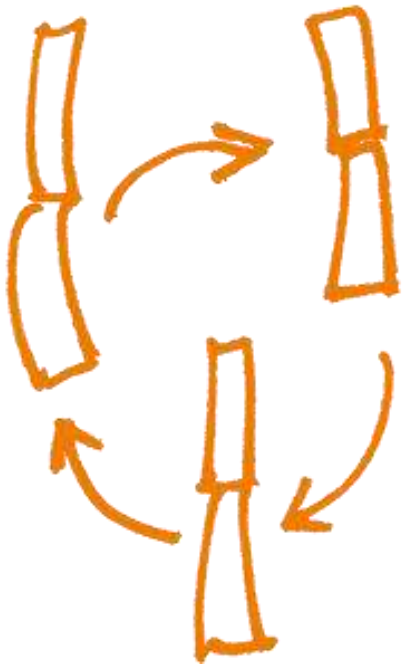
UNIVERSITY of CALIFORNIA PRESS

Ummul-Kiram Kathawalla,Priya Silverstein,Moin Syed, Easing Into Open Science: A Guide for Graduate Students and Their Advisors, Collabra: Psychology, 2021,

Discuss with other students/staff issues surrounding reproducibility and open science

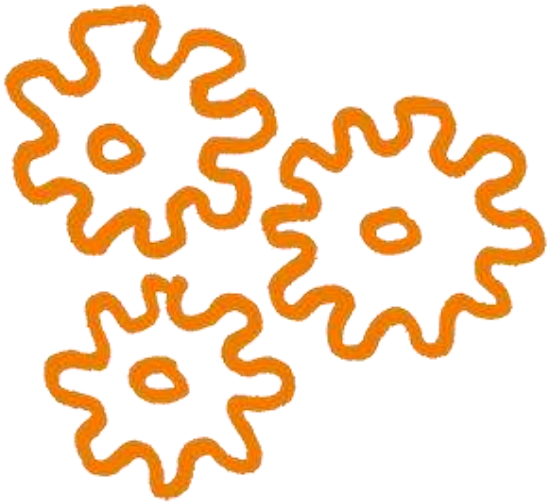
https://reproducibilitea.org

Project workflow



How you organize projects and move through the various stages of your research cycle: your **file folder structure**, **document naming conventions**, **version control**, **cloud storage**, and other details.

The choice of **who has access to the project** (e.g., collaborators, the public) and **when in the process they have access** (e.g., at all times, upon publication).



Research data lifecycle

CREATING DATA: designing research, DMPs, planning consent, locate existing data, data collection and management, capturing and creating metadata

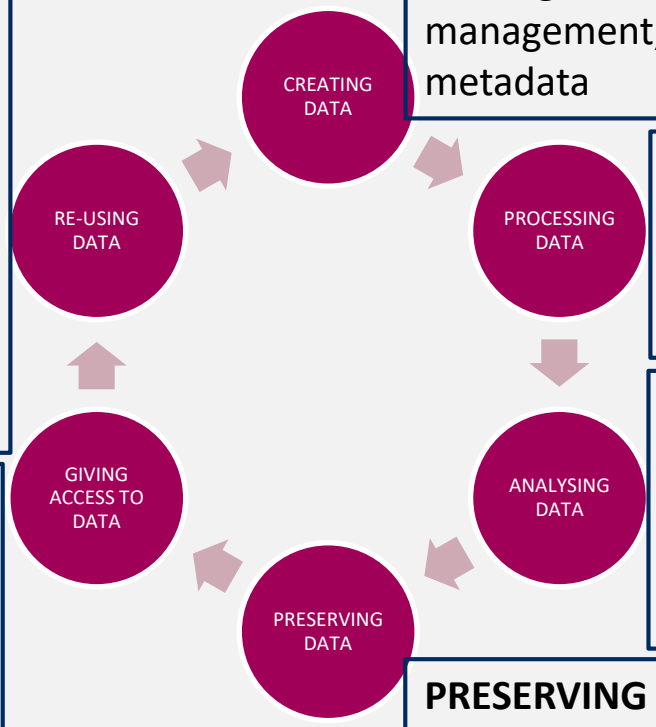
PROCESSING DATA: entering, transcribing, checking, validating and cleaning data, anonymising data, describing data, manage and store data

ANALYSING DATA: interpreting, & deriving data, producing outputs, authoring publications, preparing for sharing

PRESERVING DATA: data storage, back-up & archiving, migrating to best format & medium, creating metadata and documentation

ACCESS TO DATA: distributing data, sharing data, controlling access, establishing copyright, promoting data

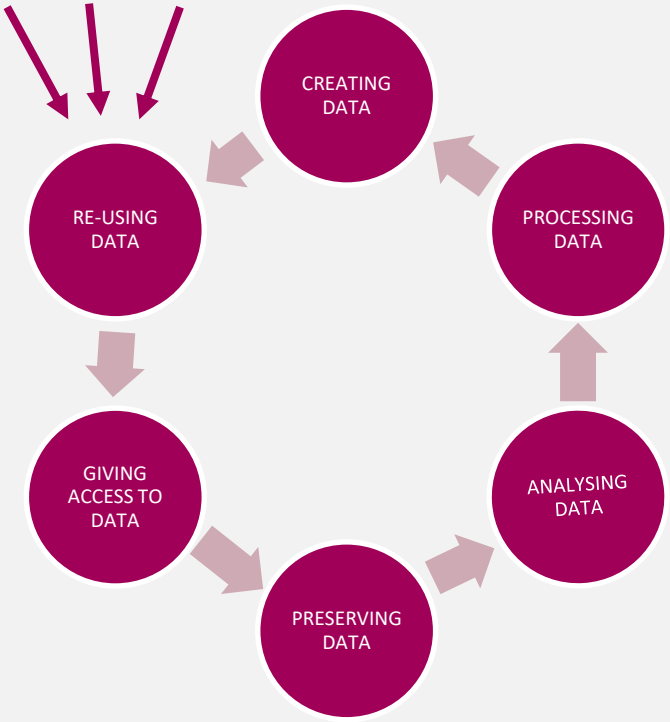
RE-USING DATA: follow-up research, new research, undertake research reviews, scrutinising findings, teaching & learning

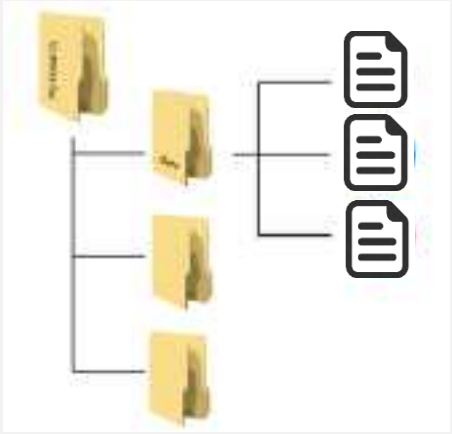


Ref: UK Data Archive: http://www.data-archive.ac.uk/create-manage/life-cycle

Planning trick: think backwards

What data organisation would a re-user like?





Data organisation

Meaningful file names

Below are tips on meaningful and consistent file names. Read more in *'Choosing a file name'*.[2]

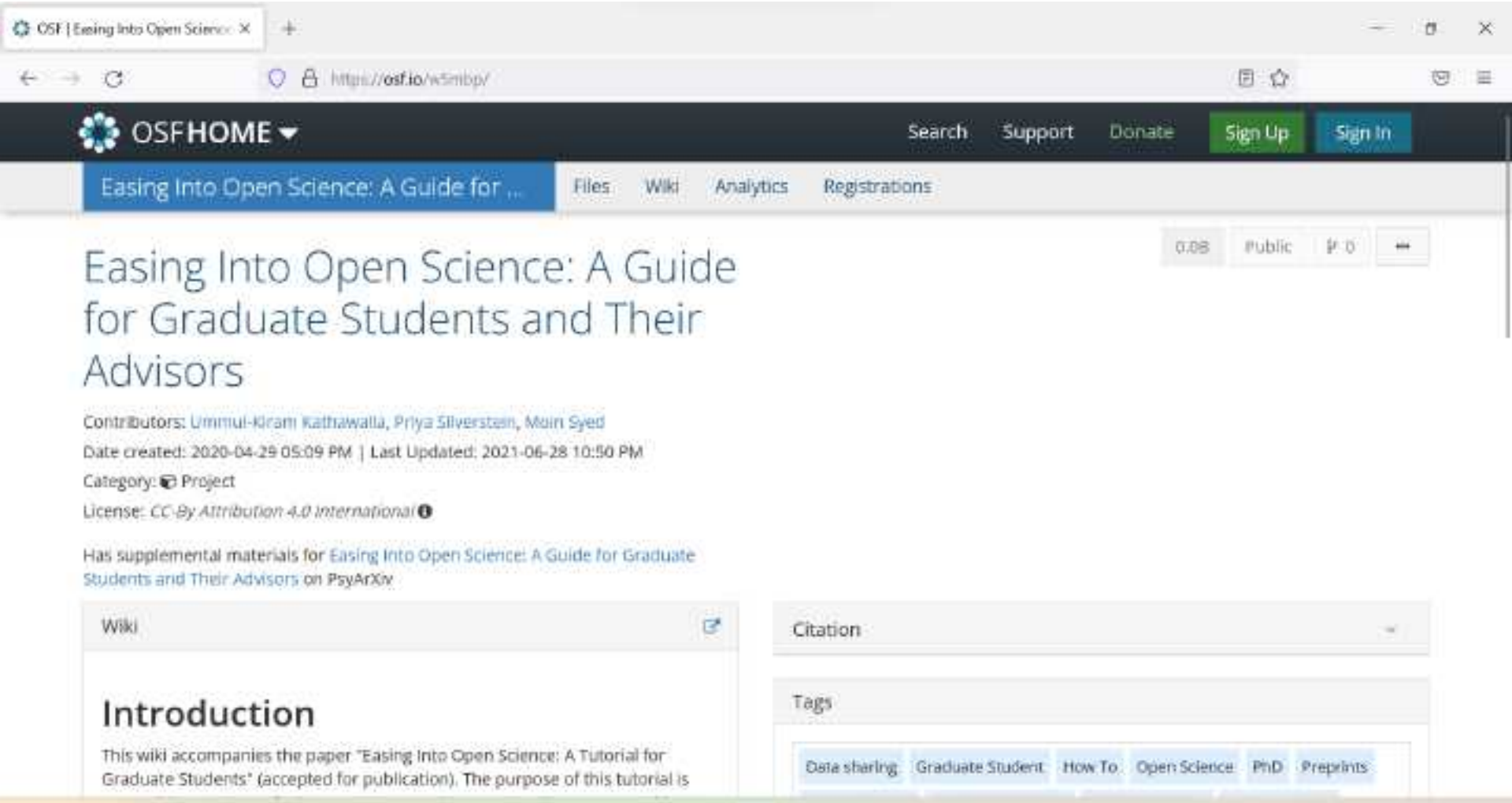
- Make sure to use consistent file names. When you use a date in the file name, choose a notation (for instance, YYYYMMDD of yymmdd).
- Do not use strange characters like ?\!@*%{[<> in the file name.
- Use traceable file names, such as Project_Instrument_locatie_YYYYMMDD.ext.
- Make sure to only use each file once in the folder structure. If you store a file in more than one place, several versions of the same file can unwillingly be created.
- See also version management.

It is good practice to note the file naming and its meaning in a readme.txt.

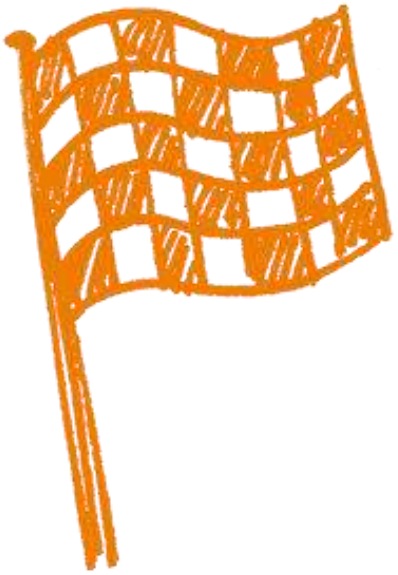
File naming and version management

Even if a researcher is well underway with his project consistent file naming is still an option by using a *bulk file rename utility*.[3] It is important, however, to check if this bulk renamer delivers on its promises.

http://datasupport.researchdata.nl/en/start-de-cursus/iii-onderzoeksfase/organising-data



https://osf.io/w5mbp



Preregistration

Preregistration

https://www.cos.io/initiatives/prereg?_ga=2.224561726.55150...

Search

Future-proof your research. Preregister your next study.

What is Preregistration?

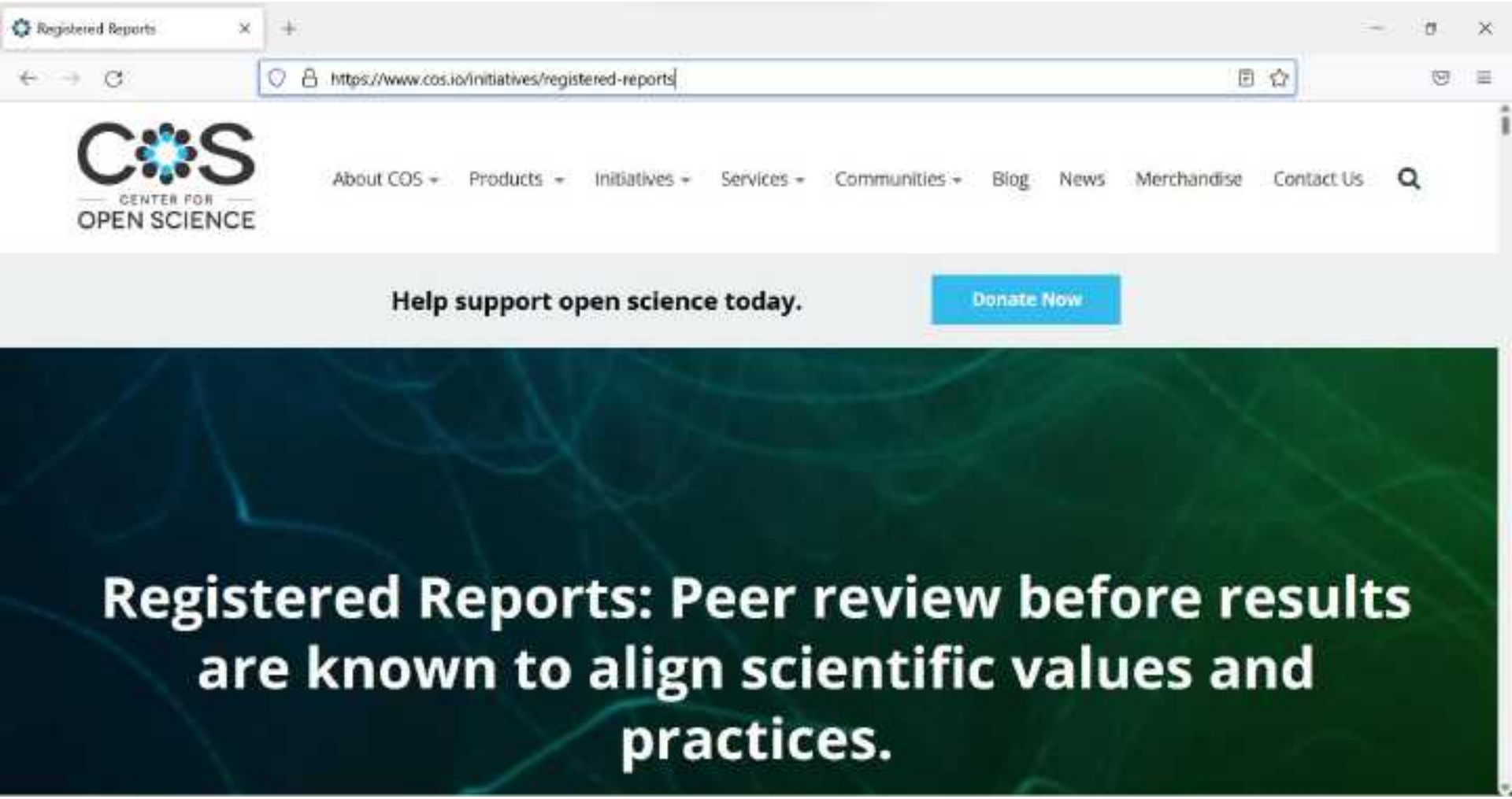
When you preregister your research, you're simply specifying your research plan in advance of your study and submitting it to a registry.

Preregistration separates *hypothesis-generating* (exploratory) from *hypothesis-testing* (confirmatory) research. Both are important. But the same data cannot be used to generate *and* test a hypothesis, which can happen unintentionally and reduce the credibility of your results. Addressing this problem through planning improves the quality and transparency of your research. This helps you clearly report your study and helps others who may wish to build on it.

For additional insight and context, you can read The Preregistration Revolution. (preprint)

Get Started Now

Registered reports



https://www.cos.io/initiatives/registered-reports

Registered Reports

https://www.cos.io/initiatives/registered-reports

Registered Reports | Participating Journals | Details & Workflow | Resources for Editors | For Funders | FAQ | Allied Initiatives

Registered Reports is a publishing format that emphasizes the importance of the research question and the quality of methodology by conducting peer review prior to data collection. High quality protocols are then provisionally accepted for publication if the authors follow through with the registered methodology.

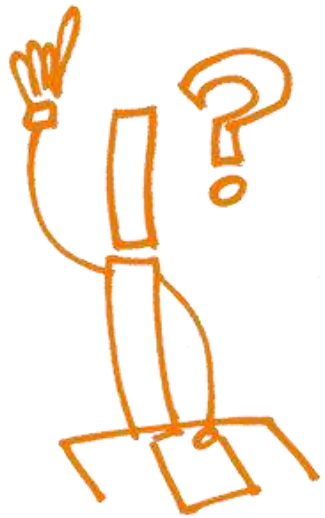
This format is designed to reward best practices in adhering to the hypothetico-deductive model of the scientific method. It eliminates a variety of questionable research practices, including low statistical power, selective reporting of results, and publication bias, while allowing complete flexibility to report serendipitous findings.

"Registered Reports eliminates the bias against negative results in publishing because the results are not known at the time of review."

"Because the study is accepted in advance, the incentives for authors change from producing the most beautiful story to the most accurate one."

https://www.cos.io/initiatives/registered-reports

Preprints



Why should I care?

Priority claim

By posting a preprint researchers can disclose their completed study immediately and without access barriers.[1]

Increase citations

Articles get 36% more citations if they have a prior associated preprint.[2]

Receive feedback

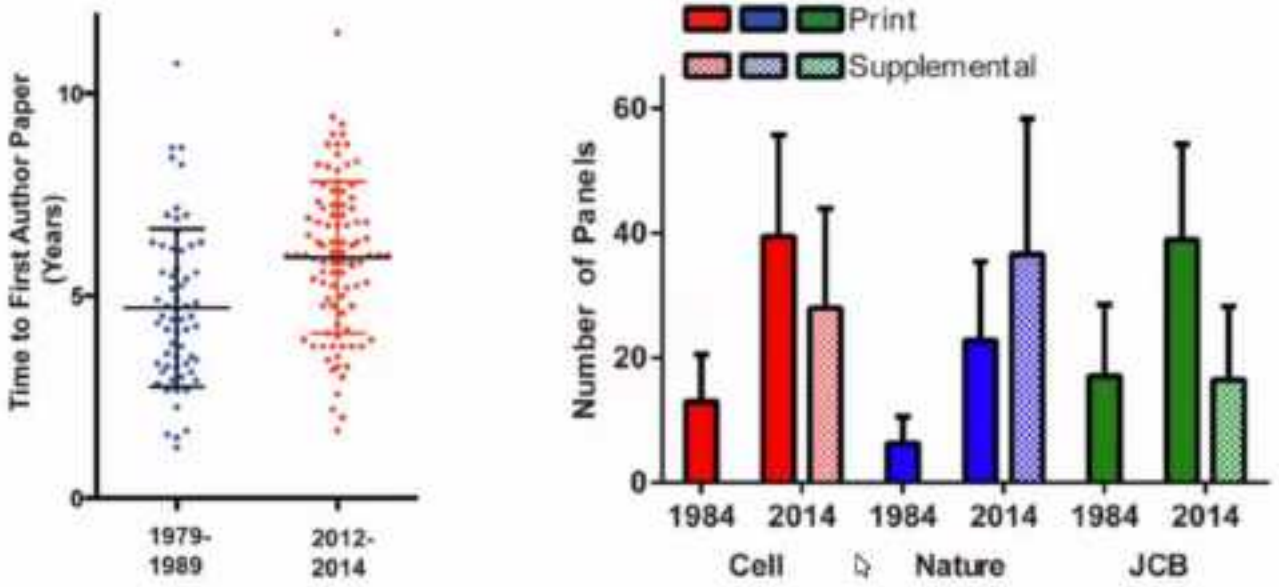
Improve your manuscript by getting valuable comments on your research prior to publication.[3]

Proof of productivity

A preprint provides funders and hiring committees with public evidence of your work.[4]

Infographics by ASAPbio Fellows:
Ana Dorrego-Rivas (@adorrego_r), Carrie Iwema and Mafalda Pimentel (@Maf_Pimentel)

Creating a publishable unit is slower than ever



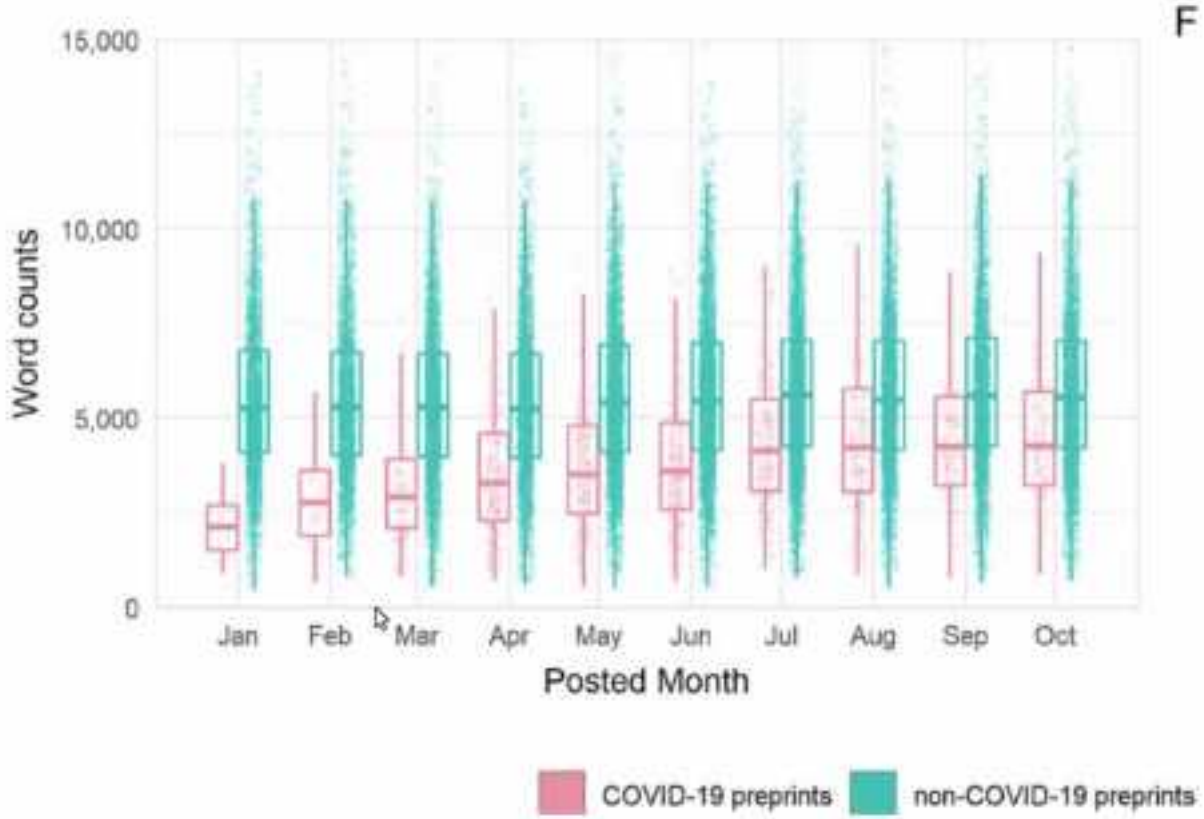
Accelerating scientific publication in biology. Ronald D. Vale
Proceedings of the National Academy of Sciences Nov 2015, 112 (44) 13439-13446; DOI: 10.1073/pnas.1511912112

Iratxe Puebla @ASAPbio Community Call: Preprints in Progress

Preprints of different forms in the response to COVID-19

COVID preprints were short (early on, <50% of length of other preprints) and were revised more often

Fraser N, Brierley L, Dey G, Polka JK, Pálfy M, Nanni F, et al. (2021) The evolving role of preprints in the dissemination of COVID-19 research and their impact on the science communication landscape. PLoS Biol 19(4): e3000959. https://doi.org/10.1371/journal.pbio.3000959



Iratxe Puebla @ASAPbio Community Call: Preprints in Progress

Preprint fact checking

Scoop protection

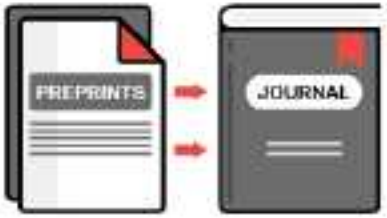
Preprints allow you to establish priority for your discoveries. 99.3% of preprint authors reported no scoop problems.[1]

Preprints are journal compatible

Over 1,200 journals operate policies compatible with preprints.[2]

Preprints are good quality

Two thirds of bioRxiv preprints appear in a journal within two years.[3] Quality of reporting is within a similar range as that of peer-reviewed articles.[4]



Smoother path to publication

Many journals allow preprint transfers directly from servers.[1] Some editors scout preprints and invite submissions to their journal.

https://asapbio.org/wp-content/uploads/2021/01/ASAPbio-fact-check-preprints-english-v2.pdf

ASAPbio

Guiding principles for researchers to aid the responsible media reporting of research posted as preprints

When communicating about their work in social media, blogs or with journalists, researchers should be mindful of the potential for misinterpretation of their findings and:

1. Label the research as a preprint (where that is the case).
2. Prominently state whether or not it has undergone peer review.
3. Prominently highlight the limitations of the work.
4. Provide narrow interpretations that are unlikely to be exaggerated or misconstrued when communicating research findings to a lay audience.
5. Make every effort to ensure that the research is presented so that non-experts can understand it with minimal room for misinterpretation.
6. Make every effort to anticipate the potential for their research to be propagated in ways that are far from the original intent.
7. Avoid overhyping the significance of the research findings.
8. Consider using a structured format, similar to that recommended by the UK Academy of Medical Sciences for press releases. For example, in biomedical fields, structured information to be included in social media post(s) might include the following.
   a) Brief lay summary
   b) Type of research: [Observational/interventional etc]
   c) Model system: [Humans/mice/in vitro biochemistry]
   d) Sample size: [Number of patients, etc]
   e) Peer review status [Preprint/(open) peer review etc]
   f) Other caveats/limitations
9. Be familiar with any guidelines provided by their institution on the responsible use of social media. Guiding principles for institutions to aid the responsible media reporting of research can be found at asapbio.org/public.
10. Work in collaboration with their institutional press office if approached by the media to comment on research they have carried out at the institution, regardless of whether or not the research is actively promoted by the institution.

