# Enabling reproducible research: community practices, service needs and first lessons learnt

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Reproducibility Workshop @TPDL Hanover, September 2016



# Agenda

Introduction

Terminology

Pragmatic approach

Perspectives (researcher, publisher, libraries, funder)

Use case: one research community

Service requirements

Challenges

**CERN** Open Data and Analysis Preservation

Lessons learnt





# Terminology

Repeatability

Replicability

Reproducibility

Conditions very discipline specific

Reusability

Repurposing

In order to reuse/repurpose results, you sometimes have to reproduce the original results first (to understand the exact details [1])

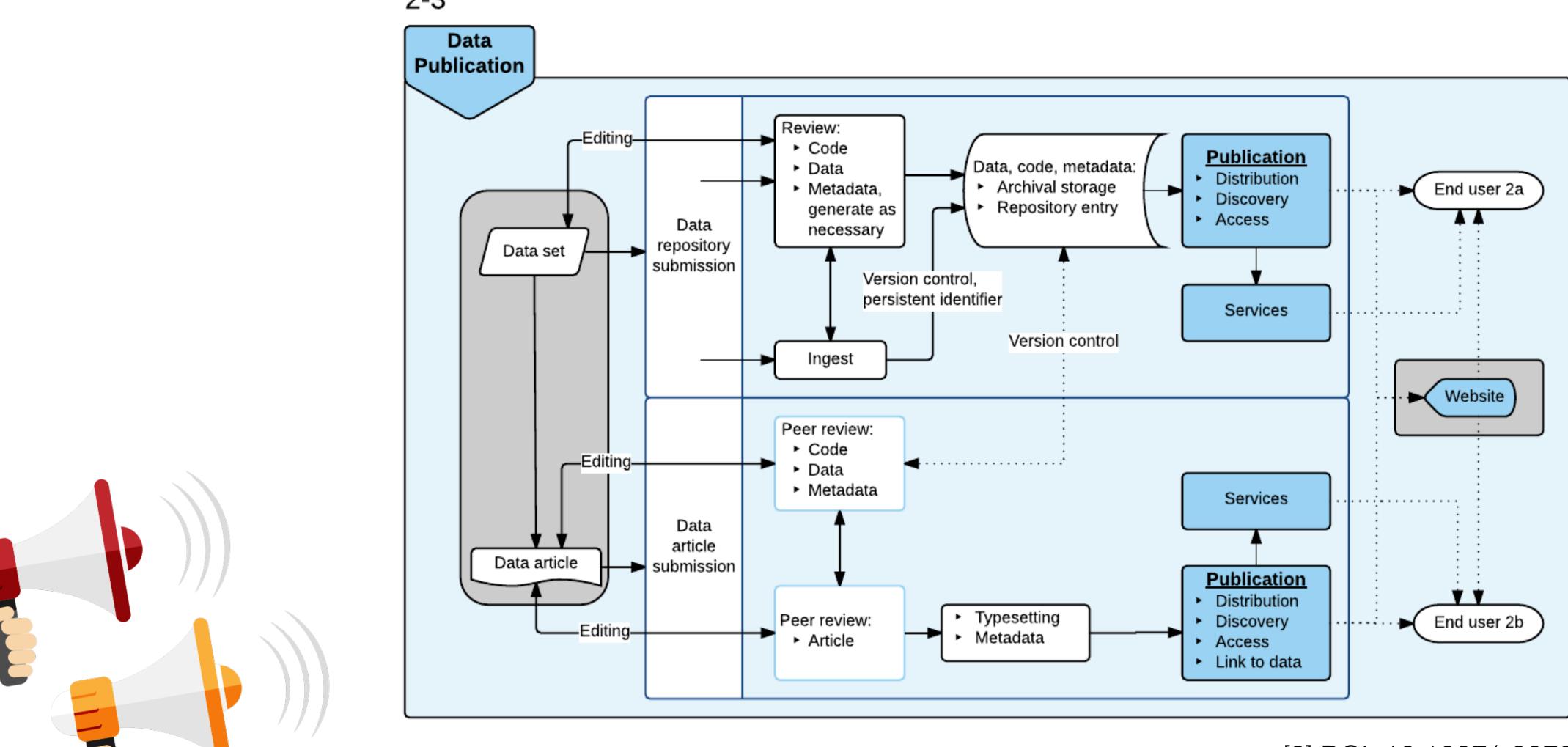


To reproduce or reuse research results a researcher needs...