ASAPbio.org

Preprints

Part of the Preprints in The Public Eye Project supported by the Open Society Foundations

https://asapbio.org/wp-content/uploads/2021/03/Preprints-in-the-Public-Eye-Researchers-infographic.pdf

'Mathematics is an unknown land': meet Fields Medal winner Maryna Viazovska

Download PDF

https://www.nature.com/articles/d41586-022-01920-8

International Mathematical Union IMU

https://www.mathunion.org/imu-awards/fields-medal/fields-medals-2022

Organization | Membership | IMU Awards | ICM | Activities | Outreach

Fields Medals 2022

The Fields Medal is awarded to recognize outstanding mathematical achievement for existing work and for the promise of future achievement.

The medals and cash p

University of Toronto, w

underfunded. In 2022, t

supplemented by gener

Foundation/Klaus Tschi

On this page

- Hugo Duminil-Copin
- June Huh
- James Maynard

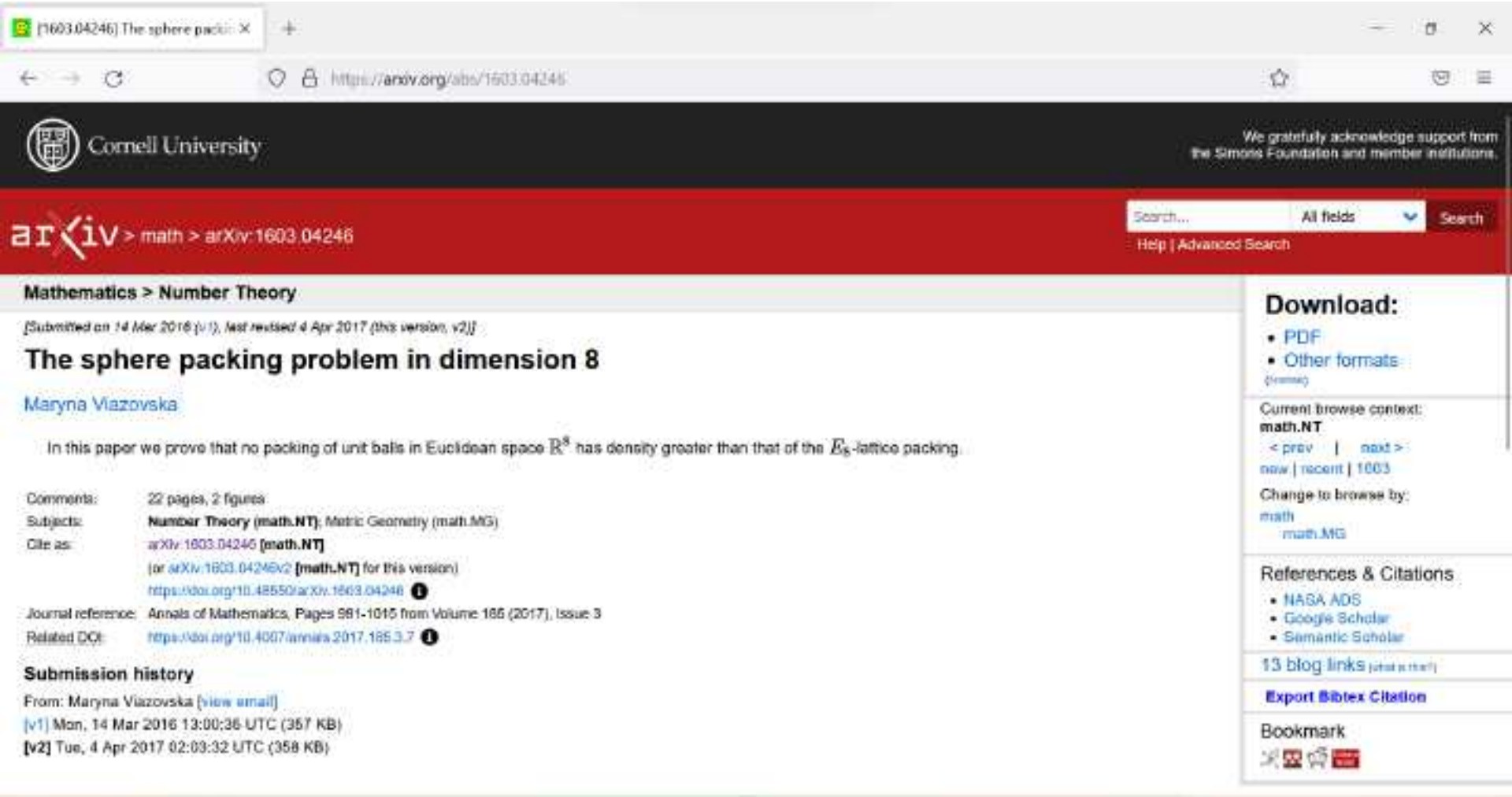
Maryna Viazovska

For the proof that the E_8 lattice provides the densest packing of identical spheres in 8 dimensions, and further contributions to related extremal problems and interpolation problems in Fourier analysis.

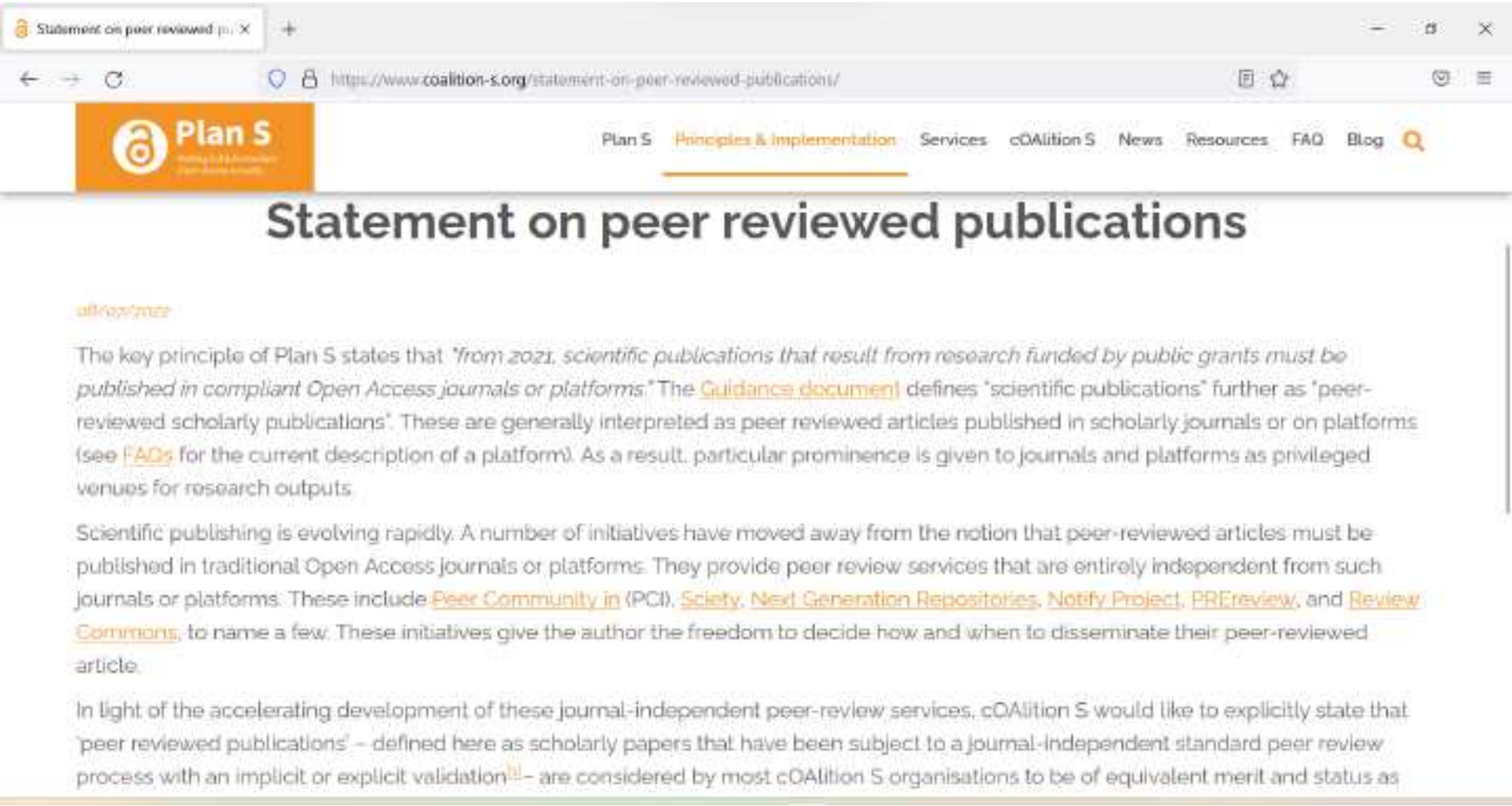
On this page

- Hugo Duminil-Copin
- June Huh
- James Maynard
- Maryna Viazovska

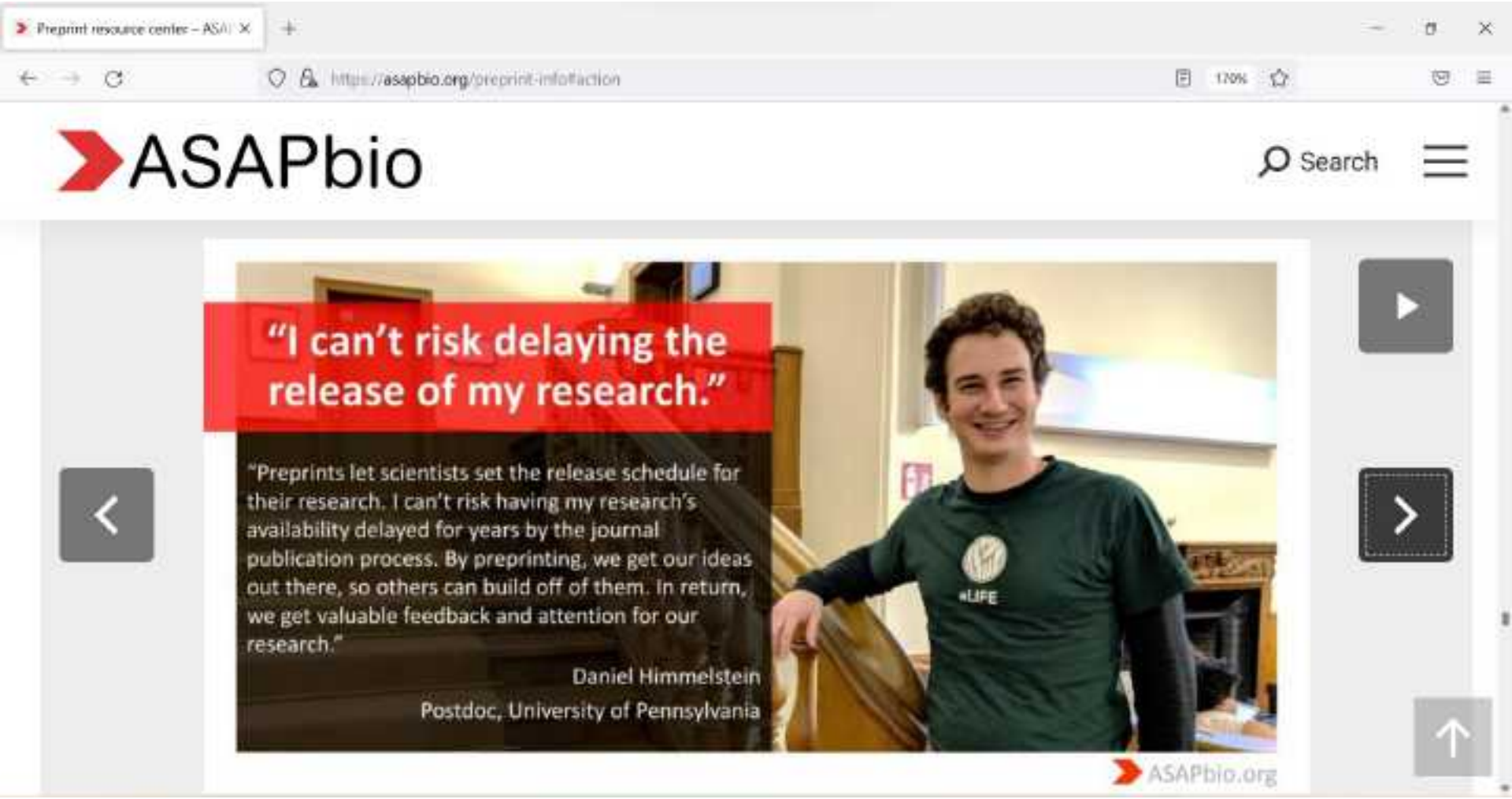
Immediate acclaim after the preprint appeared on March 14, 2016 https://arxiv.org/abs/1603.04246



https://arxiv.org/abs/1603.04246



https://www.coalition-s.org/statement-on-peer-reviewed-publications/



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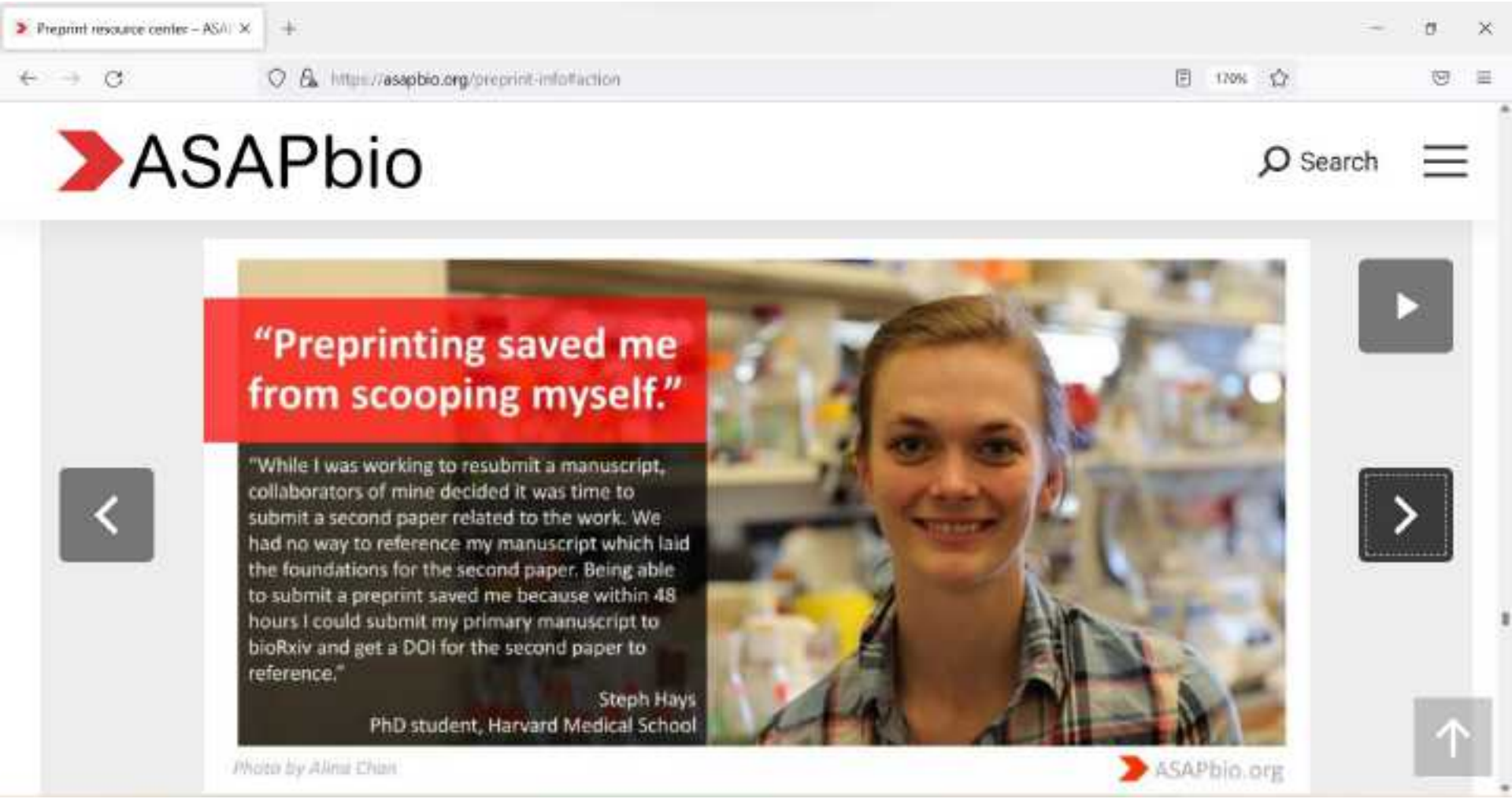

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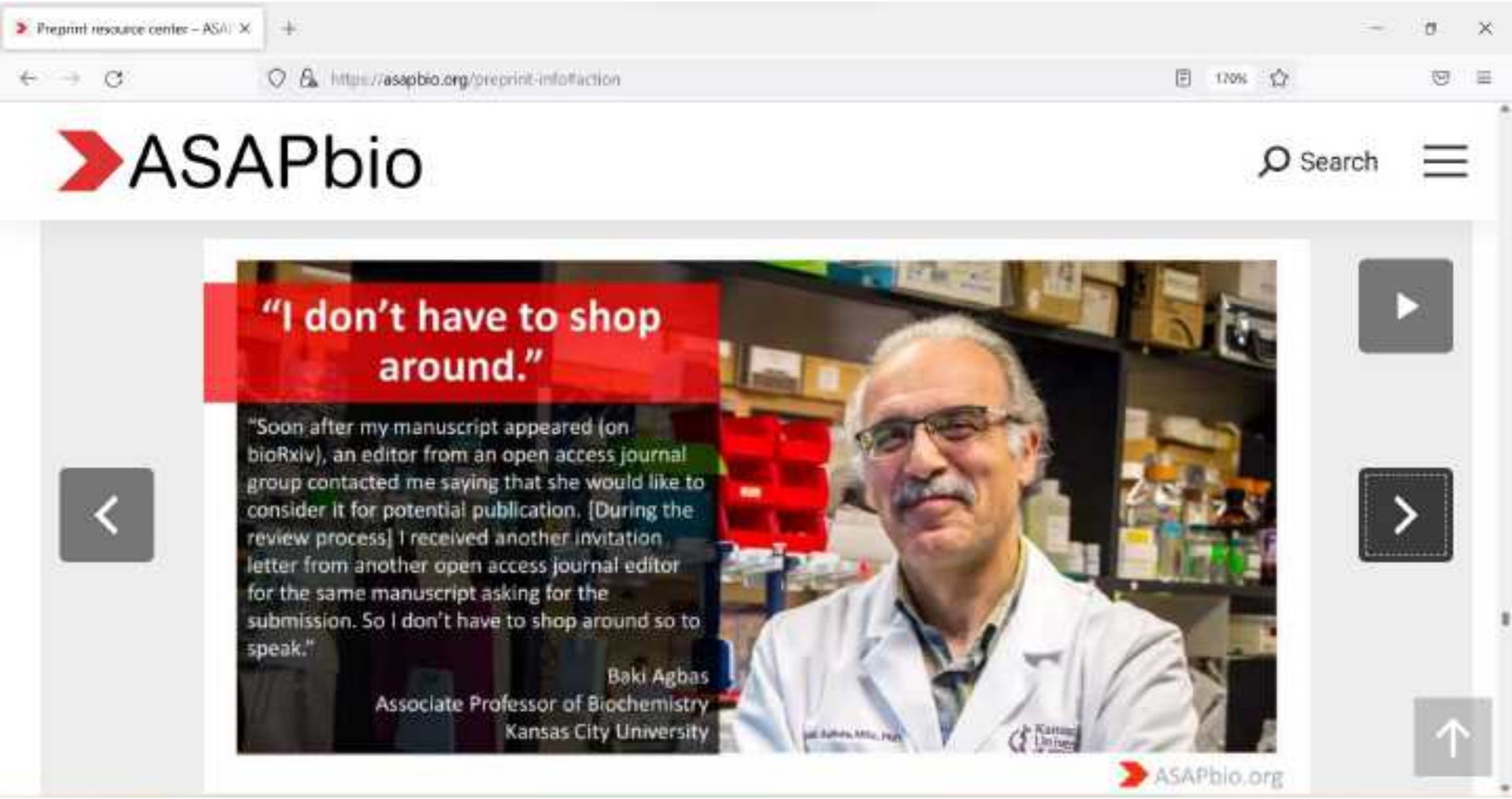

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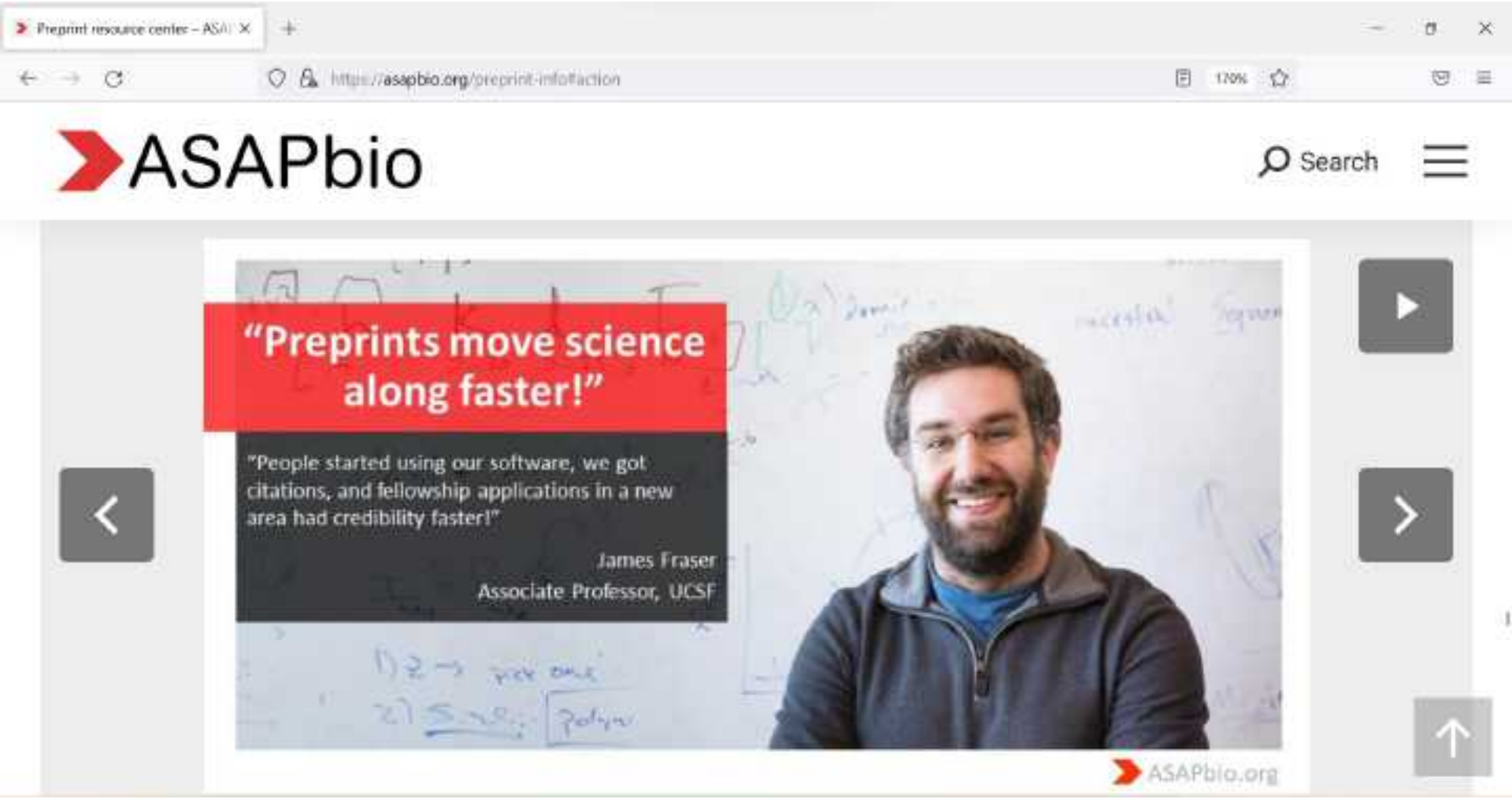

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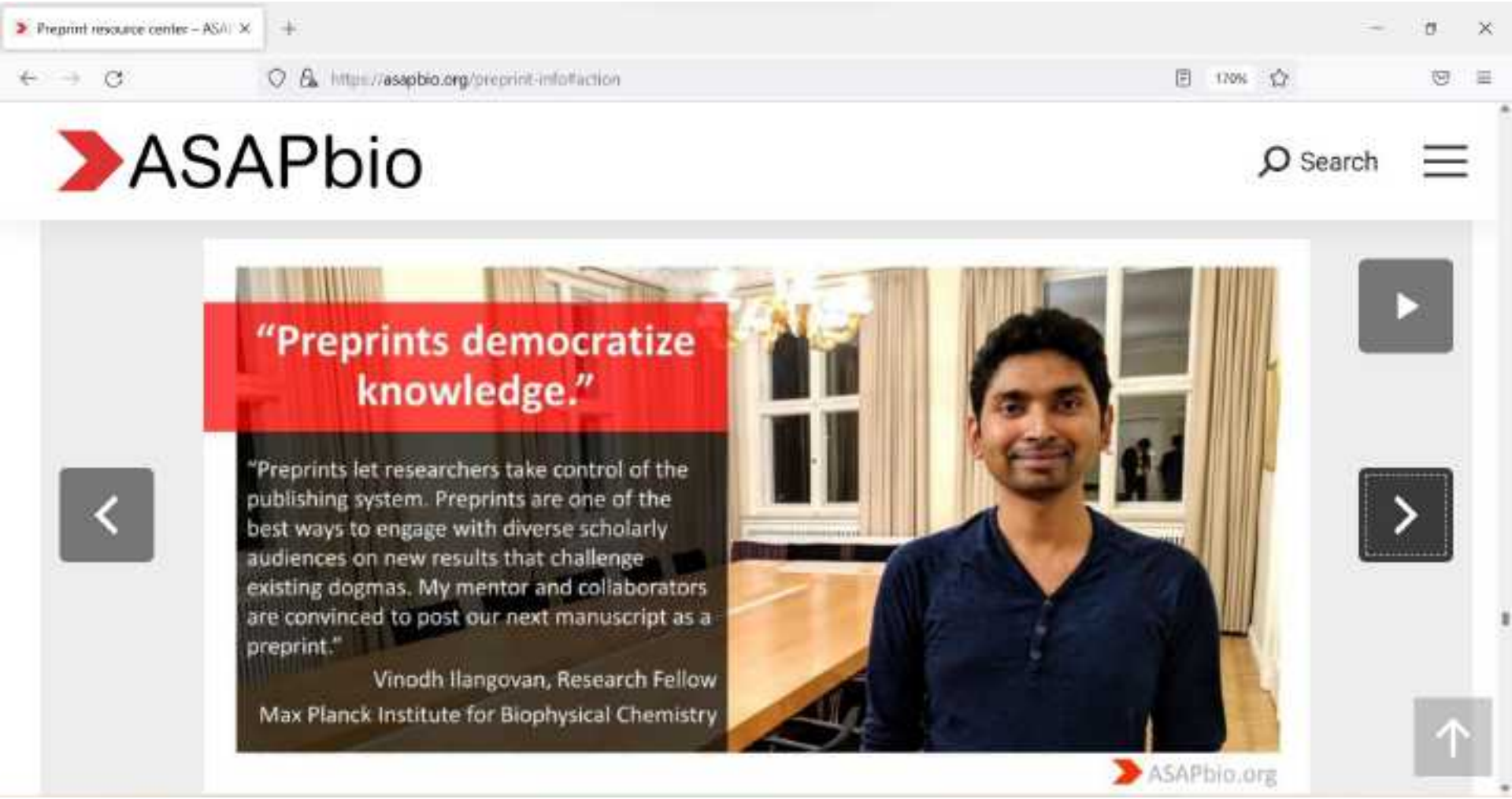

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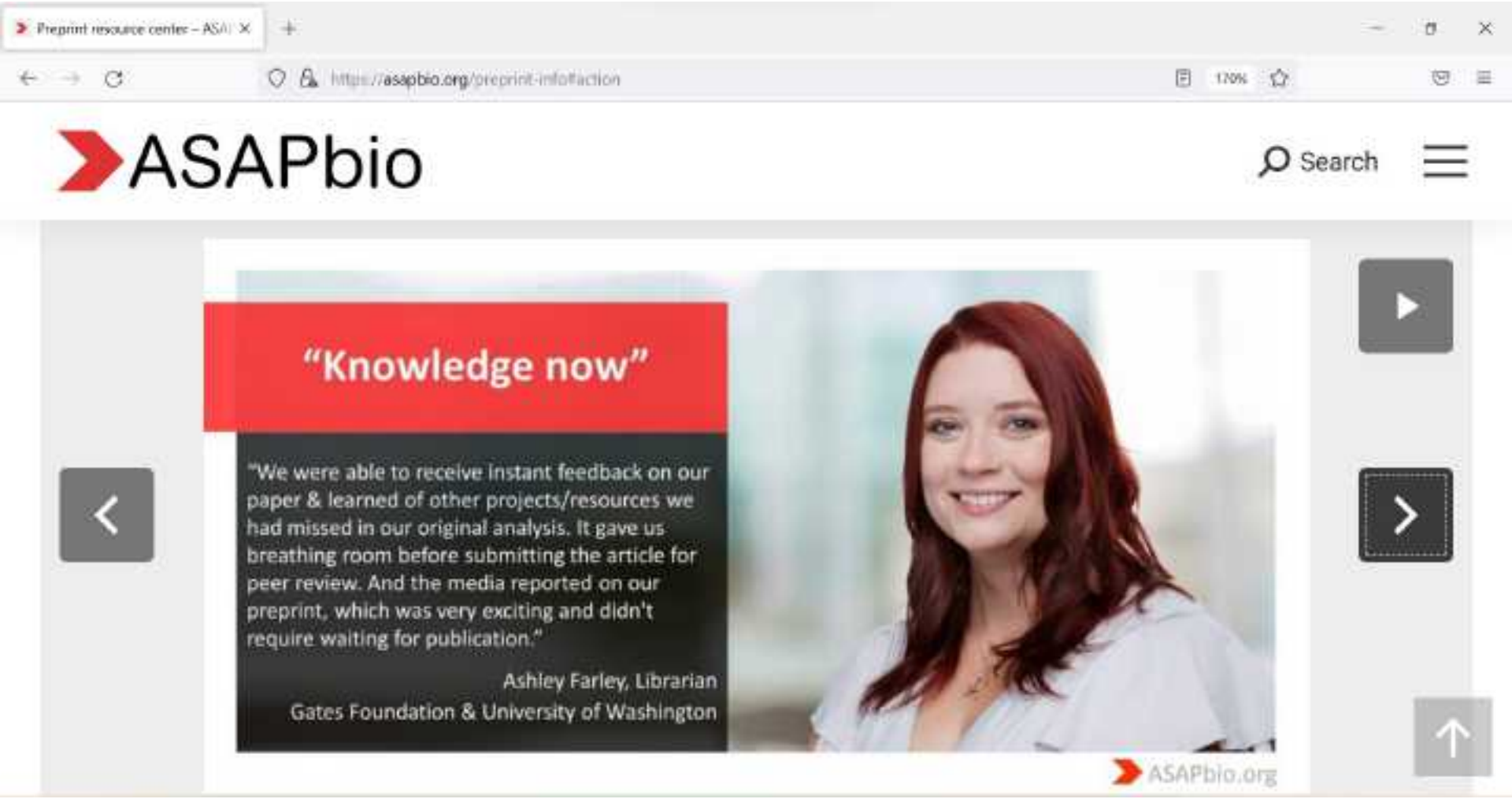

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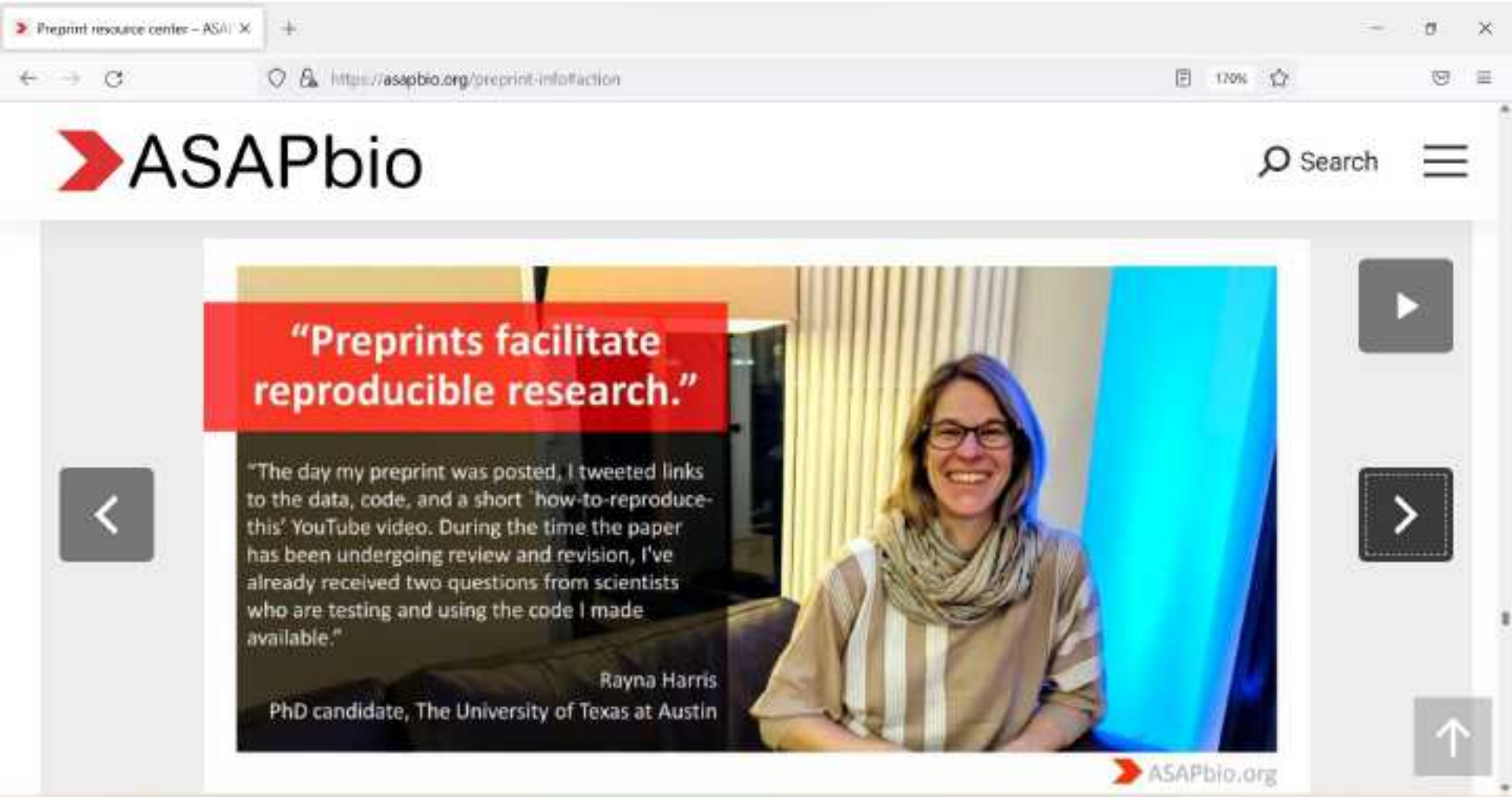

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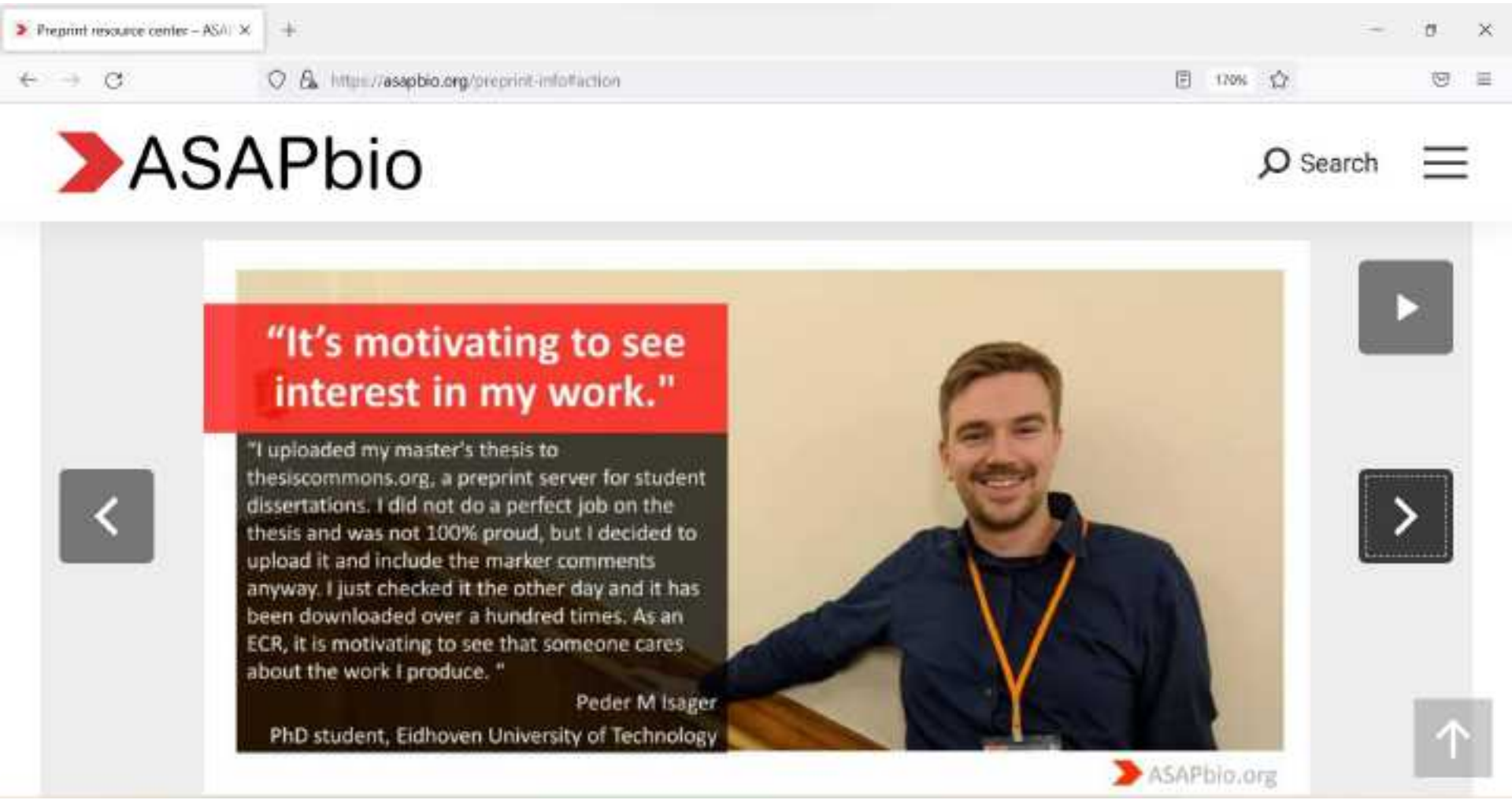

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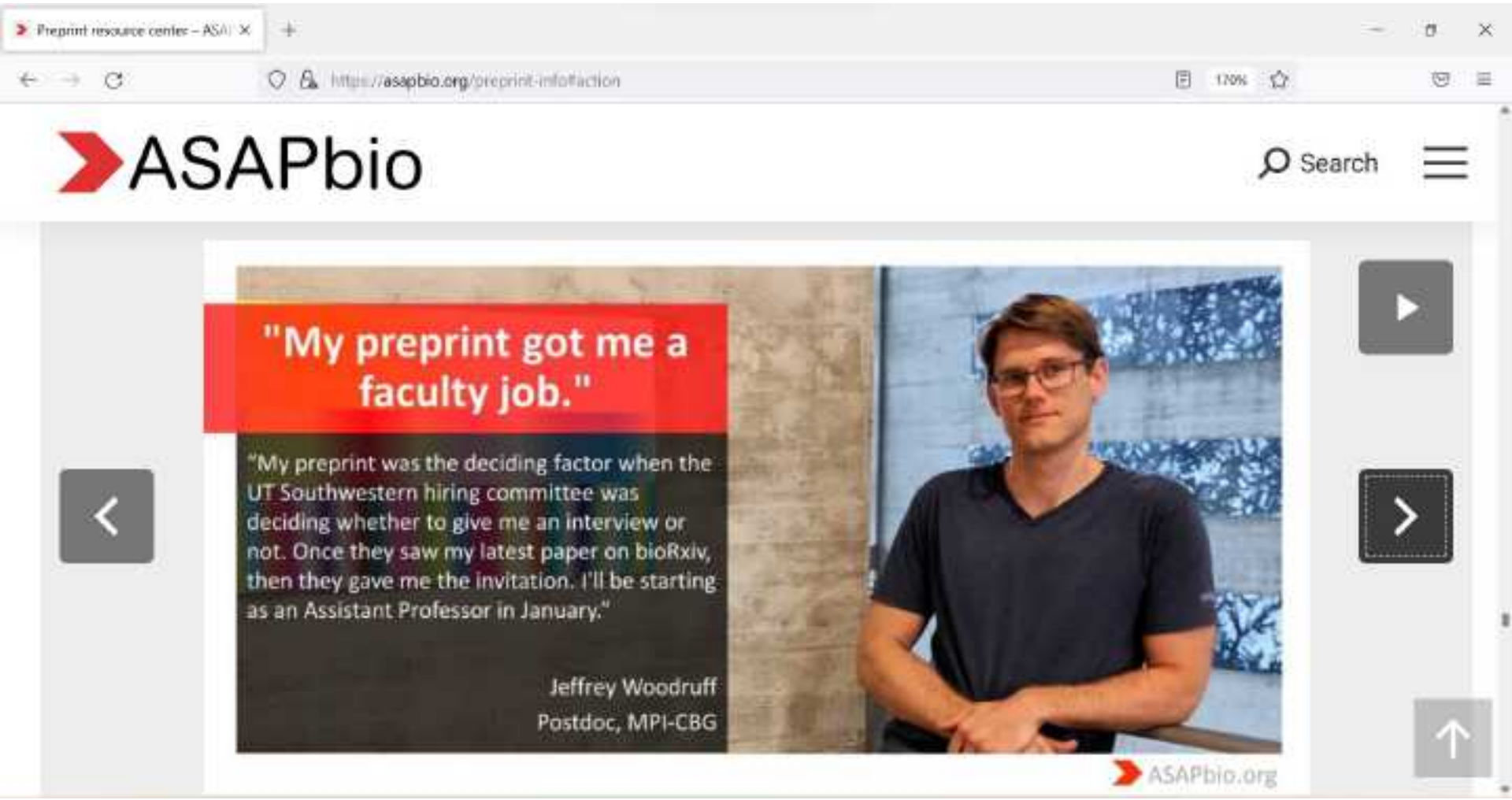
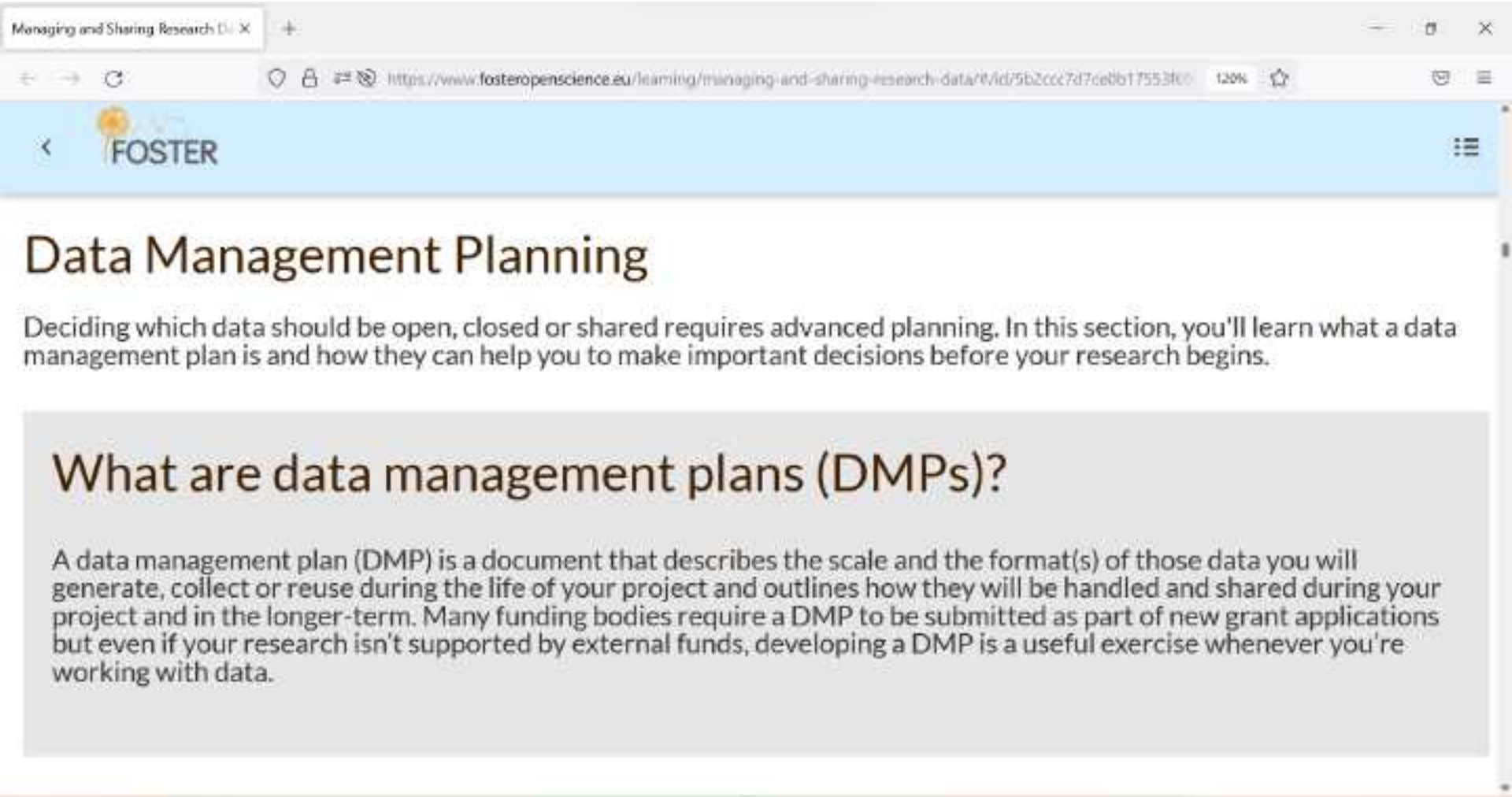


https://asapbio.org/preprint-info#action

https://doapr.coar-repositories.org/repositories/

Research Data Management



https://www.fosteropenscience.eu/learning/managing-and-sharing-research-data

Assistance: tools

- Wizards
  - Usually free for individual researchers
  - Inbuilt templates
  - Customizable (for institutions)
  - Machine readable DMPs
  - Integration with repositories
- Checklists
  - Swedish National Data Service DMP checklist
  - Customized versions are often found on the websites of academic libraries

DMPTool

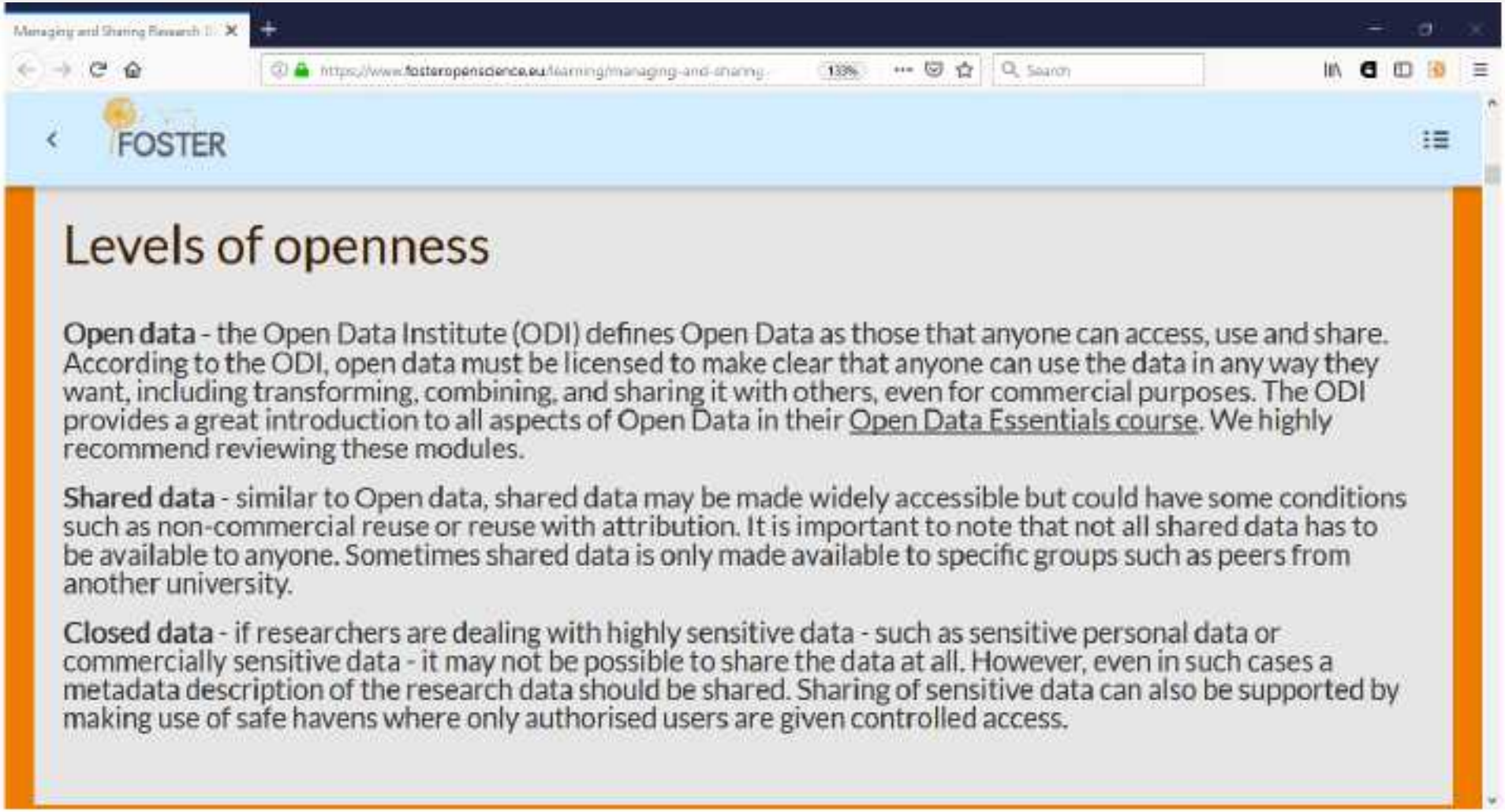
DSW

argos

DMPONLINE

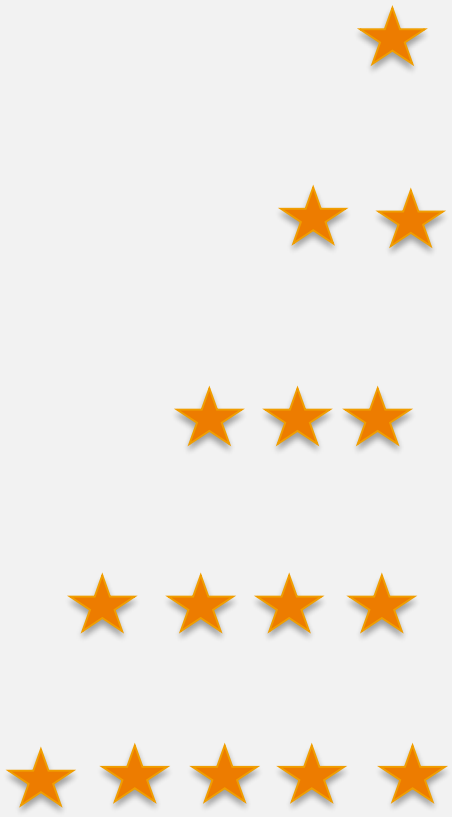
DataWiz

OpenAIRE



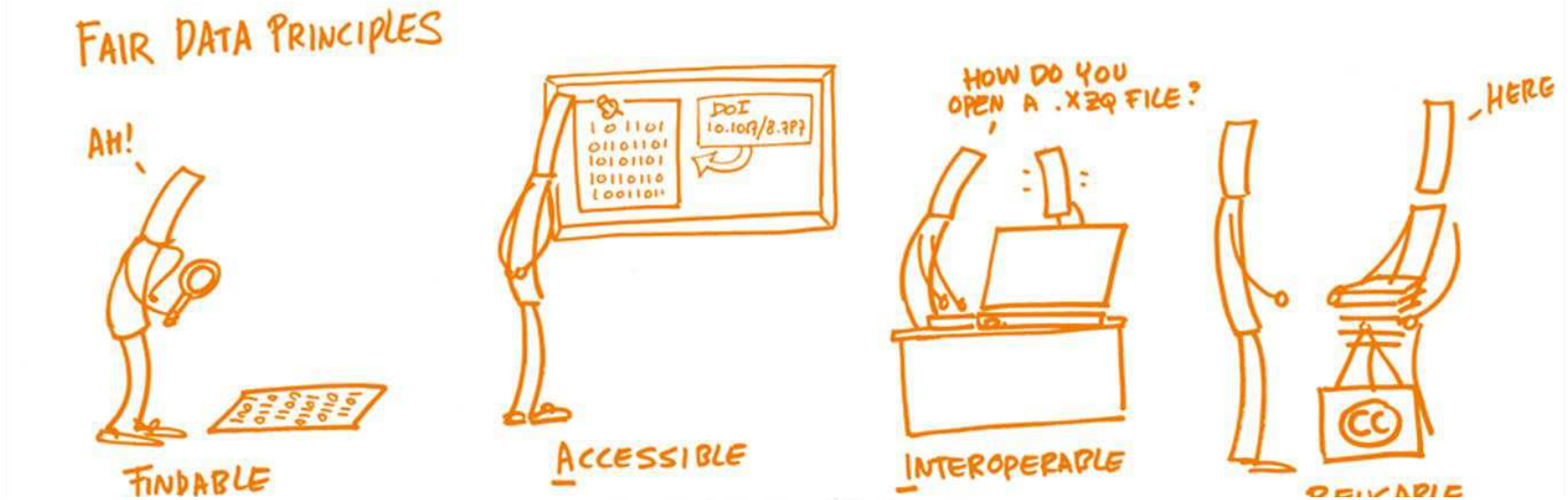
https://www.fosteropenscience.eu/learning/managing-and-sharing-research-data

Tip – use 5 Star Open Data Model to explain FAIR



- ★ make your stuff available on the Web (whatever format) under an open license
- ★★ make it available as structured data (e.g., Excel instead of image scan of a table)
- ★★★ make it available in a non-proprietary open format (e.g., CSV instead of Excel)
- ★★★★ use URIs to denote things, so that people can point at your stuff
- ★★★★★ link your data to other data to provide context

Tim Berners-Lee's proposal for five star open data - http://5stardata.info



#BeFAIRandCARE

https://www.gida-global.org/care

FAIR Guiding Principles for scientific data management and stewardship can be accessed here

What should be preserved and shared?

- The **data** needed to validate results in scientific publications (minimally!).
- The associated **metadata**: the dataset's creator, title, year of publication, repository, identifier etc.
  - Follow a metadata standard in your line of work, or a generic standard, e.g. Dublin Core or DataCite, and be FAIR.
  - The repository will assign a persistent ID to the dataset: important for discovering and citing the data.

What should be preserved and shared? (2)

- **Documentation**: code books, lab journals, informed consent forms – domain-dependent, and important for understanding the data and combining them with other data sources.
- **Software**, hardware, tools, syntax queries, machine configurations – domain-dependent, and important for using the data. (Alternative: information about the software etc.)

Basically, everything that is needed to replicate a study should be available. Plus everything that is potentially useful for others.

Tip – link data to other outputs for context (reuse)

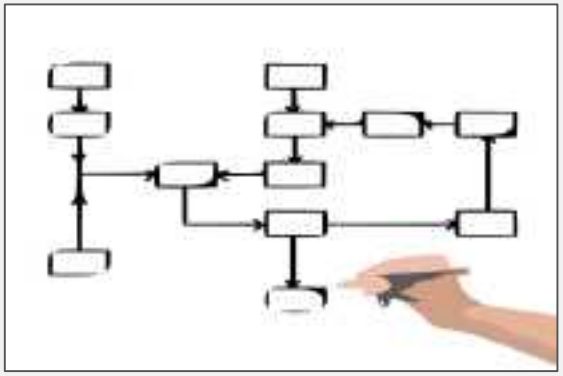
Open Data

To support validation and facilitate reuse

Open Code

Software created to analyse and/or visualise the data

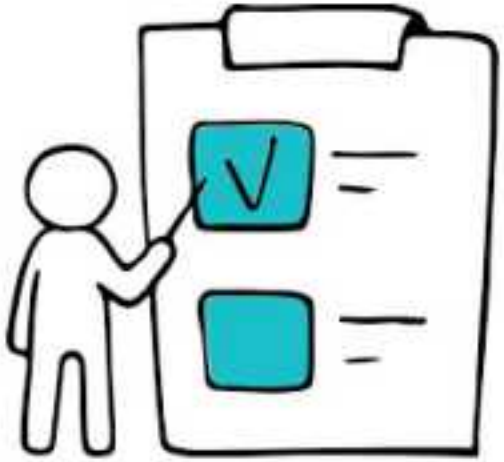
Open Workflows



What steps were taken and in what order?

PLAN FOR SHARING

- **Desirebly at data creation**
- Identify which bits of personal data will be collected
- Do you really need to collect personal data?
  - (eg. irrelevant questions in questionnaires)
- Consider how will anonymization costs be covered



"As Open as possible, as closed as necessary"

SHARING AND PUBLISHING IS ALSO RELATED WITH...

ETHICS AND RESEARCH

- Any recorded **interviews** (either video or audio)
- Surveys or **questionnaires** that collect personal information (date/place of birth or anything else that could identify the participant).
- Research where the participant is asked to **reveal or reflect on instances from their past** (e.g. oral histories...)
- Anything that involves the participation of minors
- Anything in which the participant is asked to **reveal something** that might cause them or others physical or mental harm or embarrassment if made public.
- Any research in which the participant is asked to **complete tests**, or test-like scenarios.

INFORMED CONSENT

- **Informed consent is the process by which a researcher discloses appropriate information** about the research so that a participant may make a voluntary, informed choice to accept or refuse to cooperate." (CESSDA Expert Tour Guide RDM)
- **When creating consent forms, researchers should make sure to:**
  - inform participants about their rights
  - introduce relevant aspects of the research in an understandable, transparent, and precise way
  - explain data protection measures that will be taken
  - be clear about plans for data sharing in the consent form

Consider who else has a say about sharing data

Collaborators

Research participants

Commercial partners

Data repository

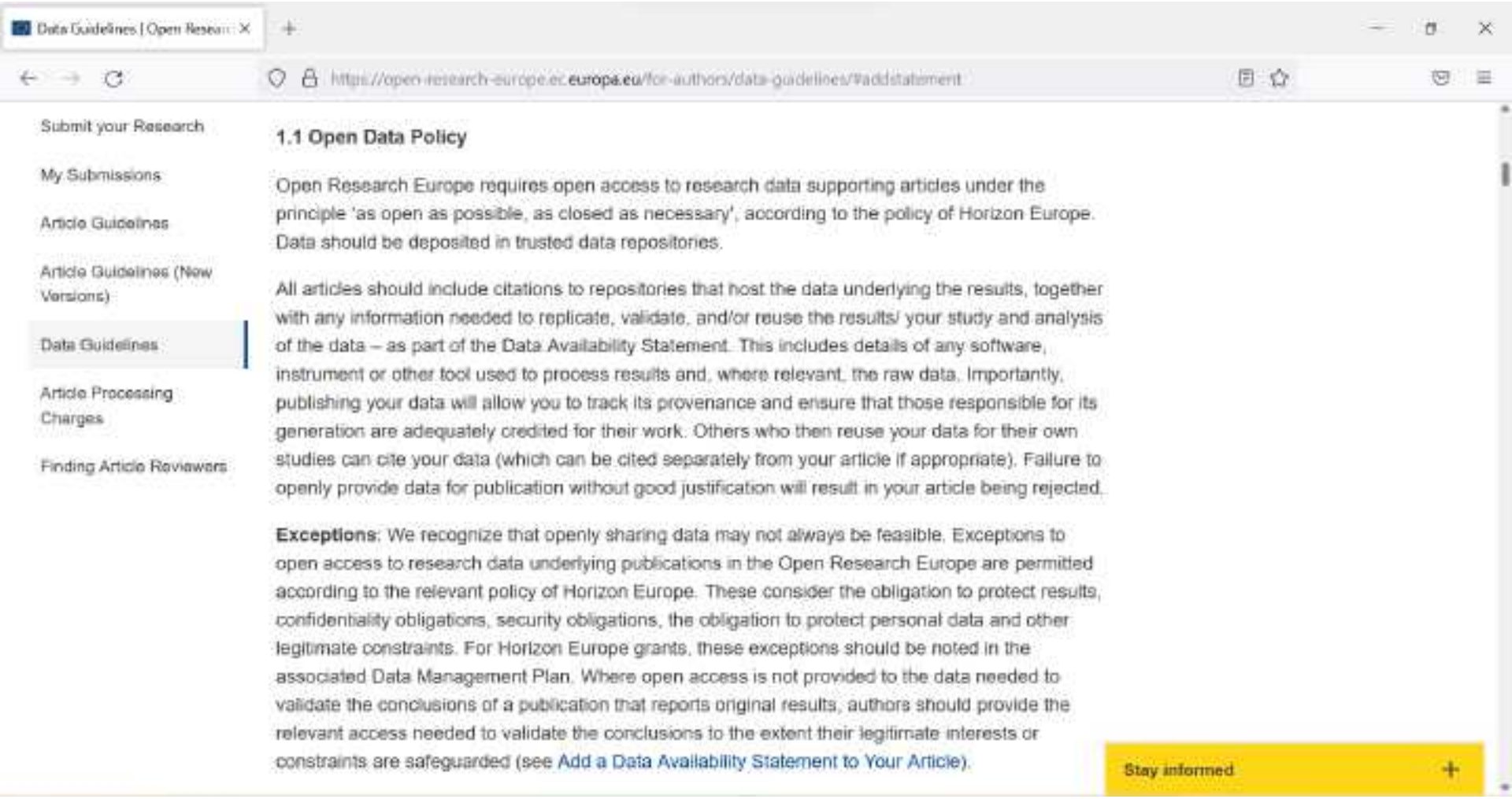
Publishers

Institutions, funders

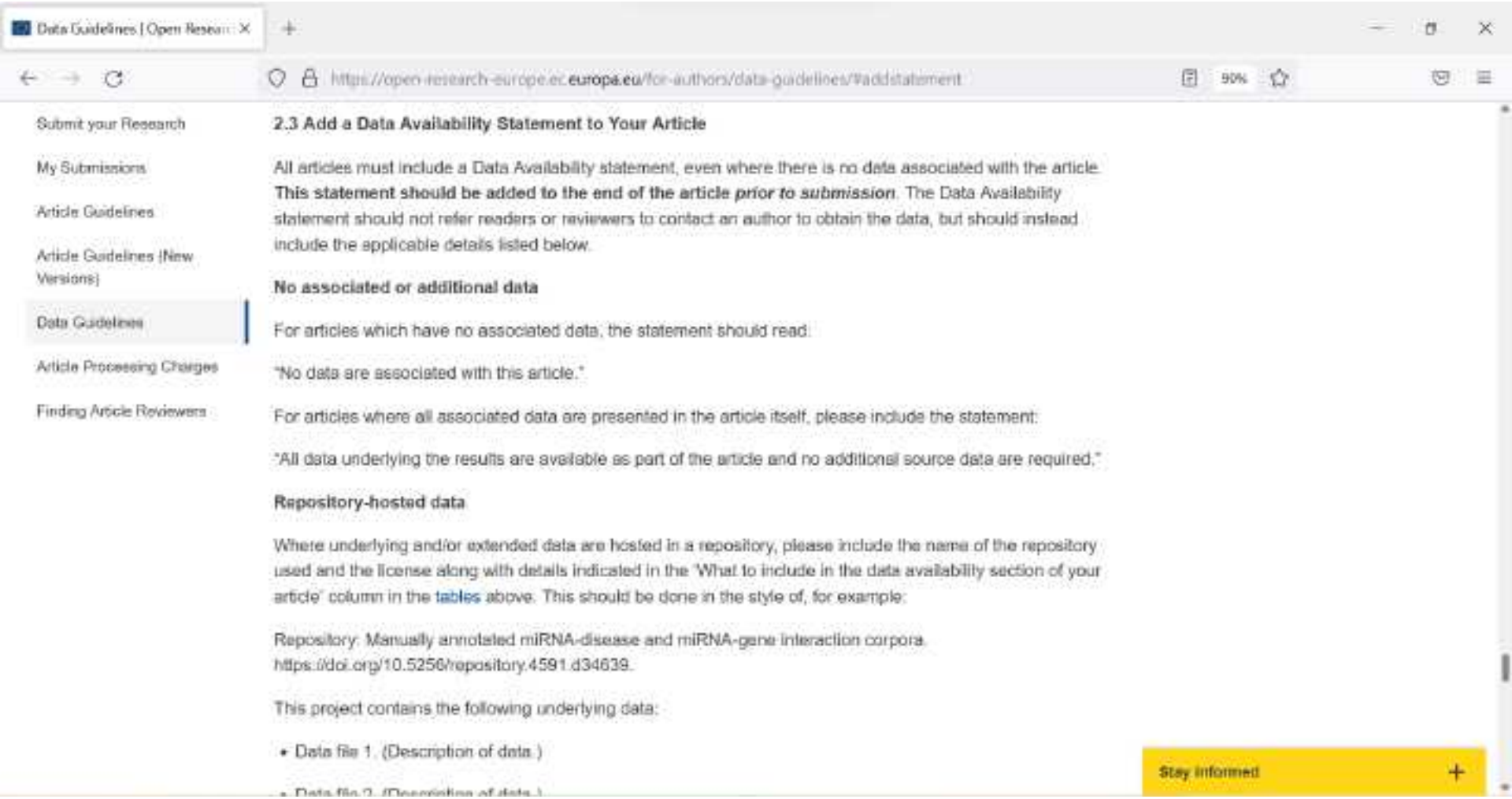
Where to find a repository?

Zenodo: http://www.zenodo.org

Re3data.org: http://www.re3data.org



https://open-research-europe.ec.europa.eu/for-authors/data-guidelines/#addstatement



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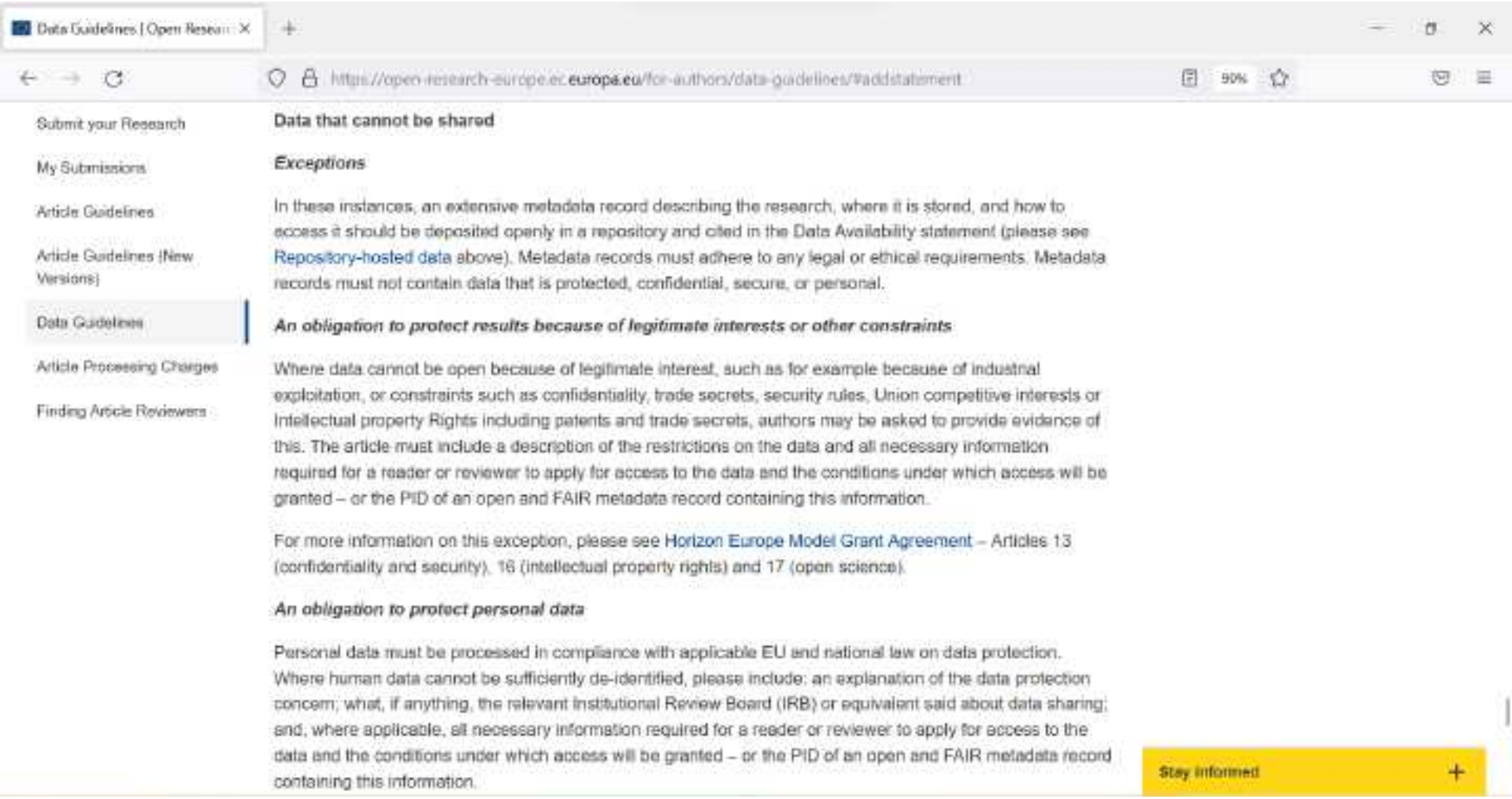


https://open-research-europe.ec.europa.eu/for-authors/data-guidelines/#addstatement

Data reuse

stories & use cases

https://www.openaire.eu/data-reuse-use-cases

In OpenAIRE we are collecting a series of stories, use cases and other relevant resources that report the process of data reuse, trying to demonstrate and describe experiences (successful or not) of reuse of a variety of research data, as well as associated assumptions and implications. This work is being developed by the RDM Task Force - Data Reuse Working Group. The number of use cases will expand over time.

FAIR4Health

Sensitive data: FAIR4Health

Data reuse use case

Edinburgh DataShare

Enabling data reuse: Edinburgh DataShare

Data reuse use case

IZTECH University's view on Research Data

Data reuse use case

binder zenodo

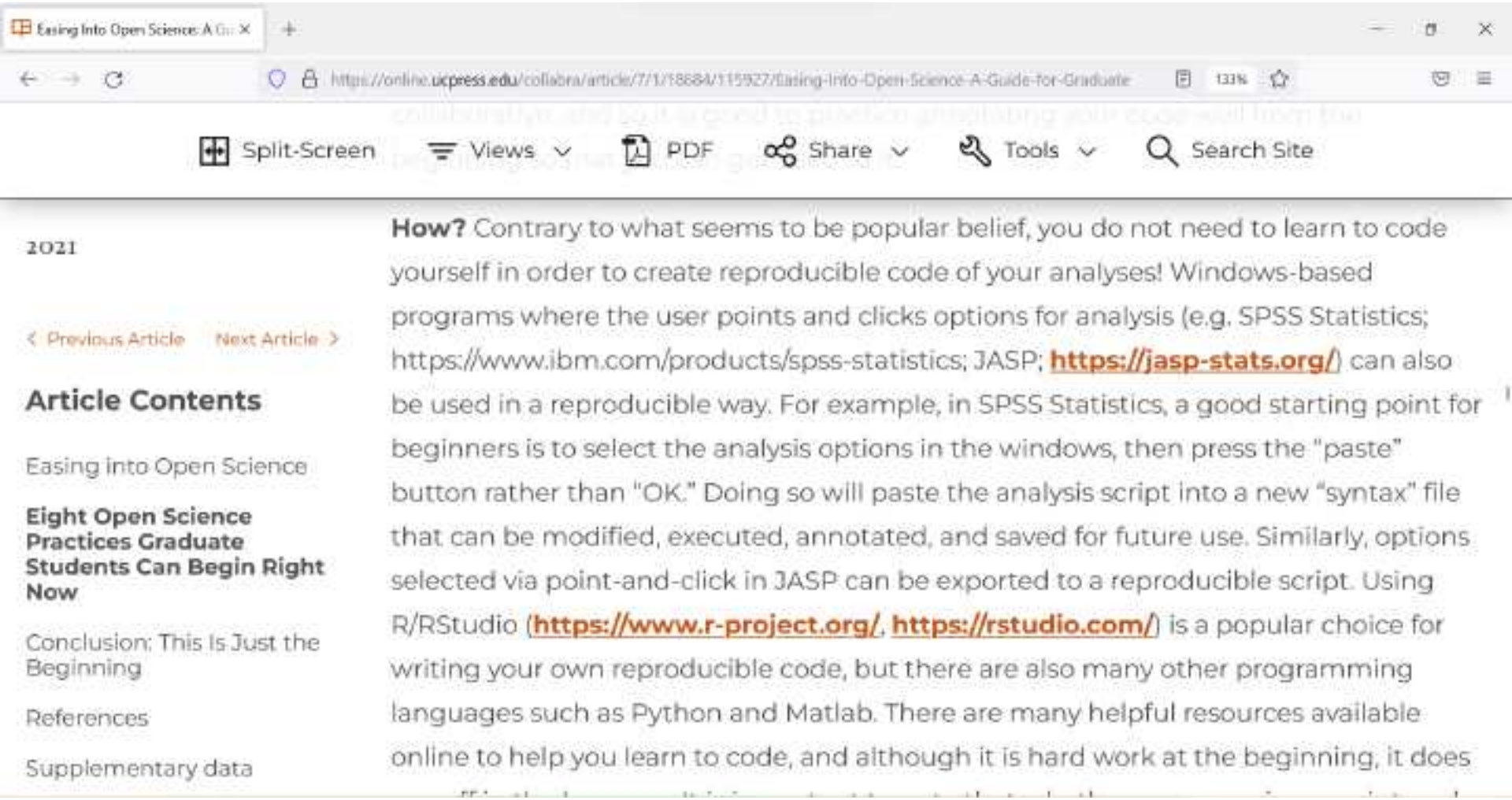
Evidence of data reuse: Binder + Zenodo

Data Reuse Stories involving several institutions and consortia in Europe

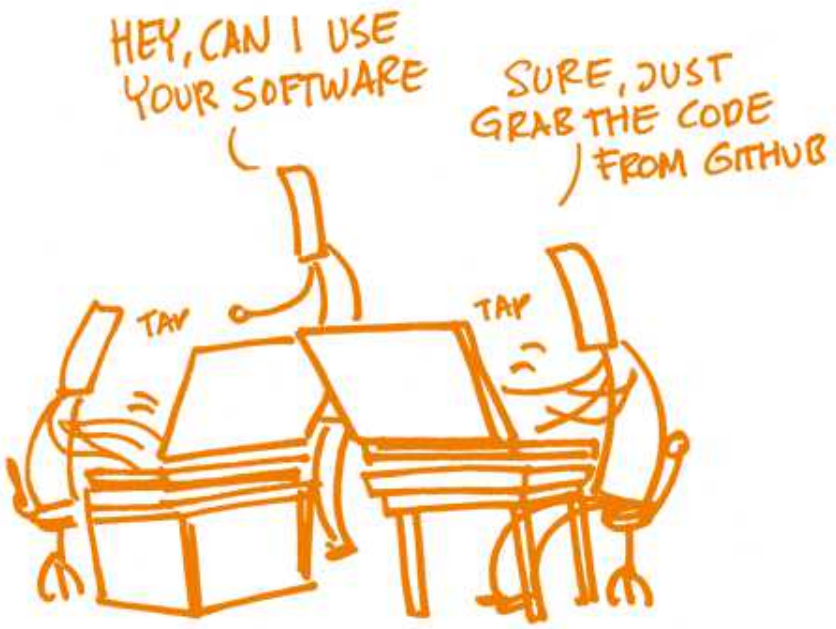
Stay tuned!

Reproducible code and open research software

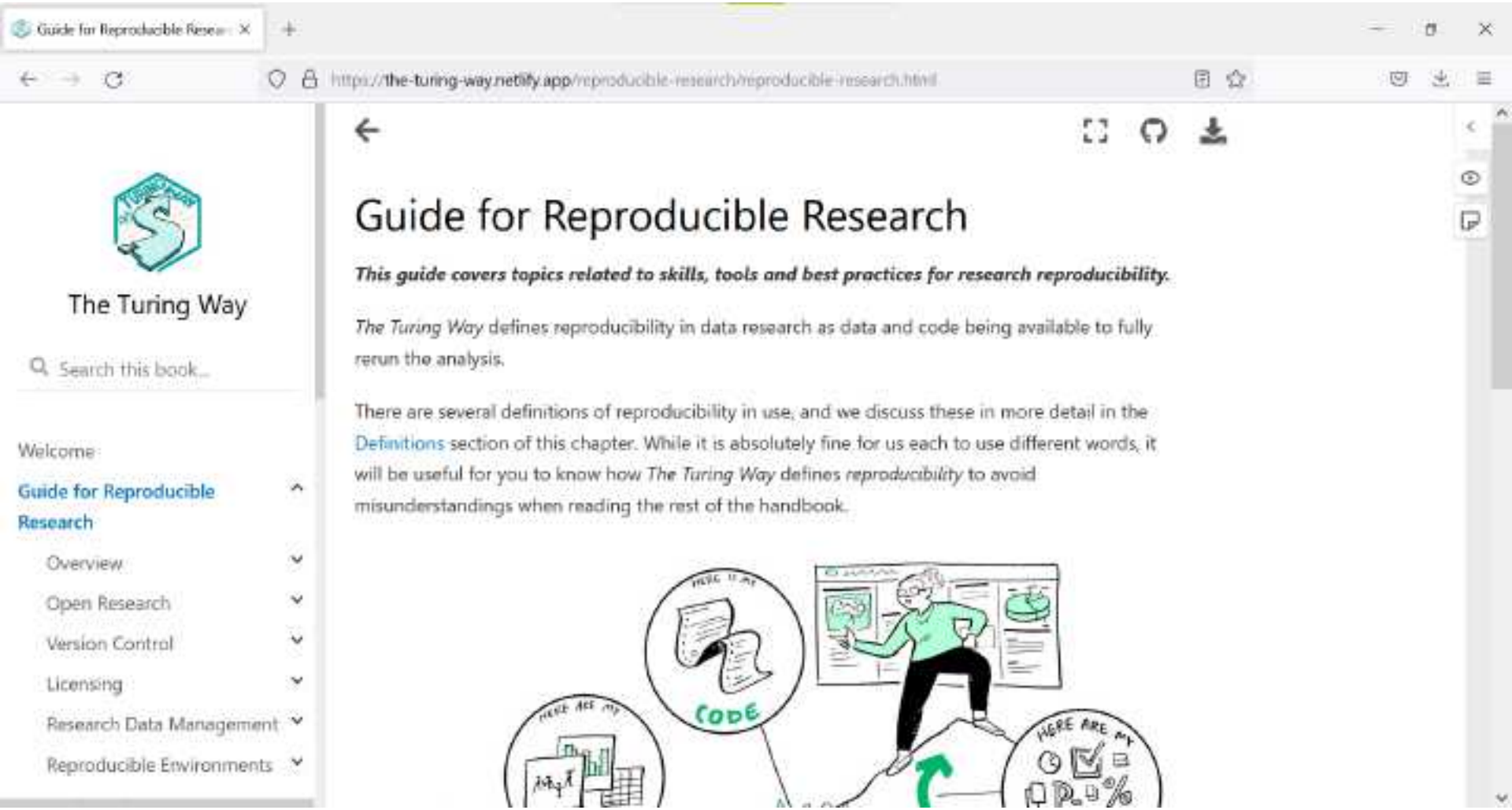
Reproducible code



OPEN SOURCE vs CLOSED SOURCE

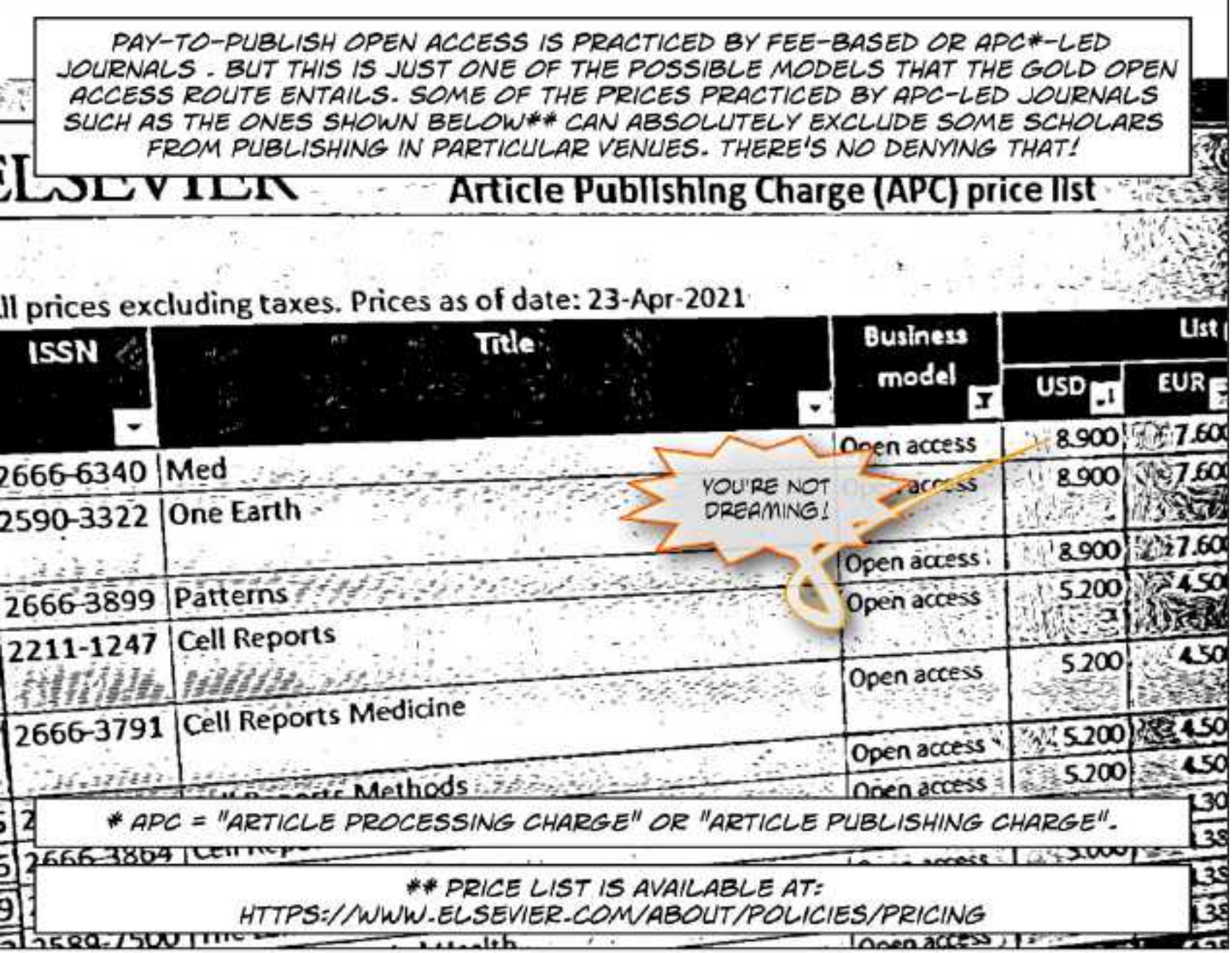


The Turing Way Community, & Scriberia. (2020, November). Illustrations from the Turing Way book dashes. Zenodo. http://doi.org/10.5281/zenodo.4323154

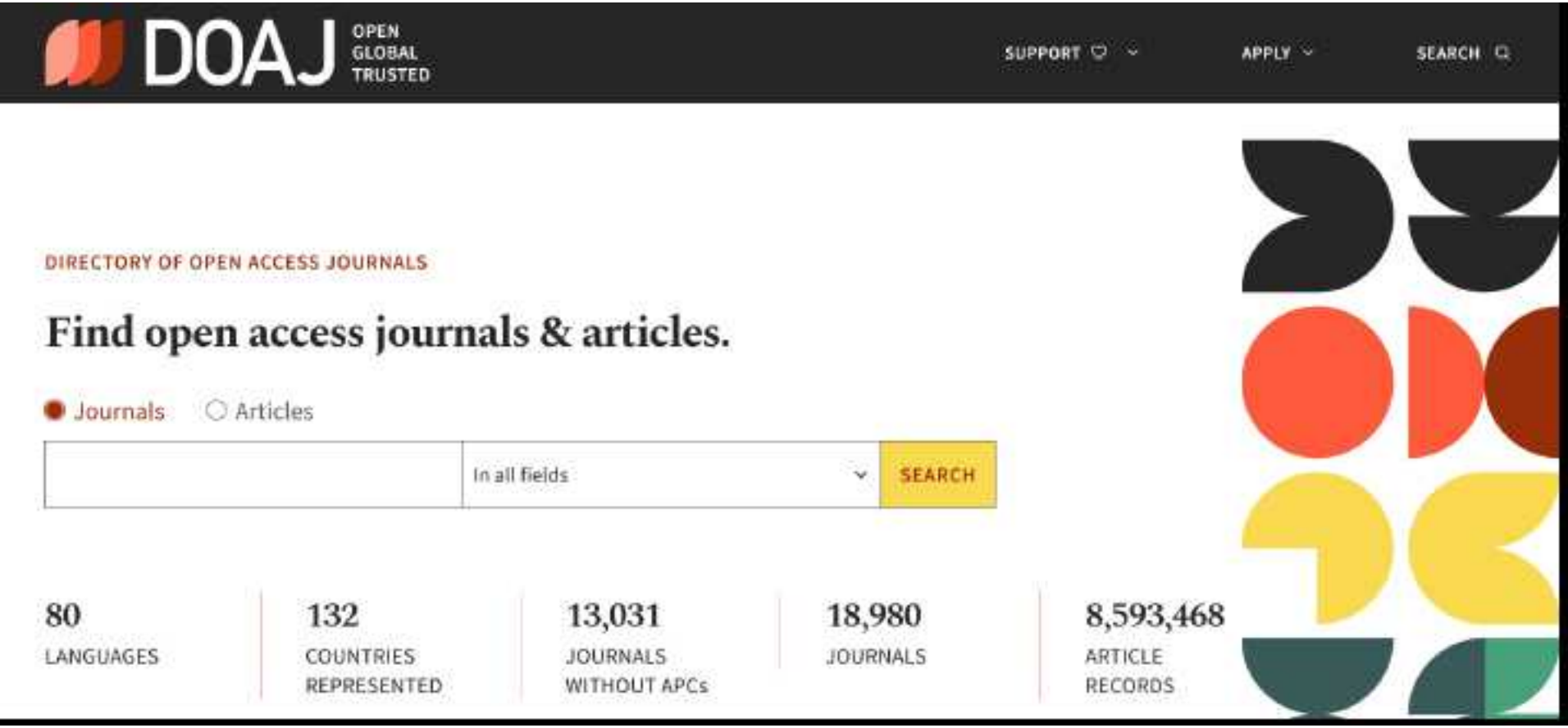


https://the-turing-way.netlify.app/reproducible-research/reproducible-research.html

Open access publishing



Christophe Dony. (2021, May 16). The Scholcomm Chronicles #1. Rambling about Misconceptions of Open Access. Zenodo. http://doi.org/10.5281/zenodo.4765798



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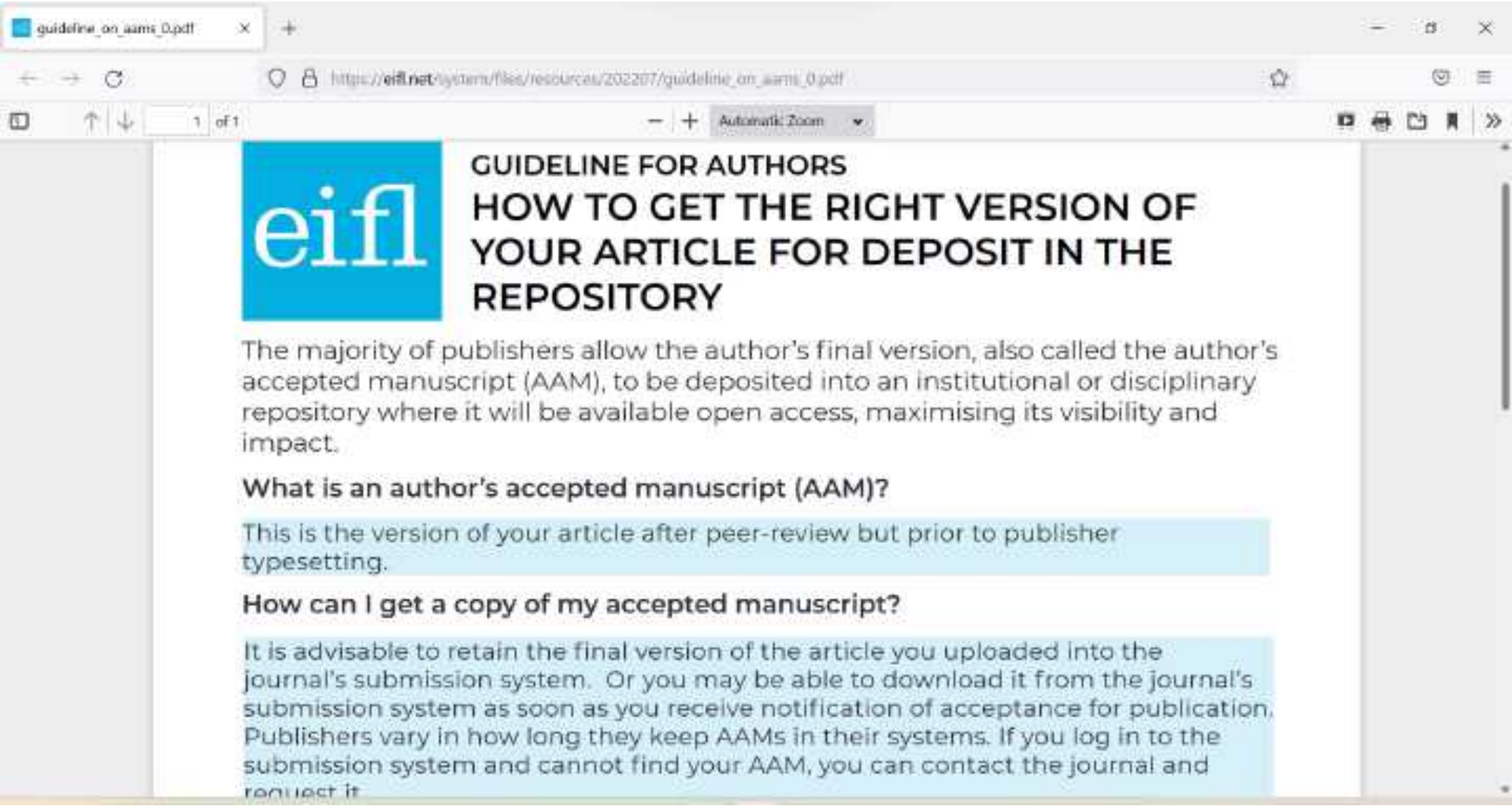
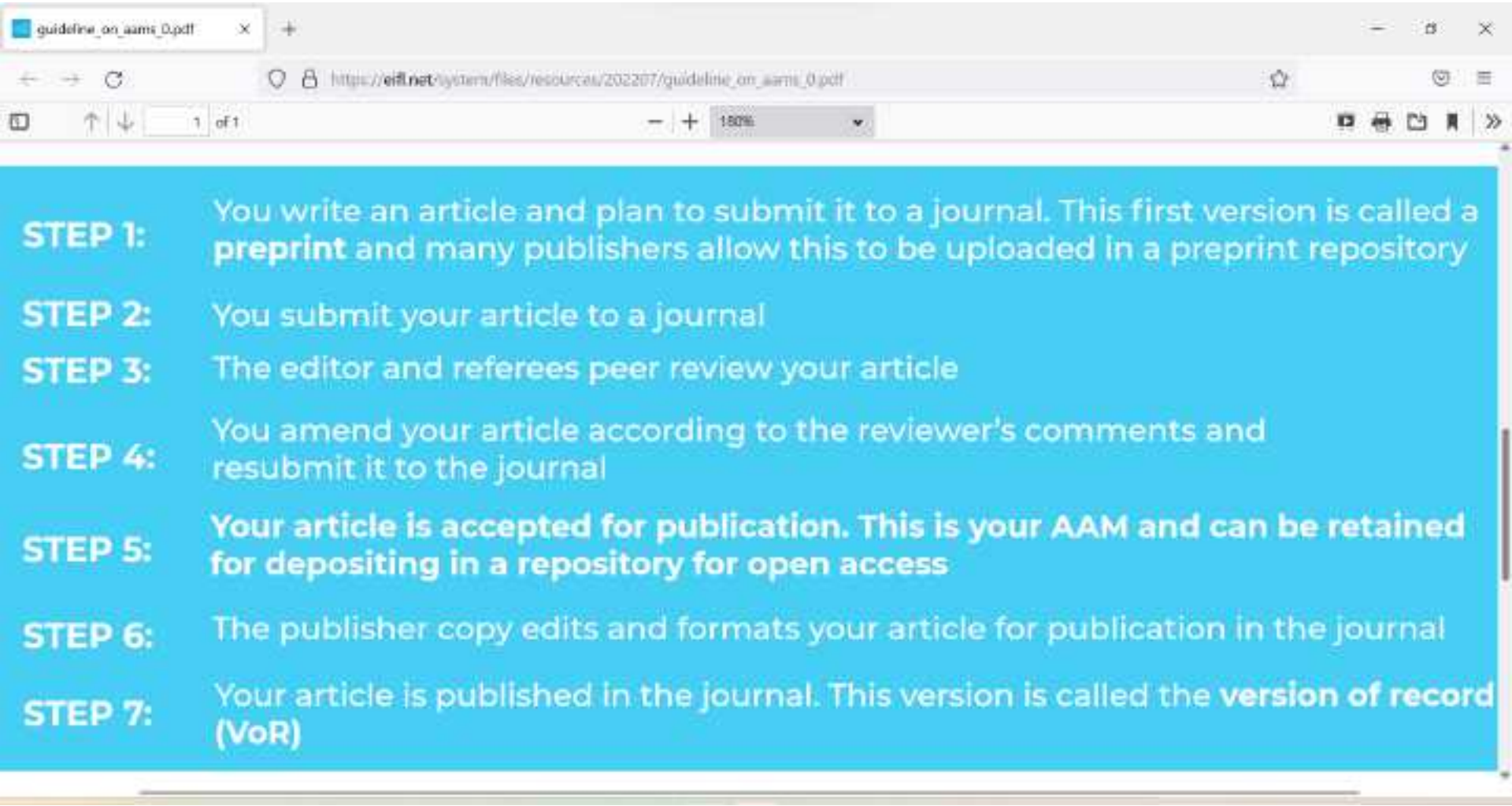


https://eifl.net/resources/authors-how-get-right-version-your-article-deposit-repository



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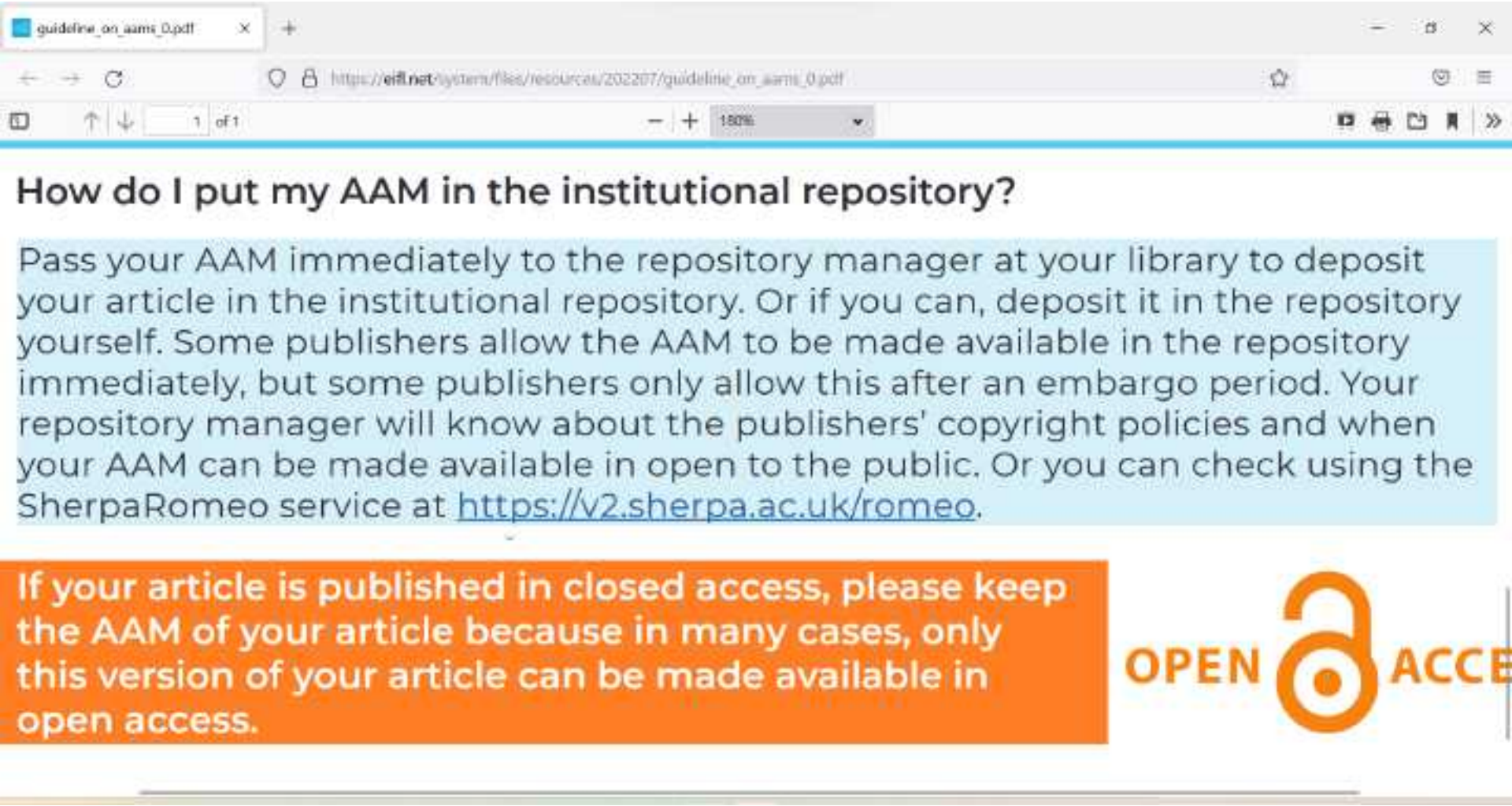

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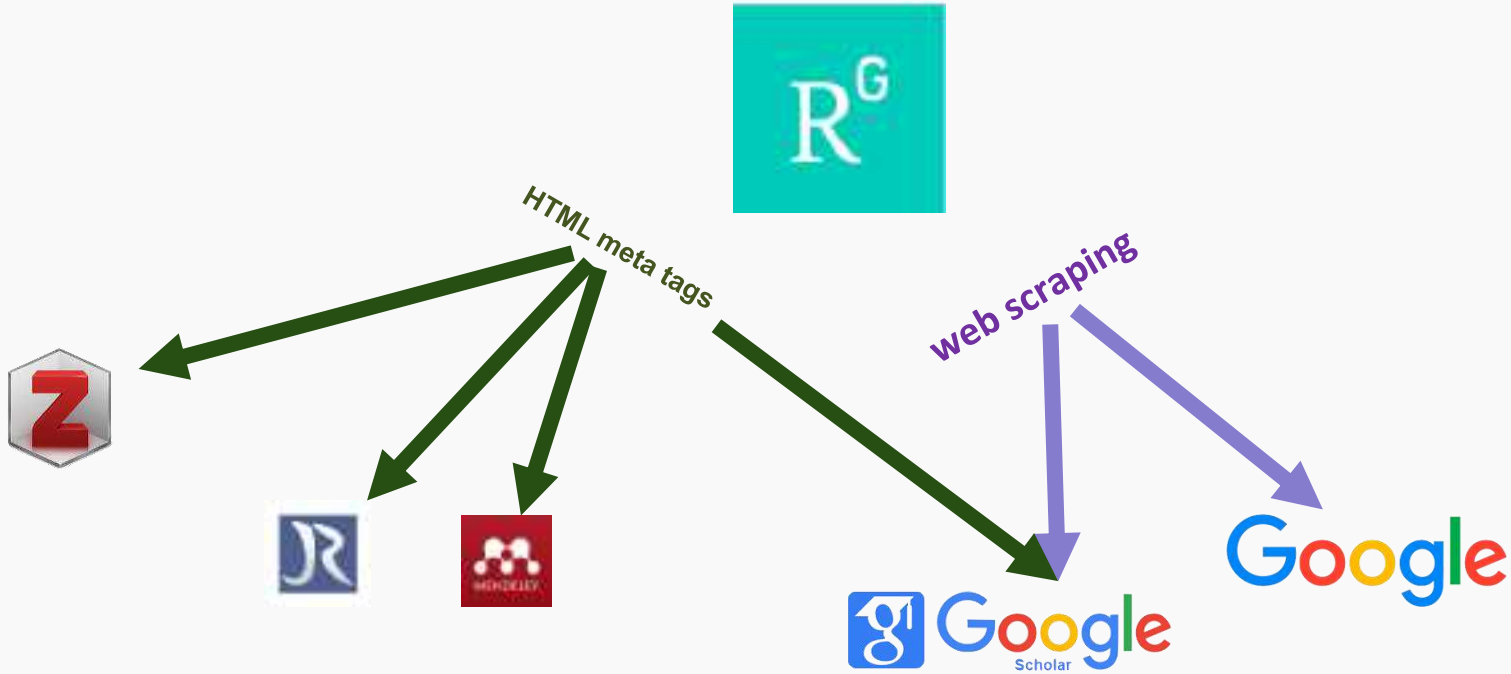
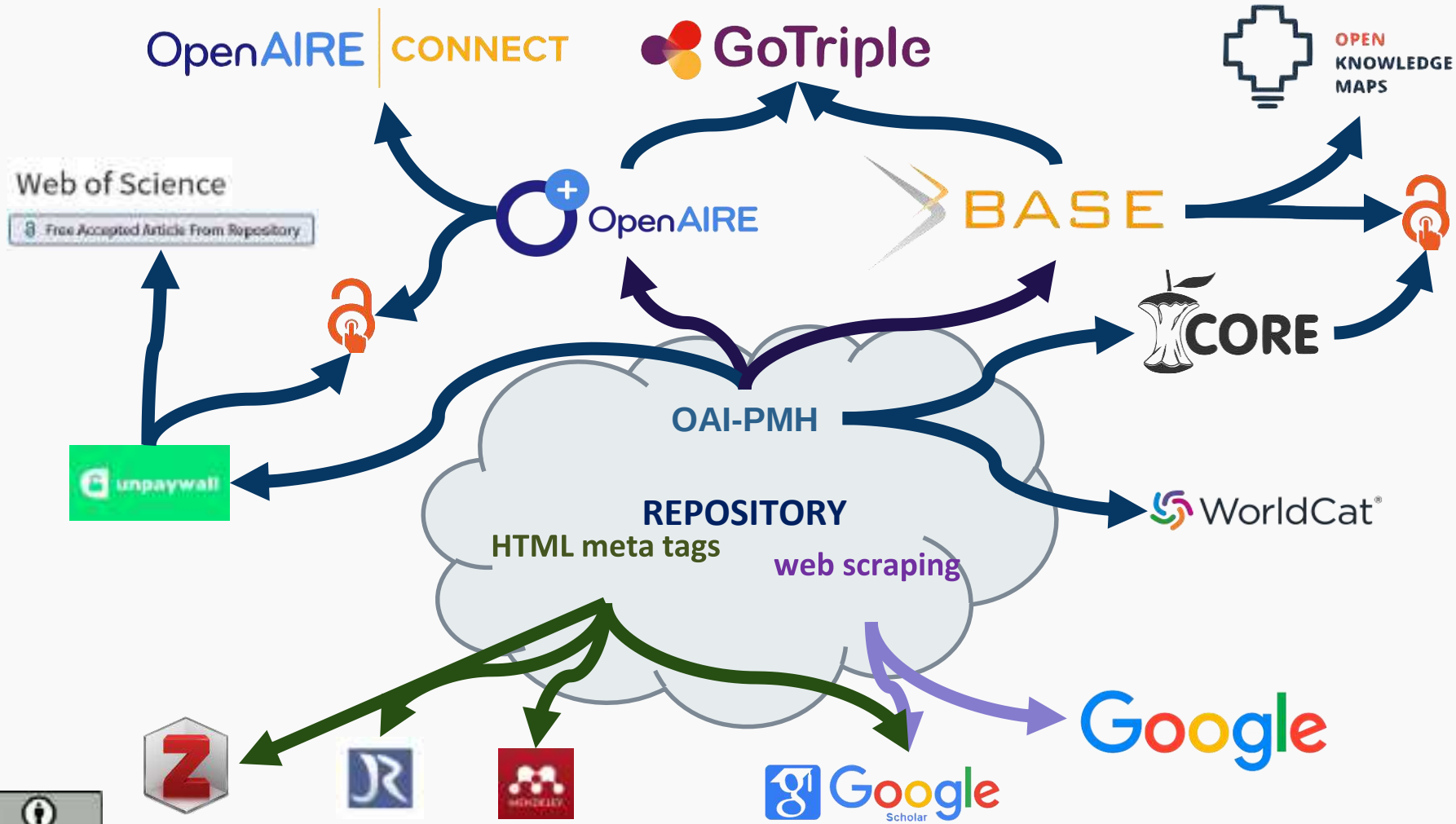


Based on https://www.napd.lu.lv/fileadmin/user_upload/lu_portal/projekti/napd/Zinas/2_EOSC_20191105_MSevkusic.pptx.pdf



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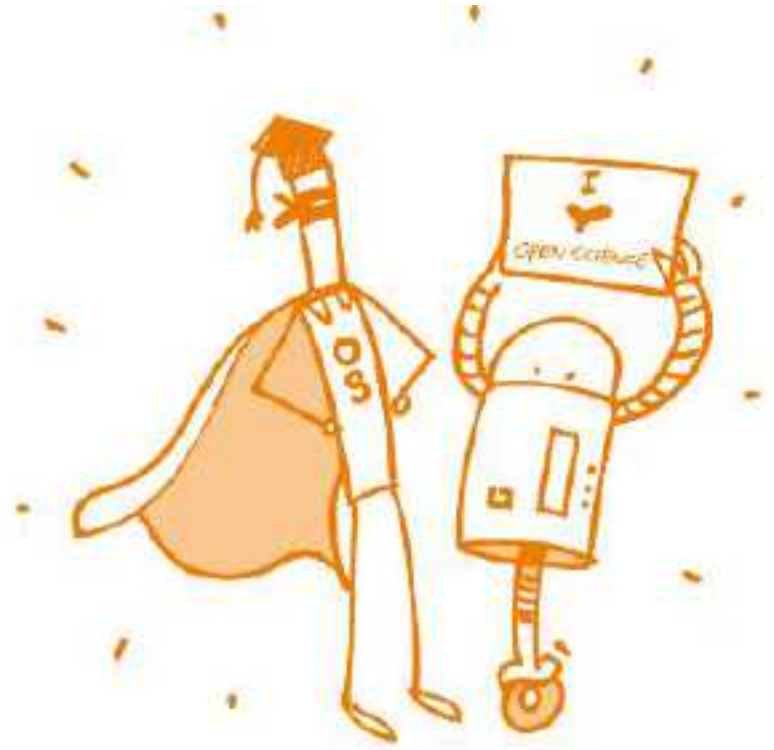
Irena Njezic on the benefits of repositories

	Open access repositories	Academia.edu	ResearchGate
Supports export or harvesting	Yes	No	No
Long-term preservation	Yes	No	No
Business model	Nonprofit (usually)	Commercial. Sells job posting services, hopes to sell data	Commercial. Sells ads, job posting services
Sends you lots of emails (by default)	No	Yes	Yes
Wants your address book	No	Yes	Yes
Fulfills requirements of UC's OA policies	Yes	No	No

https://osc.universityofcalifornia.edu/2015/12/a-social-networking-site-is-not-an-open-access-repository/

Open Peer Review

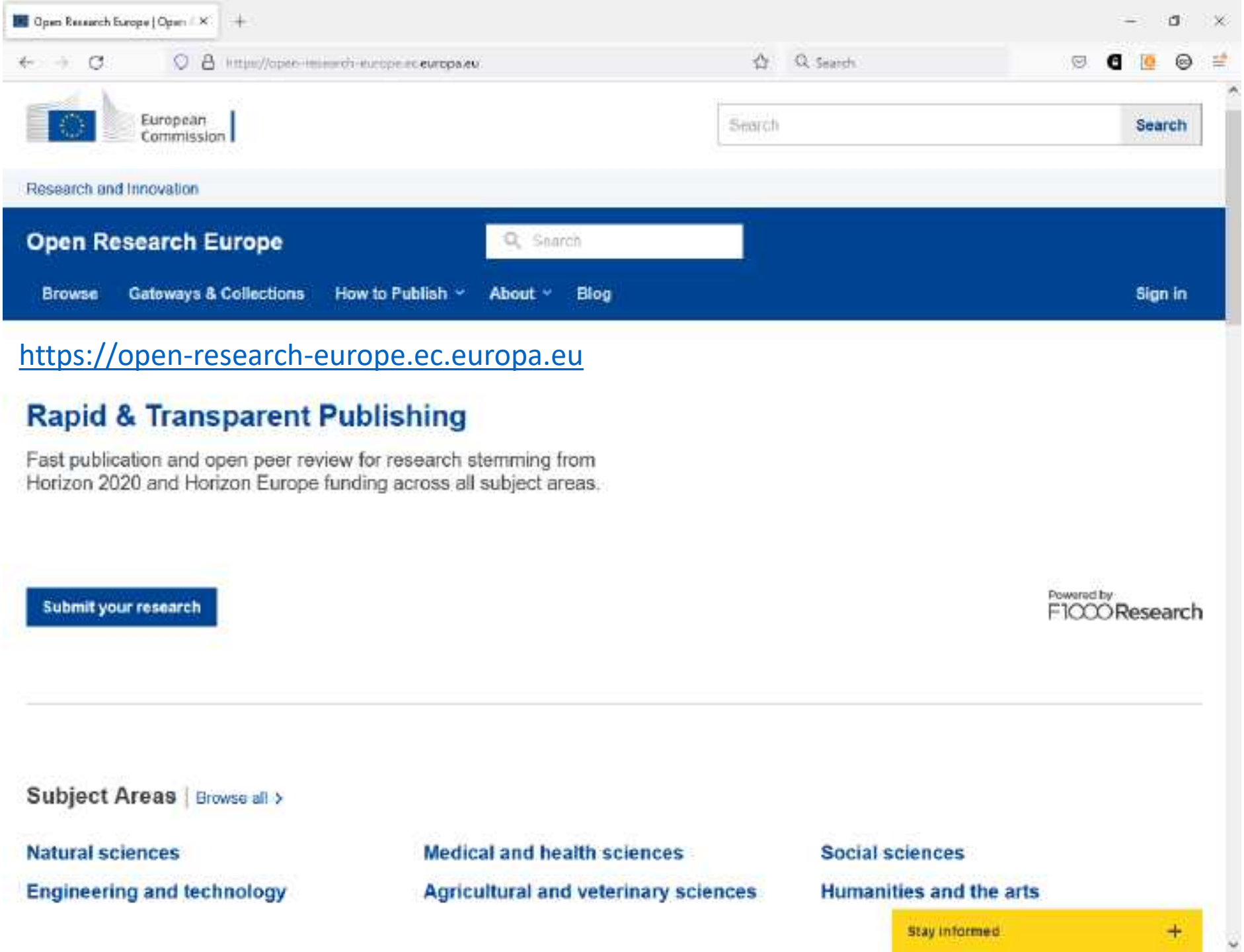


MODES OF PEER REVIEW:

BLIND PEER REVIEW

OPEN IDENTITIES

OPEN REPORTS


Open Research Europe | Open
https://open-research-europe.ec.europa.eu
Search
European Commission
Search
Search
Research and Innovation
Open Research Europe
Search
Browse
Gateways & Collections
How to Publish
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Rapid & Transparent Publishing
Fast publication and open peer review for research stemming from Horizon 2020 and Horizon Europe funding across all subject areas.
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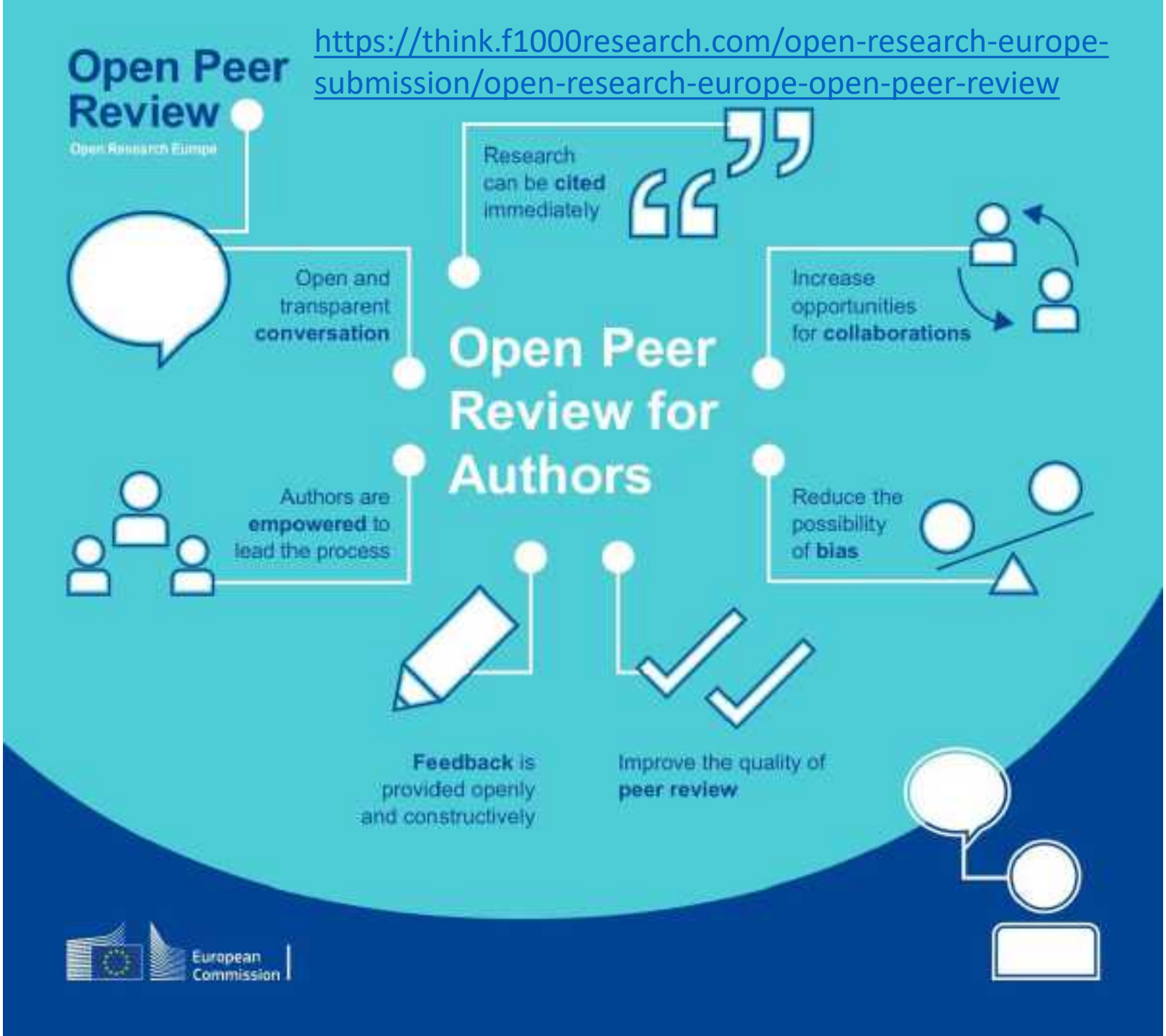
https://think.f1000research.com/open-research-europe-submission/open-research-europe-open-peer-review



How the open peer review process works

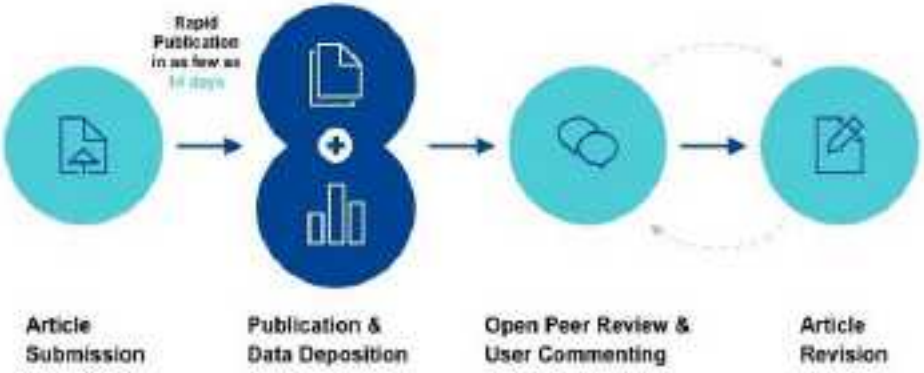
The fundamentals of post-publication peer review at Open Research Europe

At Open Research Europe, our peer review process is **formal**, **invited**, and **open** - so reports are published alongside the article, with reviewer names and affiliations.

Peer review takes place **after** the article has been published openly on the platform, so your research can be read and cited while being assessed by expert reviewers.

Reviewers assess the quality and validity of the research, not the novelty or perceived interest. We also welcome null and negative studies, and they will not be reviewed any differently.

View our detailed infographic which takes you through every step of our open, post-publication peer review process, so you know what to expect at every stage.



REVIEW

Transition from monolithic to microservice-based applications. Challenges from the developer perspective [version 1; peer review: awaiting peer review]

Antonios Makris, Konstantinos Tserpes, Theodora Varvarigou

Abstract

Microservices have taken the world of software development by storm. Application developers are struggling to understand the new concepts and make the transition by the so-called monolithic" application approach to microservices. This paper touches upon this delicate issue, providing a more concrete view of the developers' concerns together with recent responses to these concerns. The objective is to place the concept of microservices in the most up-to-date context and shed some light in the challenges that puzzle the developers the most while they attempt to make use of this development and design style.

Corresponding Author: Antonios Makris

Competing Interests: No competing interests were disclosed.

Grant Information: This work was supported by the CHARITY and ACCORDION projects that have received funding from the European Union's Horizon 2020 research and innovation program under Grant Agreement Nos. 101016509 and 871793, respectively.
The funders had no role in study design, data collection and analysis, decision to publish, or preparation of the manuscript.

First Version Published: 23 Feb 2022, **2**:24 (https://doi.org/10.12688/openreseurope.14585.1)
Latest Version Published: 23 Feb 2022, **2**:24 (https://doi.org/10.12688/openreseurope.14585.1)

REVISED

Hydrogen and deuterium charging of lifted-out specimens for atom probe tomography [version 2; peer review: 1 approved, 1 approved with reservations]

Heena Khanchandani, Se-Ho Kim, Rama Srinivas Varanasi, TS Prithiv, Leigh T. Stephenson, Baptiste Gault

Abstract

Hydrogen embrittlement can cause a dramatic deterioration of the mechanical properties of high-strength metallic materials. Despite decades of experimental and modelling studies, the exact underlying mechanisms behind hydrogen embrittlement remain elusive. To unlock understanding of the mechanism and thereby help mitigate the influence of hydrogen and the associated embrittlement, it is essential to examine the interactions of hydrogen with structural defects such as grain boundaries, dislocations and stacking faults. Atom probe tomography (APT) can, in principle, analyse hydrogen located specifically at such microstructural features but faces strong challenges when it comes to charging specimens with hydrogen or deuterium. Here, we describe three different workflows enabling hydrogen/deuterium charging of site-specific APT specimens: namely cathodic, plasma and gas charging. All the experiments in the current study have been performed on a model twinning induced plasticity steel alloy. We discuss in detail the caveats of the different approaches in order to help future research efforts and facilitate further studies of hydrogen in metals. Our study demonstrates successful cathodic and gas charging, with the latter being more promising for the analysis of the high-strength steels at the core of our work.

Corresponding Author: Baptiste Gault

Competing Interests: No competing interests were disclosed.

Grant Information: This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 771602). R.S.V was supported by an IMPRS SusMat scholarship.

Open Peer Review

Reviewer Status ✓ ?

Reviewer Reports

	Invited Reviewers	
	1	2
Version 2 (Revision) 21 Feb 22		
Version 1 14 Oct 21	✓ read	? read

1. **Maria Auger**, University of Oxford, Oxford, UK
2. **Gregory Thompson**, University of Alabama, Tuscaloosa, AL, USA

Comments on this article

All Comments (0)

Sign in to comment

REVISED **Amendments from Version 1**

The reviewers' comments have been very helpful in improving the manuscript. In response to them, the title of the manuscript is changed to emphasize that the work is focused on the lifted-out specimens. The study was conducted on a model twinning induced plasticity steel alloy. This fact has now been included in the abstract and conclusions. Figure 1 has been moved to Figure 4 as an introduction to the workflows. The first paragraph of introduction has been modified to improve its clarity.

See the detailed response from the author(s) to the review by Maria Auger
See the detailed response from the author(s) to the review by Gregory Thompson

Introduction

The ingress of hydrogen inside structural metallic materials in engineering parts in service leads to a degradation of their mechanical properties and their premature catastrophic failures[1–4]. Hydrogen that freely diffuses through the material under ambient conditions[5] can interact with crystalline defects and contributes to the deterioration of the mechanical properties[3,5–7]. A strategy to mitigate the deleterious influence of hydrogen is to design alloys with a high number density of trapping sites to limit the deleterious influence of H on moving dislocations[5,6,8]. Traps can even be irreversible traps, i.e. H is unable to re-enter the lattice under service conditions, owing to the high binding energy with H[9,10]. Trapped hydrogen has even been reported to potentially increase the resistance to hydrogen embrittlement of some materials[1,2,5]. In order to guide the design of hydrogen-resistant materials, it is necessary to study the details of the structure and composition of sites that can trap diffusible hydrogen, which are mostly defects such as stacking faults, dislocations and phase and grain boundaries[1,3]. Very few techniques have the combination of high spatial resolution and compositional sensitivity.

Atom probe tomography (APT) is a time-of-flight mass spectroscopy technique, which maps the spatial distribution of specific chemical species within a three-dimensional (3D) volume with sub-nanometre resolution[11,12]. In principle, APT is capable of detecting and quantifying hydrogen in three dimensions at near-atomic scale[13]. Yet despite some successes[14–17], and decades of work from numerous research groups, hydrogen microanalysis remains very challenging[1,2,13,14,17–20]. There are issues associated with the influence of residual gases from the analysis chamber of atom probe, specimen preparation and transport[20,21], and a strong dependence of the analytical performance on the analysis conditions[22–25]. Let us discuss these aspects in more details.

METHOD ARTICLE

Optimization and parallelization of the discrete ordinate method for radiation transport simulation in OpenFOAM: Hierarchical combination of shared and distributed memory approaches [version 1; peer review: 2 approved]

Jose Moreno-SanSegundo, Cintia Casado, David Concha, Antonio S. Montemayor, Javier Marugán

This article is included in Societal Challenges gateway

Abstract

This paper describes the reduction in memory and computational time for the simulation of complex radiation transport problems with the discrete ordinate method (DOM) model in the open-source computational fluid dynamics platform OpenFOAM. Finite volume models require storage of vector variables in each spatial cell. DOM introduces two additional discretizations, in direction and wavelength, making memory a limiting factor. Using specific classes for radiation sources data, changing the store of fluxes and other minor changes allowed a reduction of 75% in memory requirements. Besides, a hierarchical parallelization was developed, where each node of the standard parallelization uses several computing threads, allowing higher speed and scalability of the problem. This architecture, combined with optimization of some parts of the code, allowed a global speedup of x15. This relevant reduction in time and memory of radiation transport opens a new horizon of applications previously unaffordable.

Corresponding Author: Javier Marugán

Competing Interests: No competing interests were disclosed.

Open Peer Review

Reviewer Status ✓ ✓

Reviewer Reports

	Invited Reviewers	
	1	2
Version 1 24 Mar 21	✓ read	✓ read

1. **João Miguel Nóbrega**, University of Minho, Guimarães, Portugal
2. **George Karpouzas**, Engys Hellas, Athens, Greece
   Eugene de Villiers, Engys Ltd, London, UK

Comments on this article

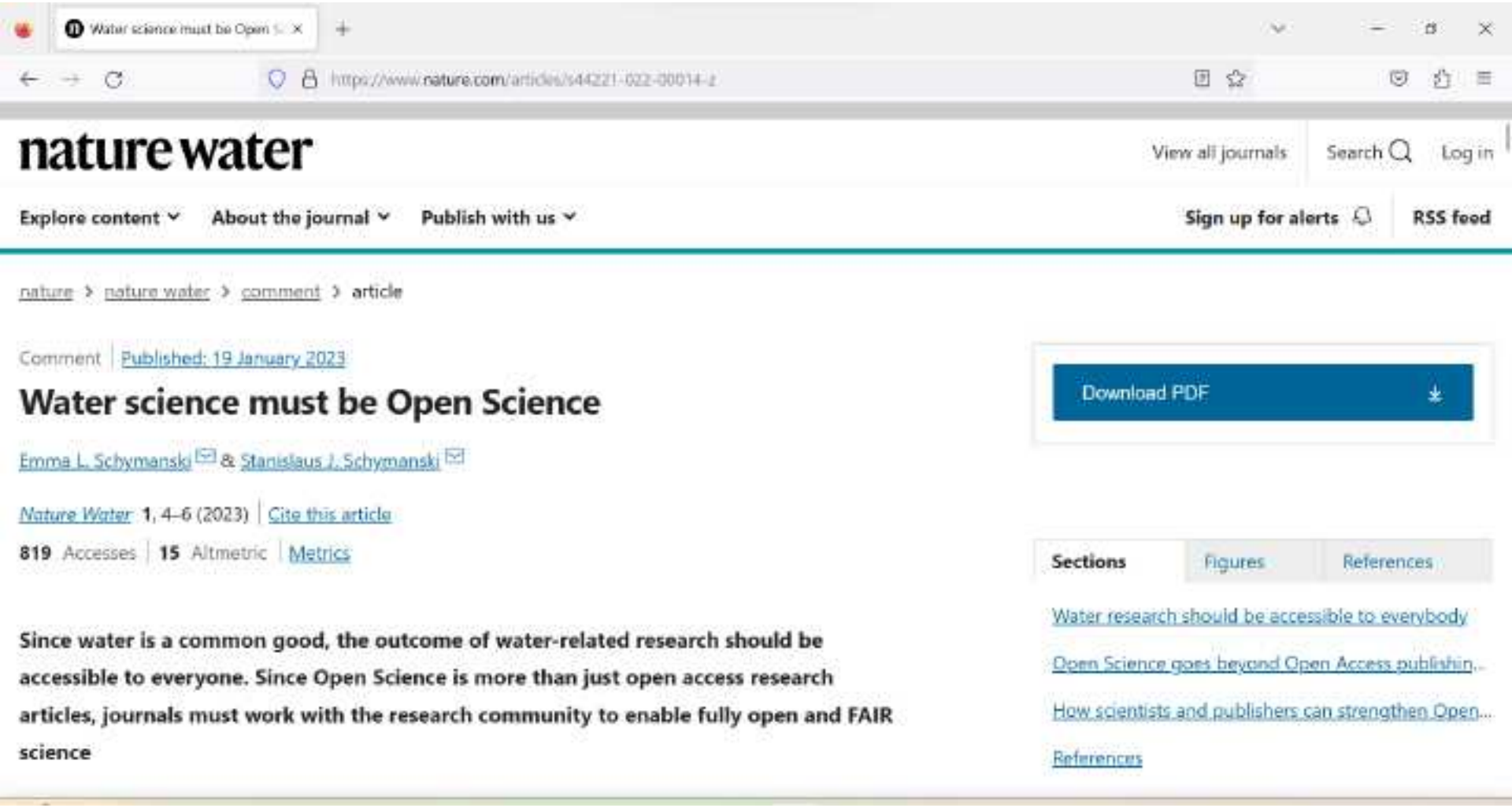
All Comments (0)

Sign in to comment

Misconception: Open Science is mainly pain with little gain

There's no denying that getting acquainted with new ways of working costs time. But at the end of the day, it will also save you time. For instance, preregistration forces you to consider issues that could otherwise have bitten you in the ass afterwards (e.g., a lack of statistical power). Moreover, a detailed plan allows for a swift analysis once the data comes in. There is an increasing number of open-source tools available that will help you make your workflow more reproducible and efficient at the same time. And there's another gain for those interested in an academic career: more and more universities and funders are seeking candidates who implement Open Science practices in their work.

https://openscience-groningen.nl/10-open-science-myths



Schymanski, E.L., Schymanski, S.J. Water science must be Open Science. *Nat Water* **1**, 4–6 (2023). https://doi.org/10.1038/s44221-022-00014-z

Open Science in Horizon Europe proposals

- PART A – Application form
  - List 5 publications, widely-used datasets, softwares, goods, services or any other achievements relevant to the call
- PART B – Project proposal – technical description
  - Under ‘Excellence’ – ‘1.2 Methodology’ (Open Science, RDM and management of other research outputs)
  - Under ‘Impact’ – ‘2.2 Measures to maximise impact’ (dissemination, exploitation and communication)
  - Under ‘Quality and efficiency of the implementation’ – ‘3.1 Work plan and resources’ and ‘3.2 Capacity of participants and consortium as a whole’

Jonathan England

Publications

- Your publications cited should be in OA
- Your publications cited will only be evaluated qualitatively (i.e. the Impact Factor is irrelevant)
- Give insights in where you are hoping to publish (e.g. Open Research Europe, full OA journals)

Jonathan England

Mandatory open science practices

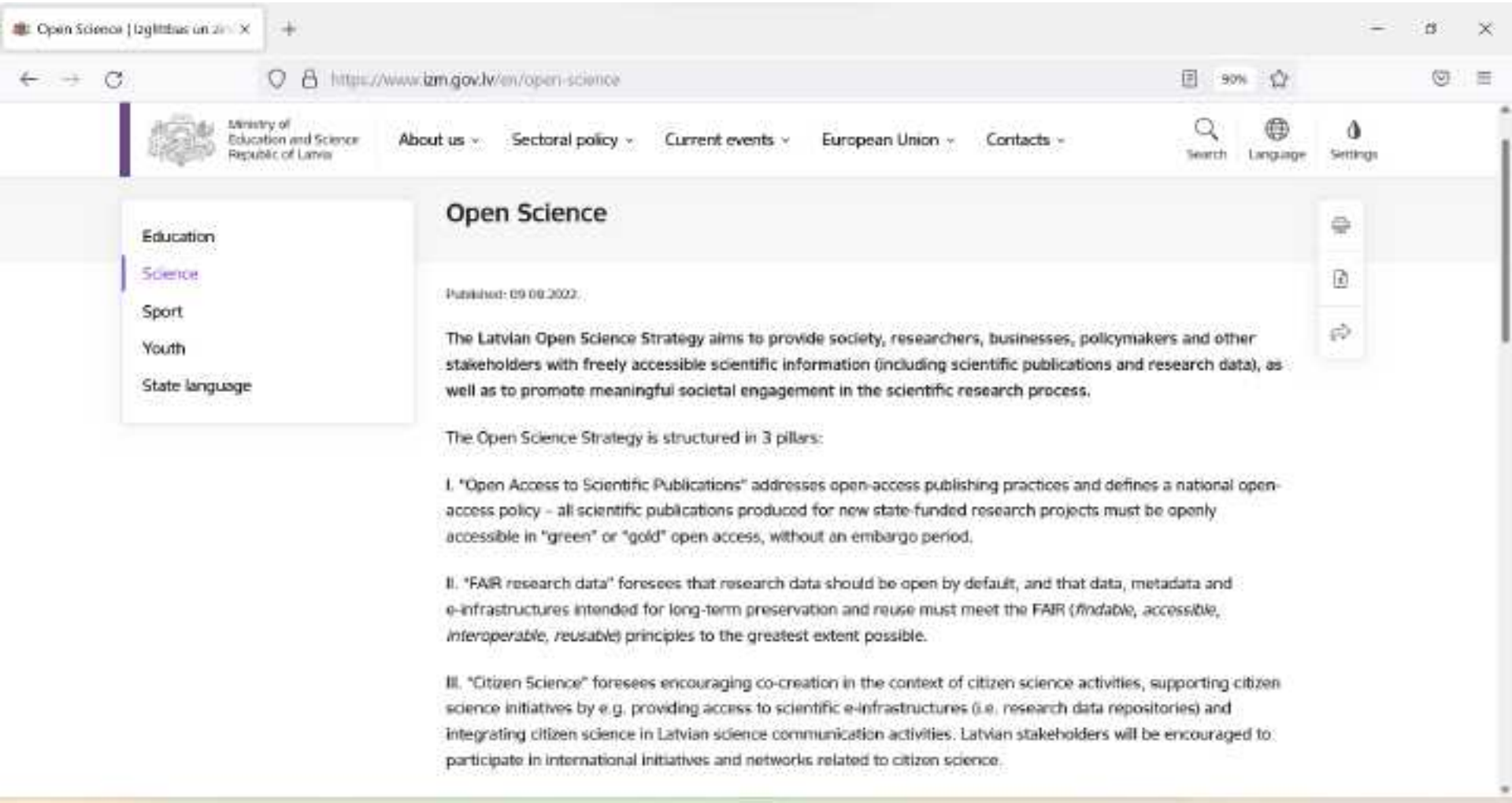
- Some open science practices are **mandatory for all beneficiaries per the grant agreement.** They concern:
  - open access to scientific publications under the conditions required by the grant agreement;
  - responsible management of research data in line with the FAIR principles of 'Findability', 'Accessibility', 'Interoperability' and 'Reusability', notably through the generalised use of data management plans, and open access to research data under the principle 'as open as possible, as closed as necessary', under the conditions required by the grant agreement;
  - information about the research outputs/tools/instruments needed to validate the conclusions of scientific publications or to validate/re-use research data;
  - digital or physical access to the results needed to validate the conclusions of scientific publications, unless exceptions apply;

https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/guidance/programme-guide_horizon_en.pdf

Recommended open science practices

- **Involving all relevant knowledge actors**, including citizens, civil society and end users in the co-creation of R&I agendas and contents (such as citizen science)
- **Early and open sharing of research**, for example, through preregistration, registered reports, pre-prints, or crowd-sourcing)
- **Research output management** beyond publications and research data
- **Measures to ensure reproducibility of research outputs**
- **Providing open access to research outputs beyond publications and research data** (for example software, models, algorithms, and workflows)
- **Participation in open peer review**

https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/guidance/programme-guide_horizon_en.pdf
https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/common/guidance/aga_en.pdf



https://www.izm.gov.lv/en/open-science

https://openclimatecampaign.org

OPEN CLIMATE CAMPAIGN

A four-year campaign to make open sharing of research outputs the norm in climate science

OPEN SOCIETY FOUNDATIONS

creative commons

SPARC

eifl KNOWLEDGE WITHOUT BOUNDARIES

ARCADIA

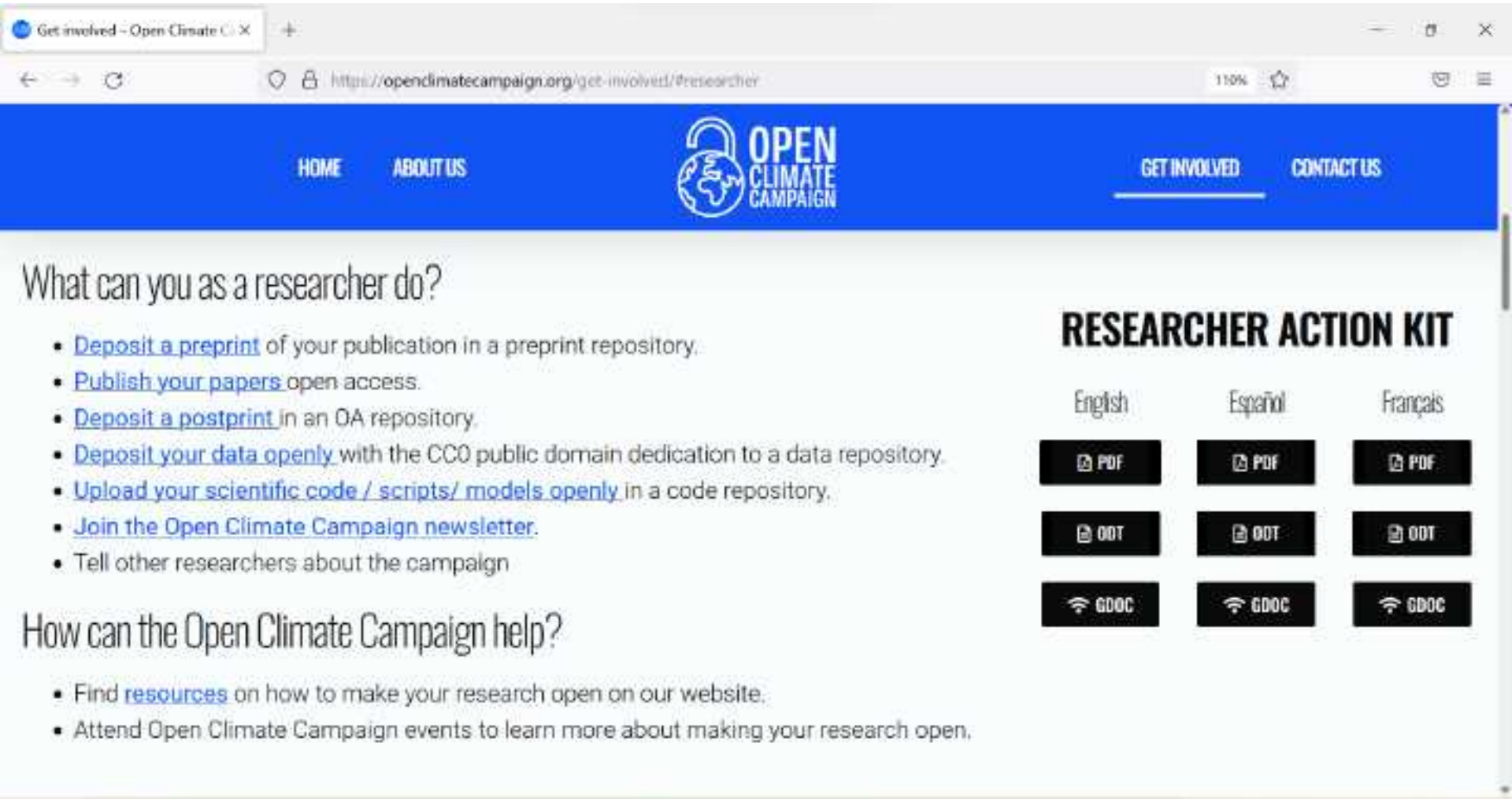
https://openclimatecampaign.org

@OpenClimateCamp

OPEN CLIMATE CAMPAIGN

- Bringing attention to the issue of access to knowledge on climate change particularly to **researchers** who are producing the knowledge and **informing them of tools that can open their research outputs**.
- Working directly with national governments, funders and environmental organizations to identify legal and policy barriers, **help governments create, adopt, implement equitable open access policies** to overcome them, and make it easier to open and share their climate change research, data and educational resources.
- Identifying, engaging, and contributing to draft **international frameworks** to include funder open access policy recommendations, and the public benefits of open access knowledge.
- Engaging with researchers, universities and policy makers from traditionally excluded groups and in geographical regions to ensure inclusive outcomes throughout.

Thabang Lehobye for ArtistsForClimate.org, CC-BY-NC-SA



https://openclimatecampaign.org/get-involved/#researcher

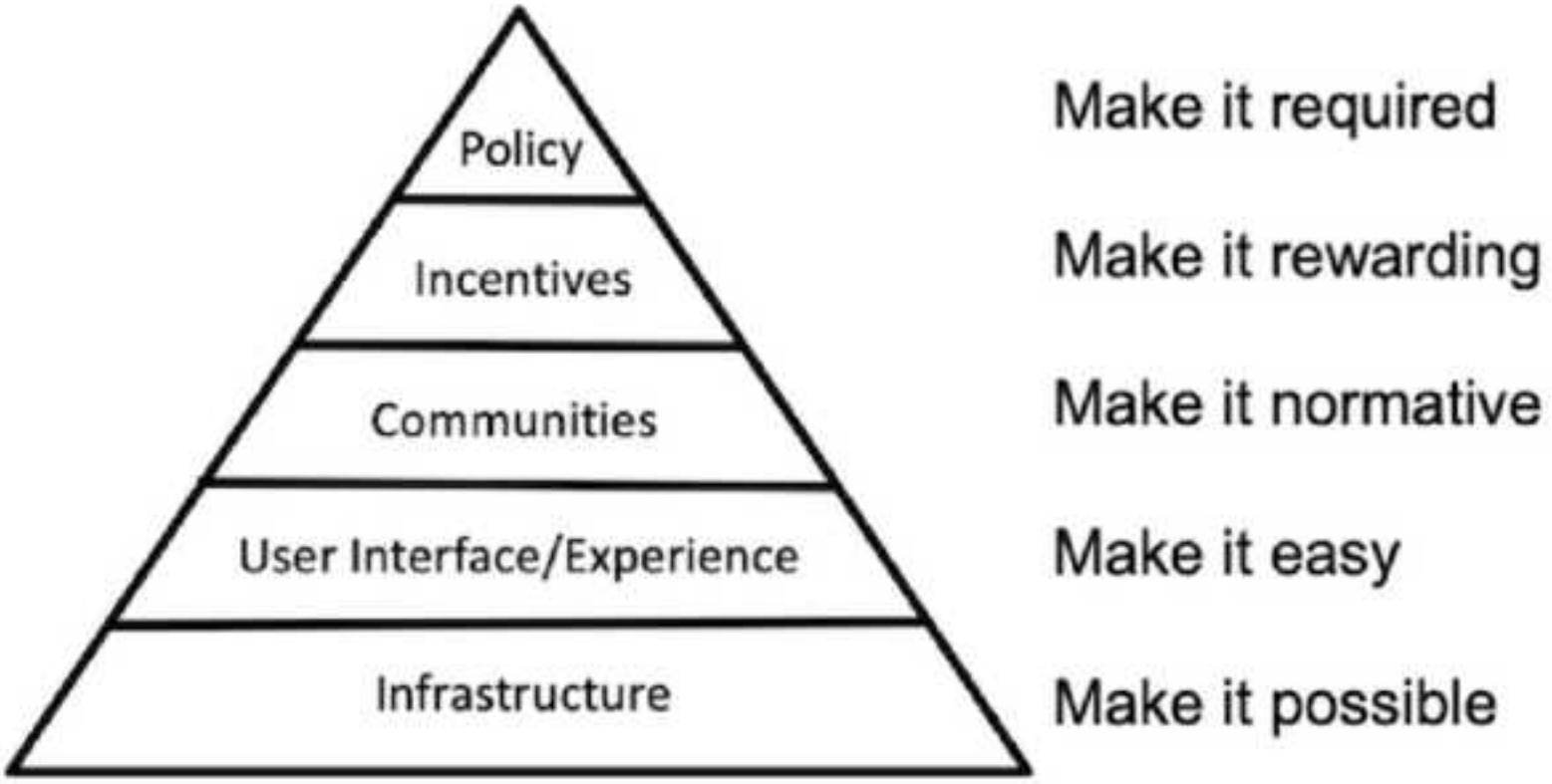
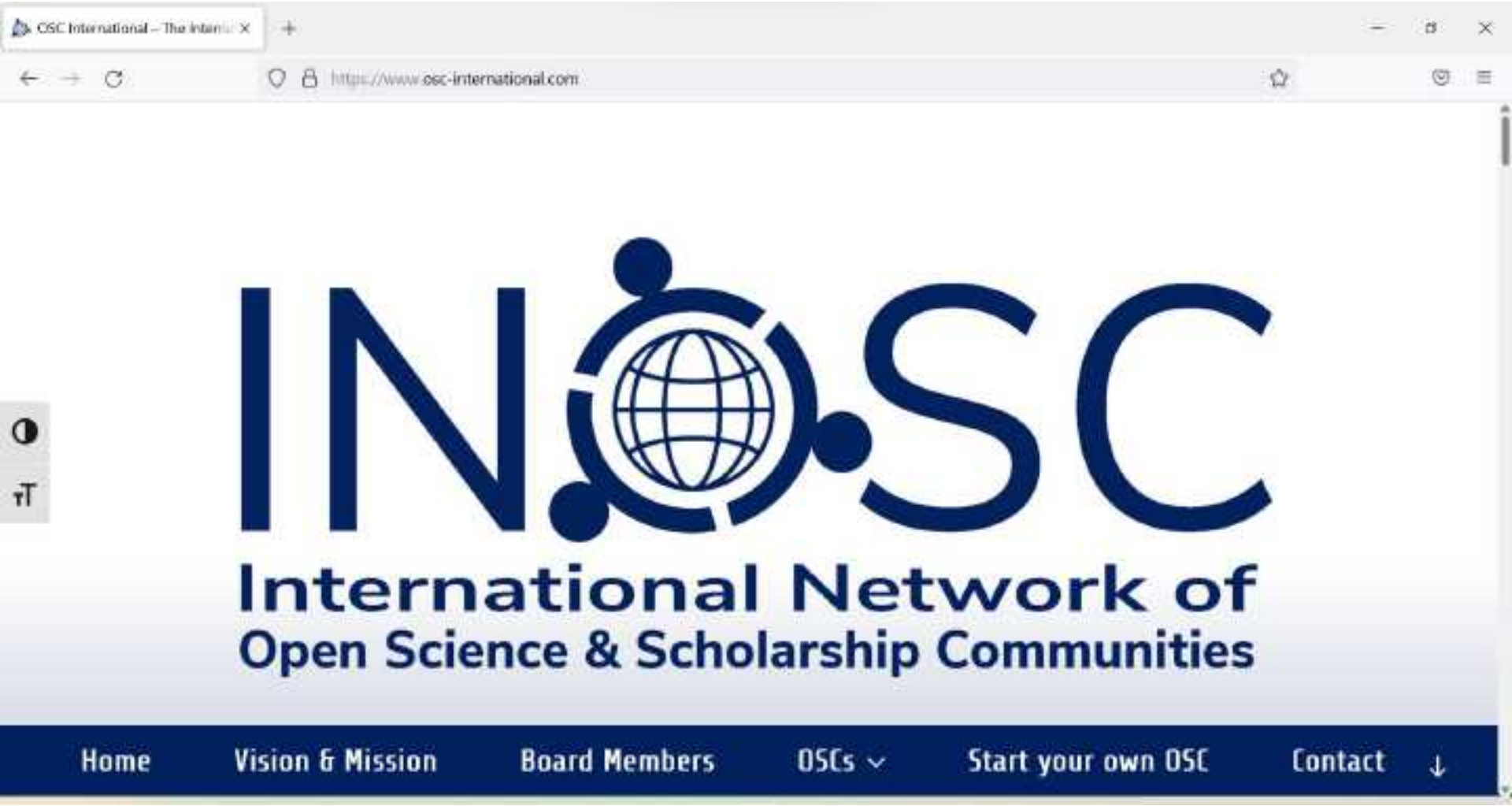
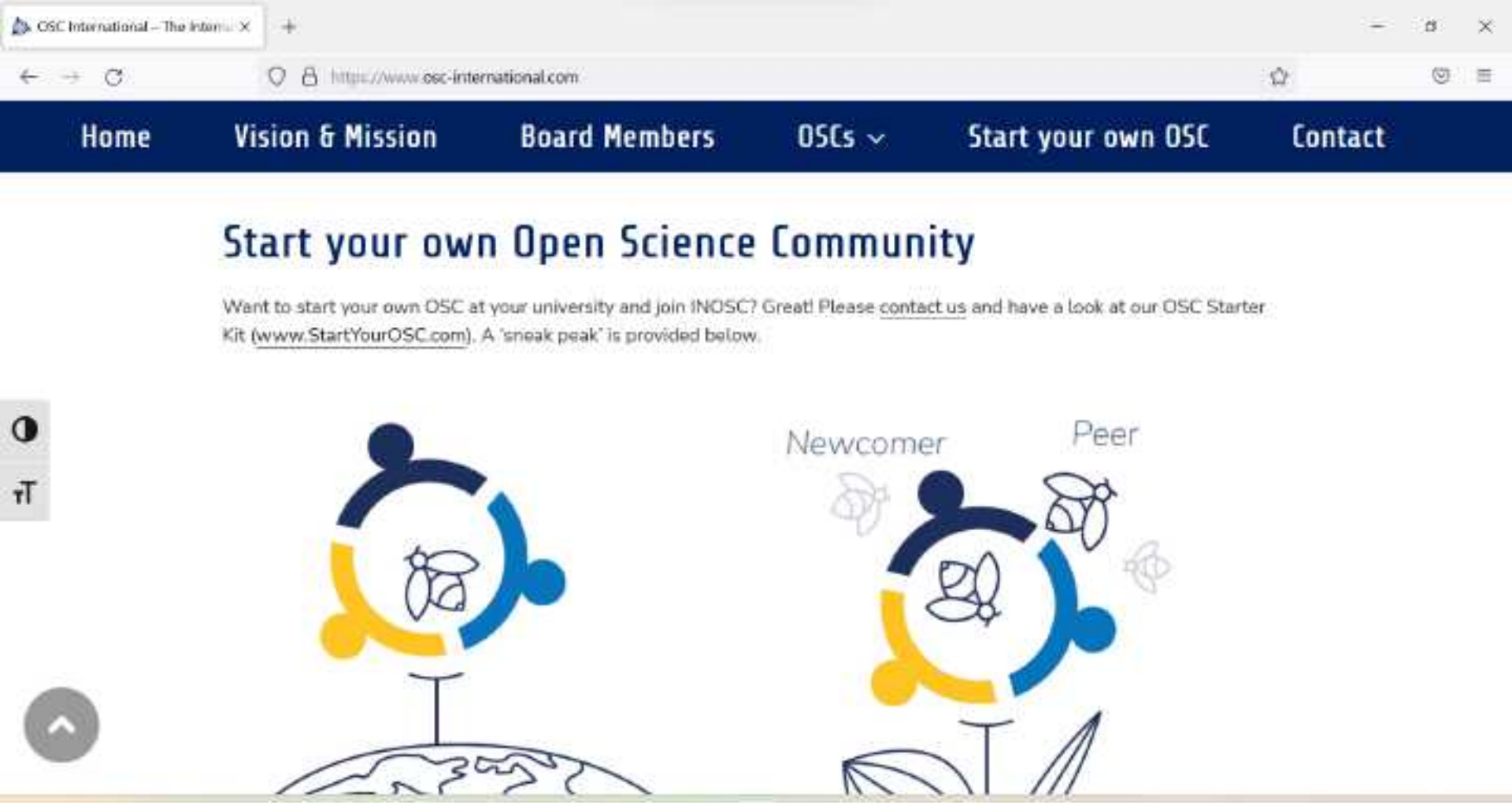


Figure 1. *The pyramid of culture change. Image by Brian Nosek (licensed under CC BY-ND 4.0), reproduced from the blog post Strategy for Culture Change.*



https://www.osc-international.com


OSC Sweden
OSC Galway
OSC the Netherlands
OSC Serbia
OSC Lisbon
OSC Saudi Arabia
OSC Nigeria



Kristijan Armeni, Loek Brinkman, Rickard Carlsson, Anita Eerland, Rianne Fijten, Robin Fondberg, Vera E Heininga, Stephan Heunis, Wei Qi Koh, Maurits Masselink, Niall Moran, Andrew Ó Baoill, Alexandra Sarafoglou, Antonio Schettino, Hardy Schwamm, Zsuzsika Sjoerds, Marta Teperek, Olmo R van den Akker, Anna van't Veer, Raul Zurita-Milla, Towards wide-scale adoption of open science practices: The role of open science communities, *Science and Public Policy*, Volume 48, Issue 5, October 2021, Pages 605–611, https://doi.org/10.1093/scipol/scab039

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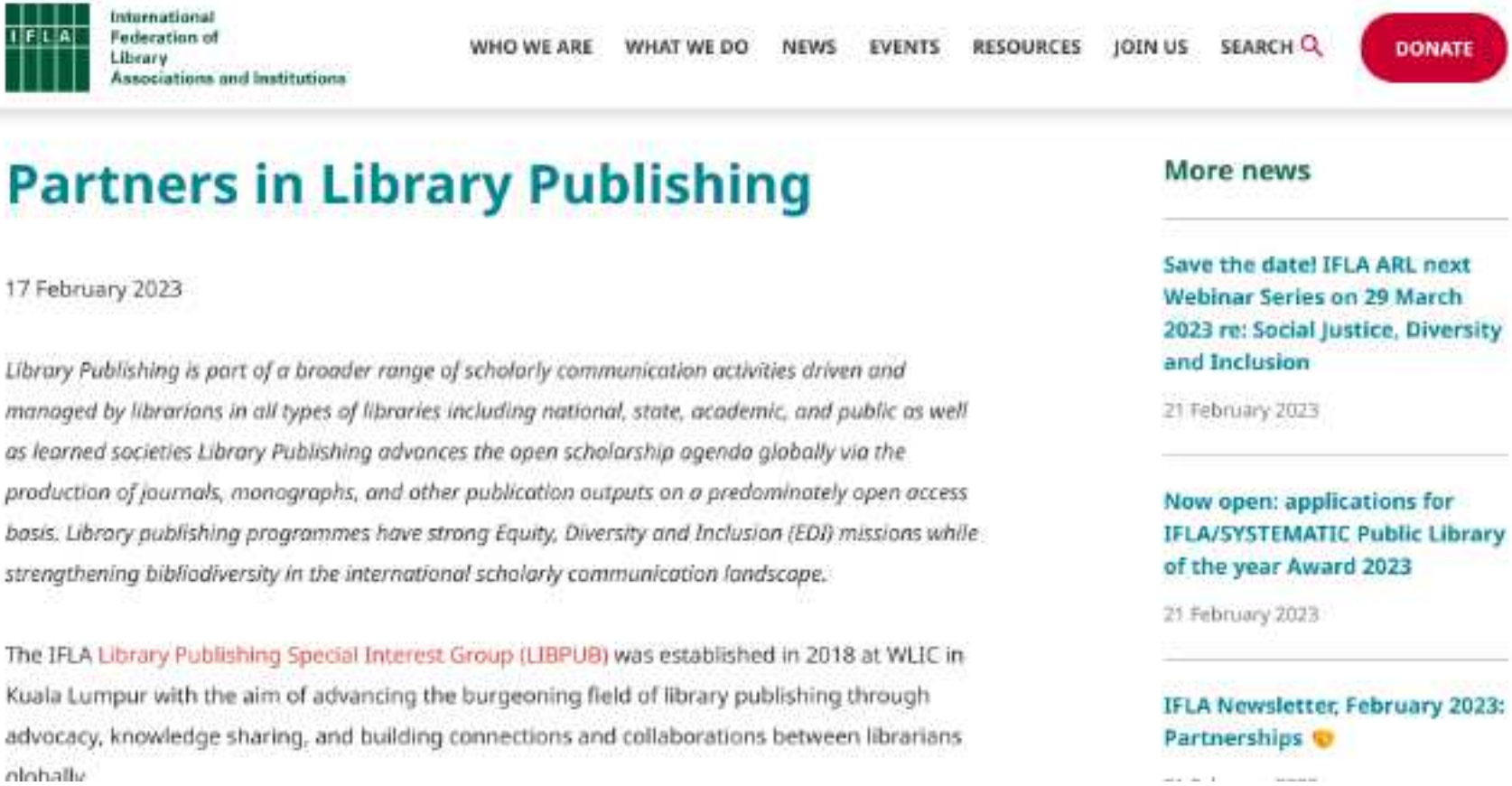
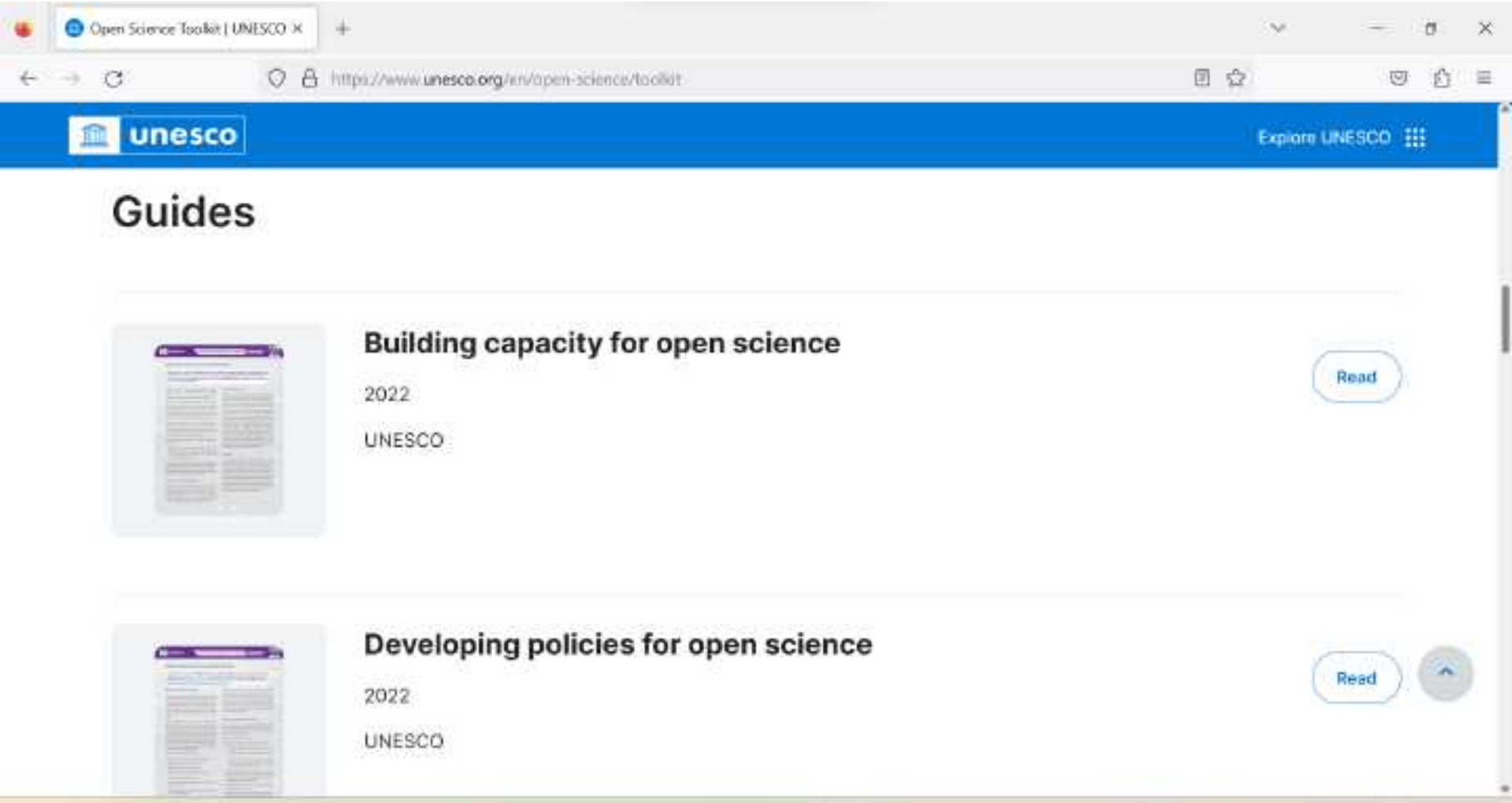
Marjan Grootveld, DANS
Pedro Principe, Minho University

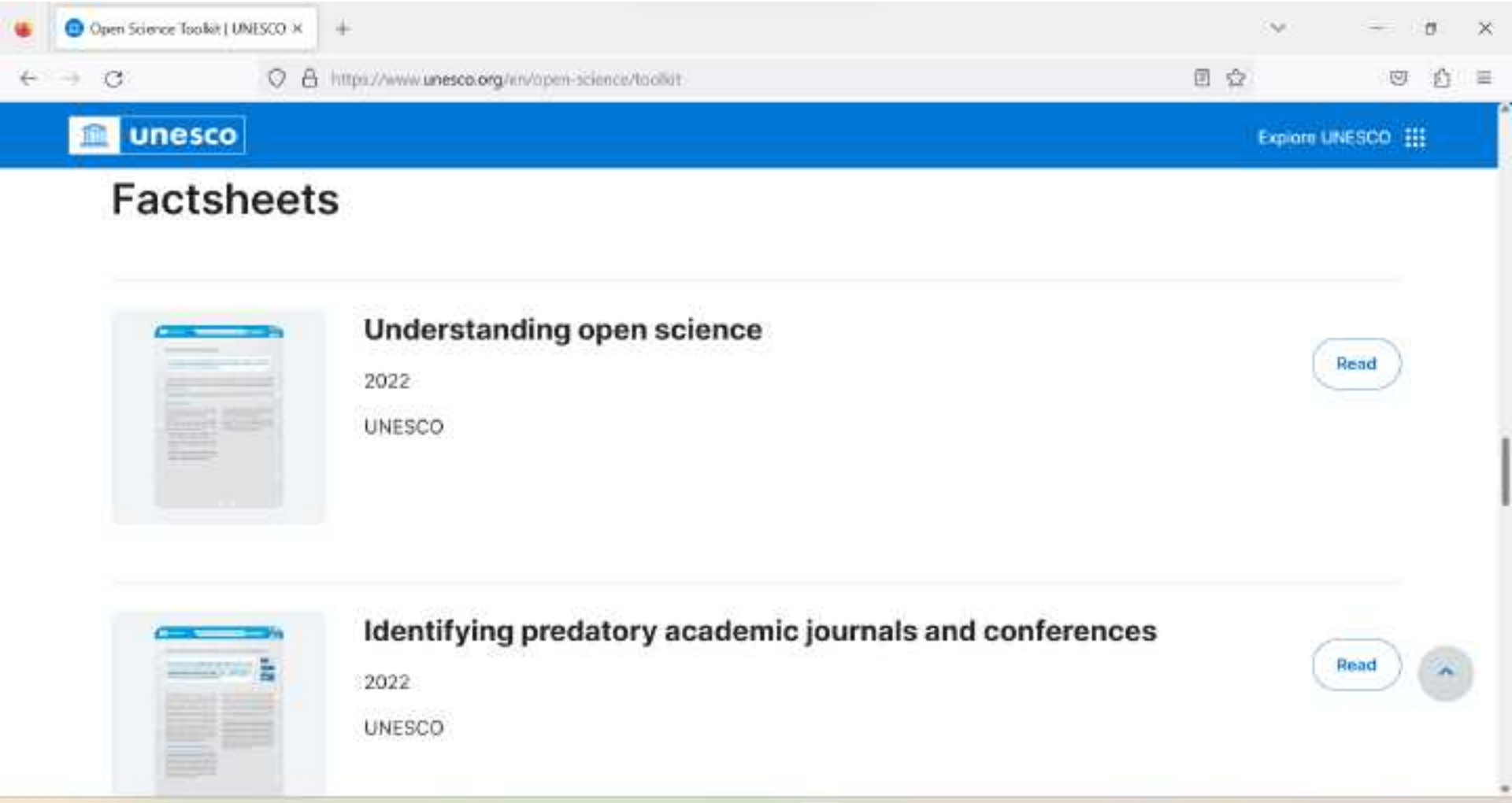
Librarians/research administrators as promoters/supporters of open science, obstacles to advocacy, finding space/resources for open science training, open science infrastructures, open access publishing support



https://www.ifla.org/news/partners-in-library-publishing/



https://www.unesco.org/en/open-science/toolkit



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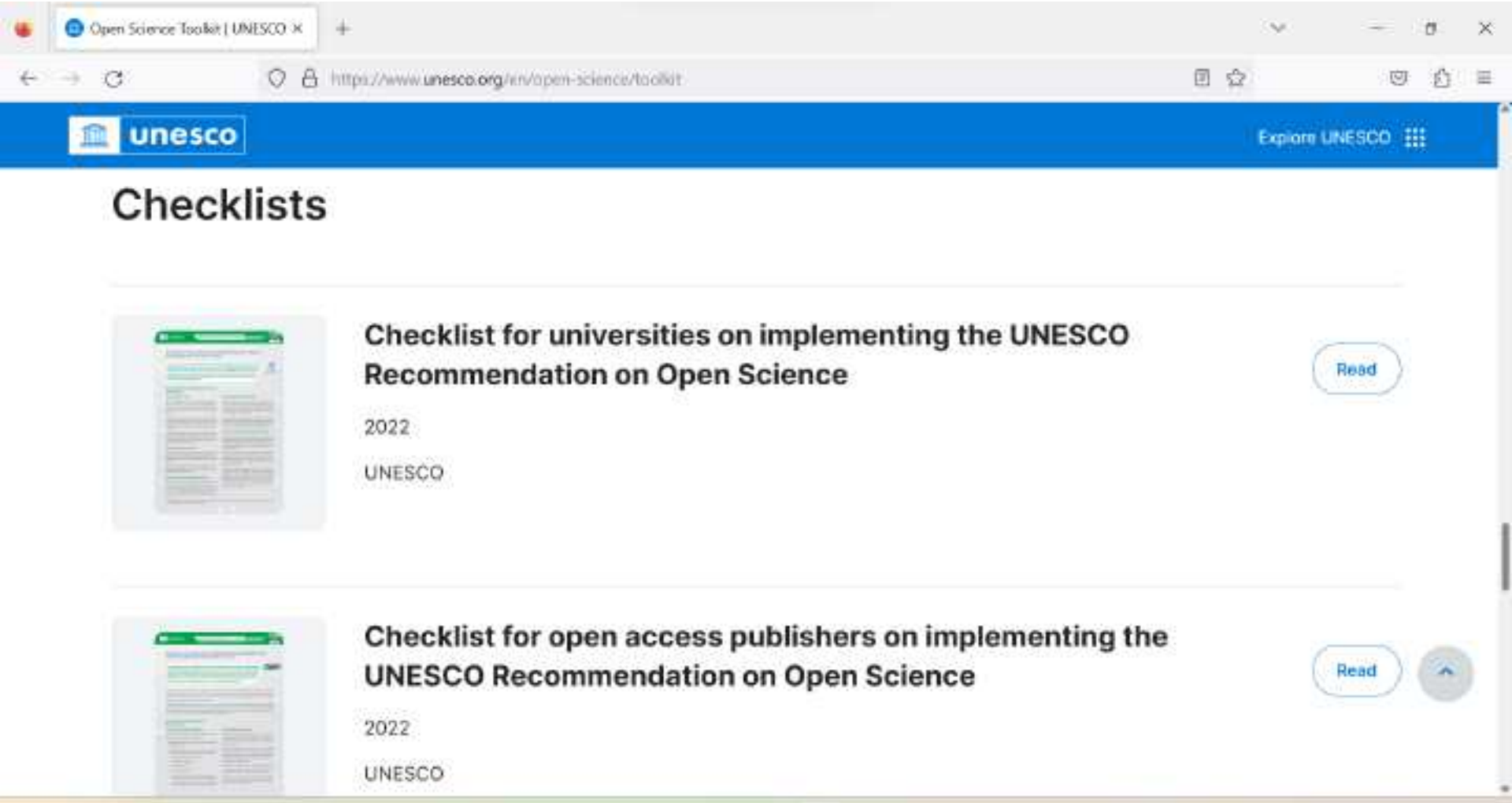
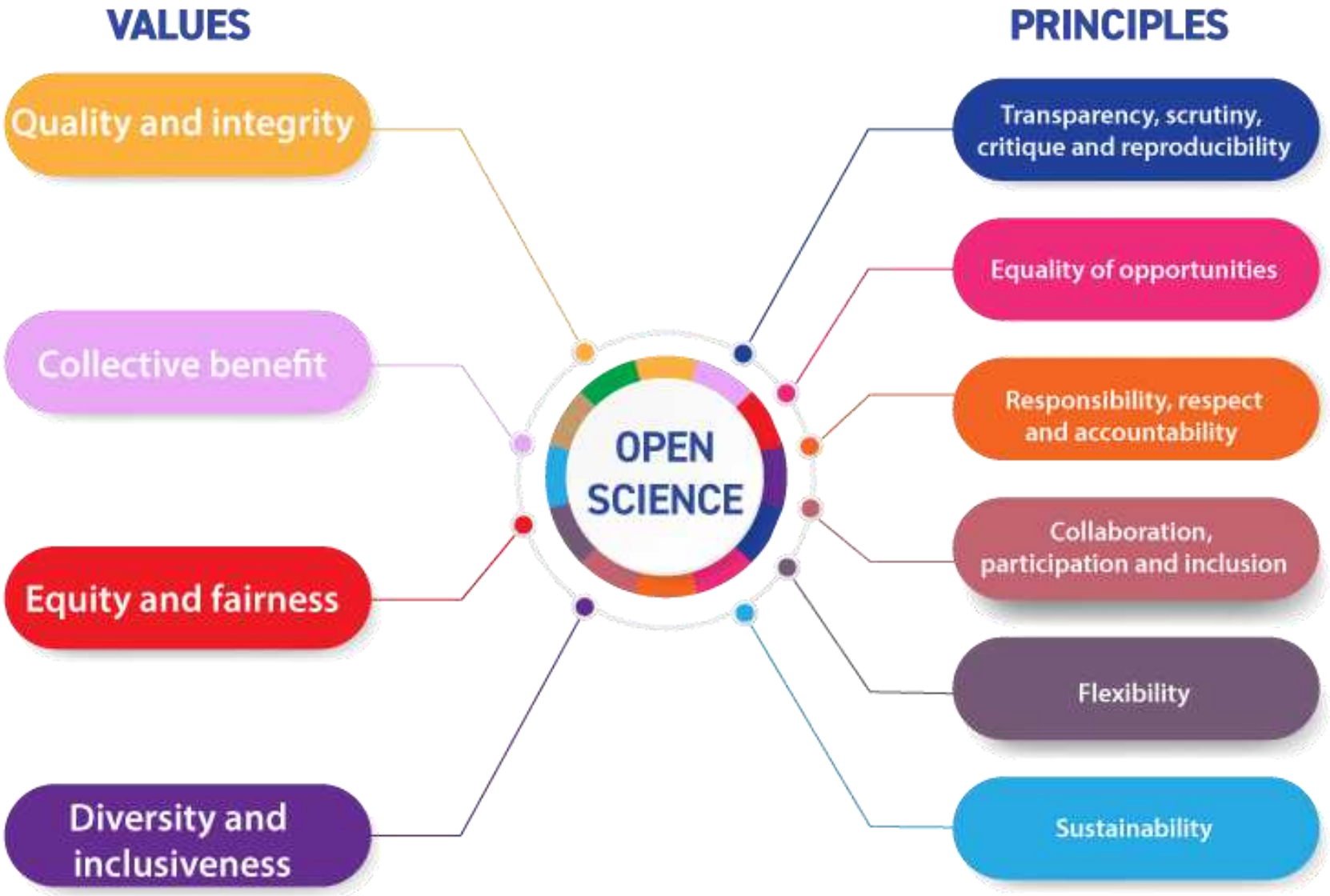


https://www.unesco.org/en/open-science/toolkit

Are your institutional values aligned with the core values of the UNESCO Recommendation on Open Science?




OPEN SCIENCE
Promoting a common understanding
Developing an Enabling policy environment
Fostering a culture of Open Science
Investing in human resources
Promoting innovative approaches
Promoting cooperation
Investing in infrastructures and services
AREAS OF ACTION

As a university practicing open science, how are you…

Nurturing open methods

Are the scientific practices at your university open by default? Are the innovators in your university encouraged and incentivized to make their practices and products open? Are newcomers to your institution introduced to open science early on?

It is possible to nurture open science from the bottom-up through capacity building and from the top-down through policy changes. Combinations of these approaches, such as mandates for training in open science, may be suitable in your context.

A clear understanding of the possibilities and risks of open science practices enable students, educators and researchers to make smarter decisions in a scientific system that is as open as possible, as closed as necessary.

Mainstreaming open practices

Rather than creating separate open science policies, it may be more efficient and effective to build openness into core policies for science, data management, educational resources and more.

Open science practices can also be mainstreamed into partnerships involving the university and external actors, including international partners.

Using and creating scientific infrastructures

Are the tools used by scientists and students at your institution openly available on open platforms? Infrastructures can be both physical and virtual. The UNESCO Recommendation on Open Science provides guidance for ensuring that access to

Thinking beyond scientific articles

Scientific practice spans far more than the production of data or articles. The Recommendation provides guidance for opening up all stages of the scientific process, from conceptualization and co-design of research projects through to post-publication communication.

Those scientific outputs related to publications[1] that are openly licensed or dedicated to the public domain should be deposited in a suitable open repository, following appropriate technical standards properly linking to the publications.

Supporting inclusive engagement and dialogue

Open science includes all scientific disciplines and aspects of scholarly practices and builds on four key pillars: open access to scientific knowledge, open science infrastructures, open engagement of societal actors and open dialogue with other knowledge systems.

There are multiple actors and stakeholders in research and innovation systems and each of them plays a role in the operationalization of open science. Similarly, universities serve many audiences in addition to academics and scientific researchers.

In practice, inclusive engagement ranges from addressing practical aspects of accessibility through to meaningful engagement with marginalized and underrepresented groups. Engagement and dialogue can inform not only education and the practices of open science but also the co-design, creation, use and production of scientific outputs in multiple formats.

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Do you incorporate the following areas of action into your university activities?

If not, have you planned a timetabled route to incorporate this area of action in the future?

The following text is from the UNESCO Recommendation on Open Science, through the lens of universities.

Promoting a common understanding of open science, associated benefits and challenges, as well as diverse paths to open science

☑ **Promote and support the common understanding of open science** as defined in this Recommendation, within the scientific community and among the different open science actors, and strategically plan and support open science awareness raising at the institutional, national and regional levels while respecting diversity of open science approaches and practices.

☑ **Ensure that publicly funded research is undertaken based on the principles of open science** in line with the provisions of this Recommendation, and that the scientific knowledge from the publicly funded research, including scientific publications, open research data, open

☑ **Enable open multi-stakeholder discussions on open science benefits and its real and apparent challenges** as regards, for example, competition, extraction and exploitation of data by more advanced technologies, links to intellectual property rights, privacy, security and inequalities between publicly and privately funded research, in order to address these challenges constructively and implement open science practices in line with the values and principles outlined in this Recommendation.

Developing an enabling policy environment for open science

☑ **Develop or encourage policy environments**, including those at the institutional, national, regional and international levels **that support operationalization of open science and effective implementation of open science practices,** including policies to incentivize open science practices among researchers. Through a transparent participatory, multi-stakeholder process that includes dialogue with the scientific community, especially early-career researchers, and other open science actors.

☑ **Develop effective institutional and national open science policies and legal frameworks** that are consistent with existing international and regional law and are in line with the definition, values and principles as well as actions outlined in this Recommendation.

software, source code and open hardware, is openly licensed or dedicated to the public domain.

☑ **Encourage bibliodiversity** through the diversity of formats and means of publications and diversity of business models, by supporting not-for-profit, academic and scientific community-driven publishing models as a common good.

☑ **Encourage multilingualism** in the practice of science, in scientific publications and in academic communications.

☑ **Ensure that the needs and rights of communities**, including the rights of indigenous peoples over their traditional knowledge, **should not be infringed on in open science practices.**

☑ **Enhance open science communication** to support the dissemination of scientific knowledge to scholars in diverse research fields, decision makers and the public at large.

☑ **Engage the private sector in the discussion** about the ways in which the scope of open science principles and priorities can be enlarged and mutually shared.

☑ **Align open science policies, strategies and actions from individual institutions to local and international levels**, while respecting the diversity of open science approaches.

☑ **Mainstream gender equality aspects** into open sciences policies, strategies and practices.

☑ **Implement policies and strategies for open science**.

☑ **Enhance the inclusion of citizen and participatory science as integral parts of open science policies and practices** at the national, institutional and funder levels.

☑ **Design models that allow co-production of knowledge with multiple actors** and establish guidelines to ensure the recognition of nonscientific collaborations.

☑ **Encourage responsible research and researcher evaluation and assessment practices**, which incentivize quality science, recognizing the diversity of research outputs, activities and missions.

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Investing in human resources, training, education, digital literacy and capacity building for open science

☑ **Provide systematic and continuous capacity building on open science concepts and practices**, including broad comprehension of the open science guiding principles and core values as well as technical skills and capacities in digital literacy, digital collaboration practices, data science and stewardship, curation, long-term preservation and archiving, information and data literacy, web safety, content ownership and sharing, as well as software engineering and computer science.

☑ **Agree on a framework of open science competencies** aligned with specific disciplines for researchers at different career stages, as well as for actors active in the private and public sectors or in civil society, who need specific competences to include the use of open science products in their professional careers; and develop recognized skills and training programmes in support of the attainment of these competencies. A core set of data science and data stewardship skills, skills related to intellectual property law, as well as skills needed to ensure open access and engagement with society, as appropriate, should be regarded as part of the foundational expertise of all researchers and incorporated into higher education research skills curricula.

☑ **Support science communication accompanying open science practices** with a view to the dissemination of scientific knowledge to scholars in other research fields, decision-makers and the public at large. Dissemination of scientific information through scientific journalism and media, popularization of science, open lectures and various social media communications builds public trust in science while increasing the engagement of societal actors beyond the scientific community. To avoid misinterpretation and dissemination of misinformation, the quality and appropriate citation of original sources of information are of paramount importance to science communication as regards open science.

Fostering a culture of open science and aligning incentives for open science

☑ **Engage actively in removing the barriers for open science, particularly those relating to research and career evaluation and awards systems**. Assessment of scientific contribution and career progression rewarding good open science practices is needed for operationalization of open science. Attention should also be given to preventing and mitigating the unintended negative consequences of open science practices, such as predatory behaviours, data migration, exploitation and privatization of research data, increased costs for scientists and high article processing charges associated with certain business models in scientific

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☑ **Invest in and promote advanced education and the professionalization of roles in data science and data stewardship.** Enabling open science also requires data governors capable, in cooperation with the scientific community, of setting strategic directions for data management and openness at the national or local levels and advanced and professional data stewards who manage and curate data according to agreed principles, notably FAIR and CARE principles, within trusted institutions or services. In order to take advantage of the opportunities offered by open science, research projects, research institutions and civil society initiatives need to call on advanced data science skills including analysis, statistics, machine learning, artificial intelligence, visualization and the ability to write code and use algorithms with scientific and ethical responsibility.

☑ **Promote the use of open educational resources** (OER), as an instrument for open science capacity building. OER should therefore be used to increase access to open science educational and research resources, improve learning outcomes, maximize the impact of public funding and empower educators and learners to become co-creators of knowledge.

publishing that may be causes of inequality for the scientific communities around the world and, in some cases, the loss of intellectual property and knowledge.

☑ **Combine efforts** of many different stakeholders, including research funders, universities, research institutions, publishers and editors, and scientific societies across disciplines and countries, to change the current research culture and to recognize researchers for sharing, collaborating and engaging with other researchers and society, and to support, in particular, early-career researchers to drive this cultural change.

☑ **Review research assessment and career evaluation systems in order to align them with the principles of open science**. Considering that a commitment to open science requires time, resources and efforts that cannot be automatically converted into traditional academic output, such as publications, but which can have a significant impact on science and society, evaluation systems should take into account the wide breadth of missions within the knowledge creation environment. These missions come with different forms of knowledge creation and communication, not limited to publishing in peer reviewed international journals.

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☑ **Promote the development and implementation of evaluation and assessment systems** that:

- ☑ Build on the existing efforts to improve the ways in which the scientific outputs are evaluated, such as the 2012 San Francisco Declaration on Research Assessment, with an increased focus on the quality of research outputs rather than quantity, and by fit-for-purpose use of diversified indicators and processes that forego the use of journal based metrics such as the journal impact factor;
- ☑ Give value to all relevant research activities and scientific outputs including high-quality FAIR data and metadata, well-documented and reusable software, protocols and workflows, machine-readable summaries of findings, and teaching, outreach and engagement of societal actors;
- ☑ Take into account evidence of research impact and knowledge exchange, such as widening participation in the research process, influence on policy and practice and engaging in open innovation with partners beyond academia;
- ☑ Take into account the fact that diversity of disciplines requires different approaches in open science;
- ☑ Take into account the fact that assessment of researchers against open science criteria should be fit for different stages of careers, with particular attention to researchers at the beginning of their careers.

☑ **Ensure that the practice of open science is well known and is taken into account as a scientific and academic recruitment and promotion criterion.**

☑ **Adopt policies that require and reward open access** to scientific knowledge, including scientific publications, open research data, open software, source code and open hardware, in line with the provisions of this Recommendation

☑ **Promote materials that are in the public domain and existing open licensing schemes, copyright and other intellectual property exceptions** for research and educational uses that allow distribution and re-use of a copyright work, or work subject to other intellectual property protection, including partial or derivative use, on the condition that the creator is appropriately credited, in accordance with international law.

☑ **Promote high-quality and responsible research and explore the potential of open science practices to reduce scientific misconduct,** including the fabrication and falsification of results, violation of scientific ethical norms, and plagiarism.

Promoting innovative approaches for open science at different stages of the scientific process

☑ **Promote open science from the outset of the research process** and extend the principles of openness in all stages of the scientific process to improve quality and reproducibility, including the encouragement of community-driven collaboration and other innovative models, for example preprints clearly distinguished from final peer-reviewed publications, and respecting the diversity of scientific practices, in order to accelerate dissemination and encourage rapid growth in scientific knowledge.

☑ **Promote, as appropriate, open peer review evaluation practices** including possible disclosure of the identity of the reviewers, publicly available reviews and the possibility for a broader community to provide comments and participate in the assessment process.

☑ **Encourage and value publication and sharing of negative scientific results** and those that do not conform to the results expected by the researchers who carried them out, and data associated with them, as these results also contribute to the advancement of scientific knowledge.

EMPOWER
High-level policy/strategy

This section outlines a series of actions that university leaders can take, independently or jointly, to catalise OA throughout the institution.

Actions

1. Discuss the benefits of OA implementation (and its challenges) with university members
2. Adopt a policy that includes a Rights Retention Statement
3. Add OA criteria in academic assessment
4. Monitor APC costs. Centralise and streamline APC reporting. Assign funding for OA publishing*
5. Support non-commercial, scholar-led publishing initiatives (Diamond OA)*
6. Advocate policy change by governments and funders

BUILD CAPACITY
Libraries and consortia

This section includes a series of actions that university libraries, consortia and publishers can take to accelerate OA output, including different types of agreements.

Actions

1. Monitor APC costs. Centralise and streamline APC reporting*
2. Enter into a publishing agreement with a pure OA publisher
3. Enter into a transformative agreement (TA) with a smaller or society publisher
4. Enter into a transformative agreement (TA) with a large publisher

REINFORCE EXISTING STRUCTURES
Academic community-driven Infrastructures

This section includes a series of actions that institutions can take to support scholarly-led initiatives on OA, to accelerate OA output.

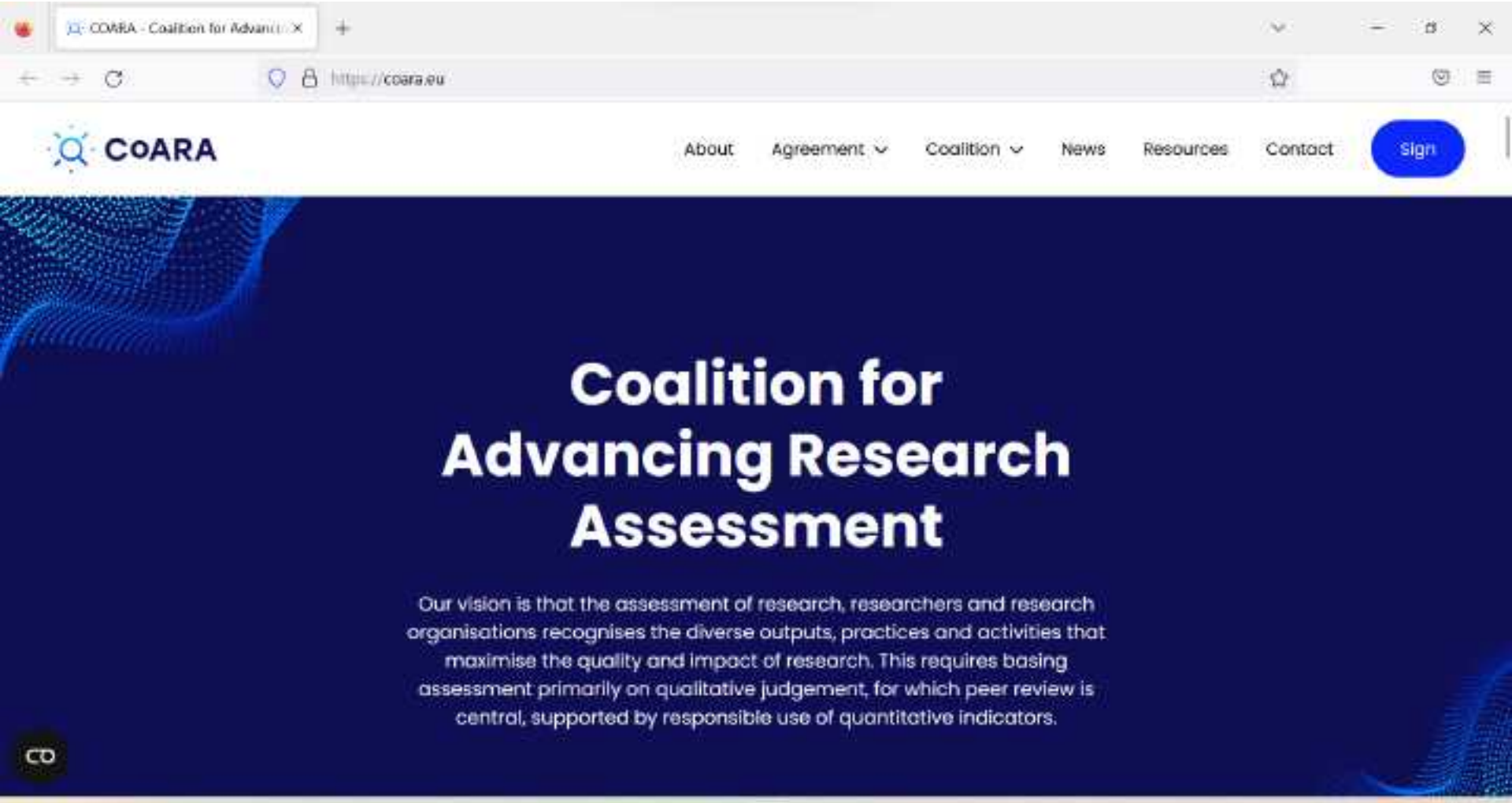
Actions

1. Support non-commercial, scholar-led publishing initiatives (Diamond OA)*
2. Support non-commercial infrastructure for scholarly communication
3. Develop and use an institutional (or shared) OA repository

* These actions fall under more than one goal. Their description has been slightly adapted to the different goals and target groups.

https://eua.eu/resources/publications/986:the-new-university-open-access-checklist.html

The EUA Open Science Agenda 2025 https://eua.eu/downloads/publications/eua%20os%20agenda.pdf



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Thank you!
Questions?

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