- More than "just" the article \_
- Context, documentation
- Links to related research objects: data, code, workflows
- Understandable method, processing, software etc.
- Steps taken during the research process (versions)



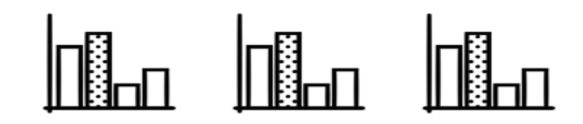
# A data publishing perspective: establishing context



<sup>2-3</sup> 

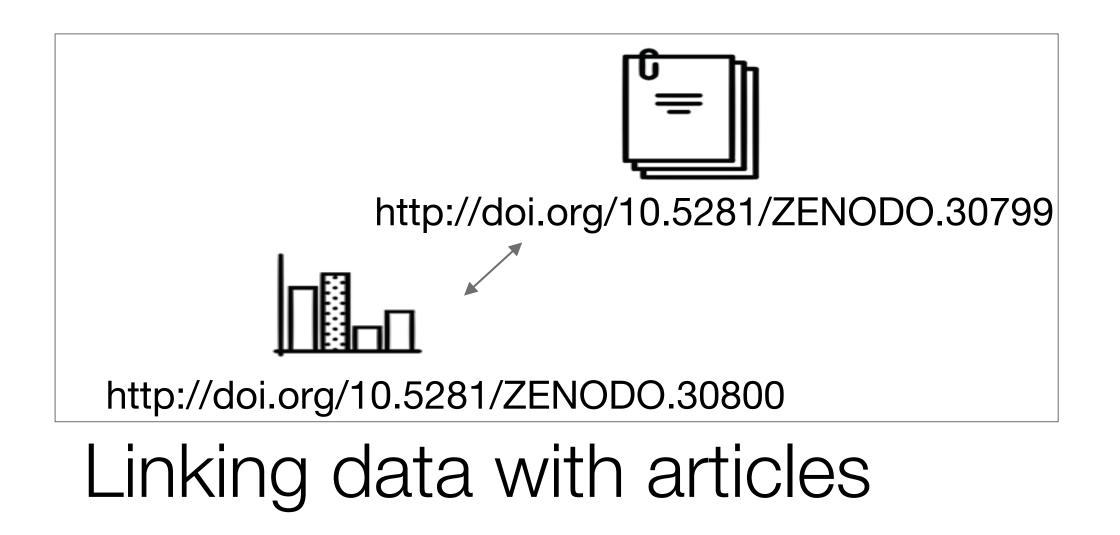
[2] DOI: 10.1007/s00799-016-0178-2

# Helicopter view: Trusted bridges across research life-cycle

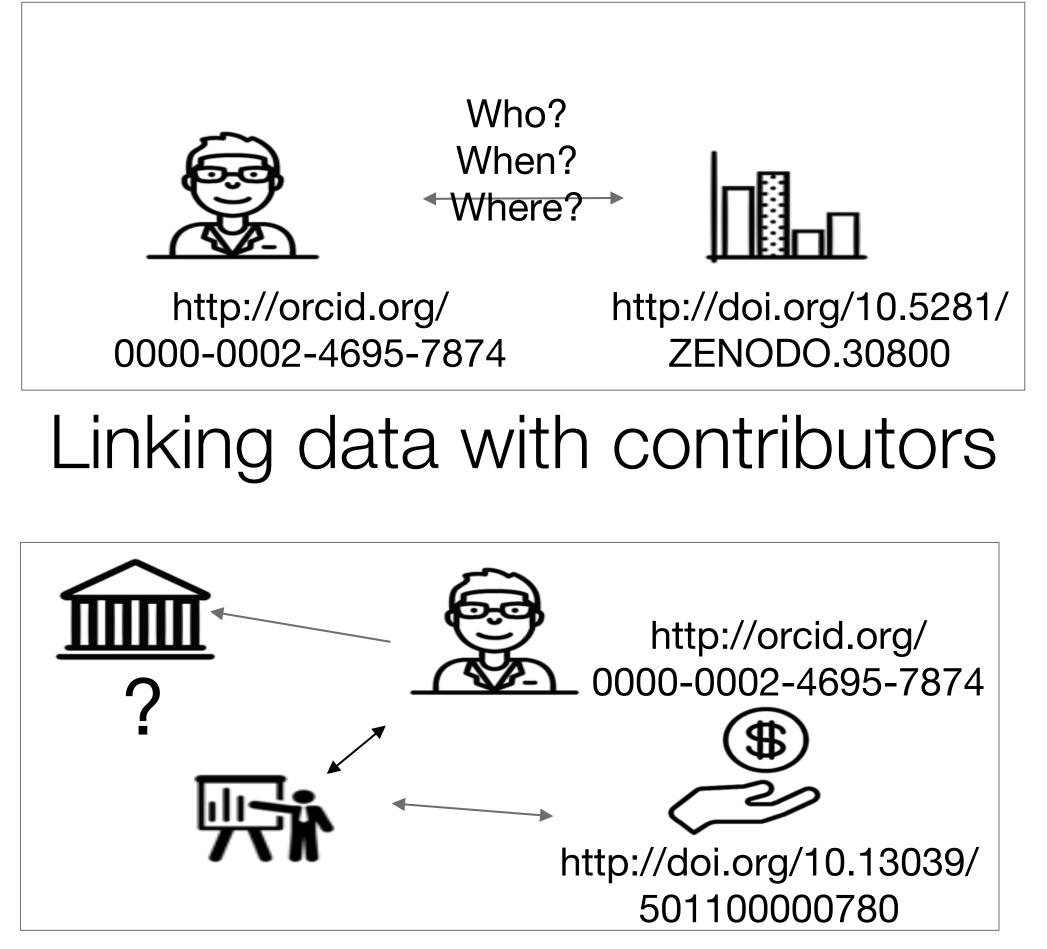


Subsets of Data Multiple Versions Dynamic Data

# Linking data with data







Linking data with institutions/funders

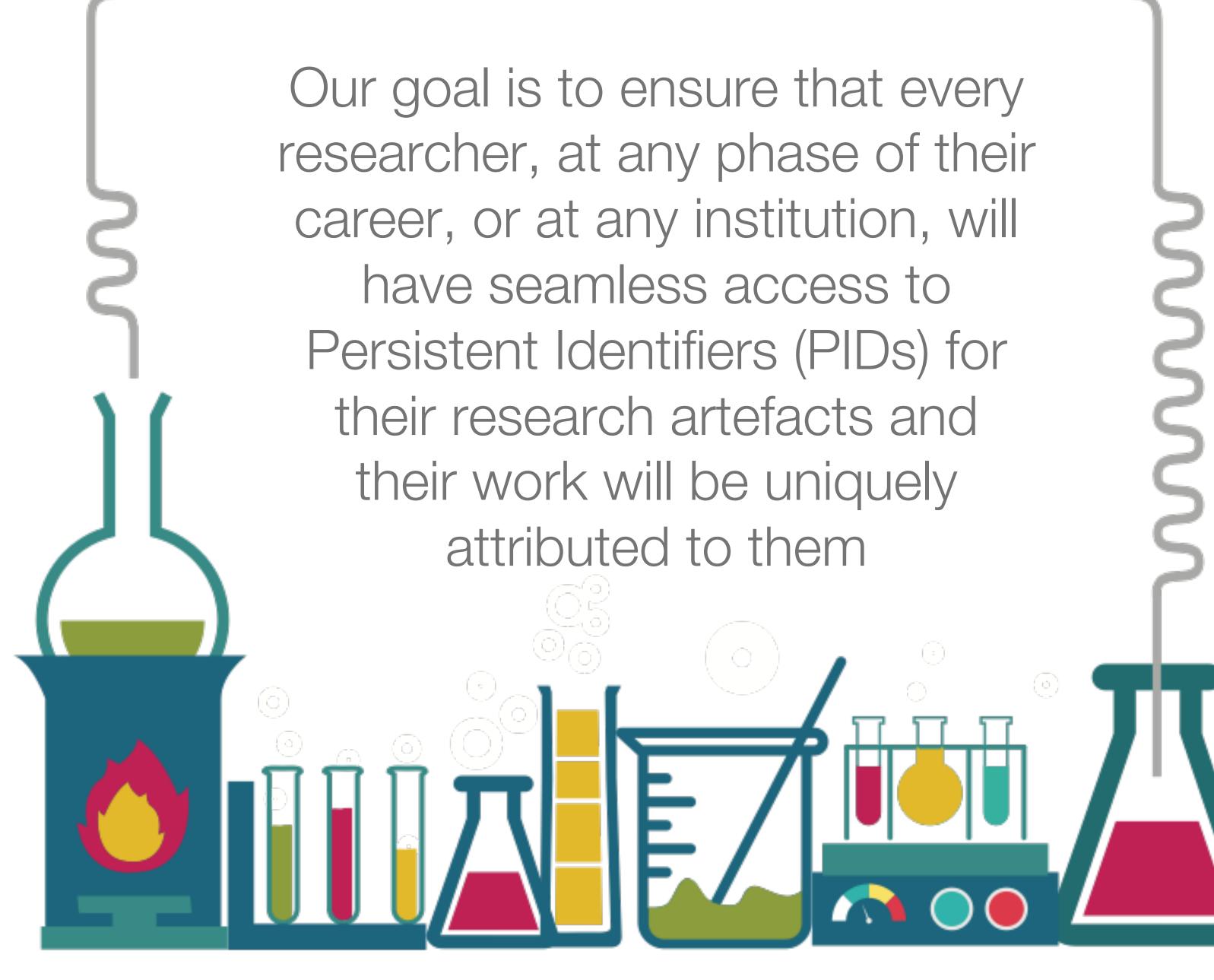
# Slide credit to Trisha Cruse, Datacite





# Technical and Human infrastructure for Open Research

https://project-thor.eu/



Our goal is to ensure that every researcher, at any phase of their career, or at any institution, will have seamless access to Persistent Identifiers (PIDs) for their research artefacts and their work will be uniquely attributed to them





# Use Case: High-Energy Physics Community

Discussions, requirements and emerging services



# CERN

#### Founded in 1954

Intergovernmental research organization

22 members states

~2500 employees

12,000 visiting scientists fromover 70 countries and with120 different nationalities

A different dimension of "collaborative research"



# A use case: High Energy Physics

- Small community, data driven
- Every experimental analysis with complex and big data and software pieces
- Experience with Open Access (it is the de facto default, in fact)
- Little or no experience with Open Science
- The usual: high throughput of personnel •

There is only one LHC in the world: What does that mean for .... reproducibility and replicability of an analysis?

- Surely it is work intensive, lots of dependencies
- What is needed? What makes sense for science?



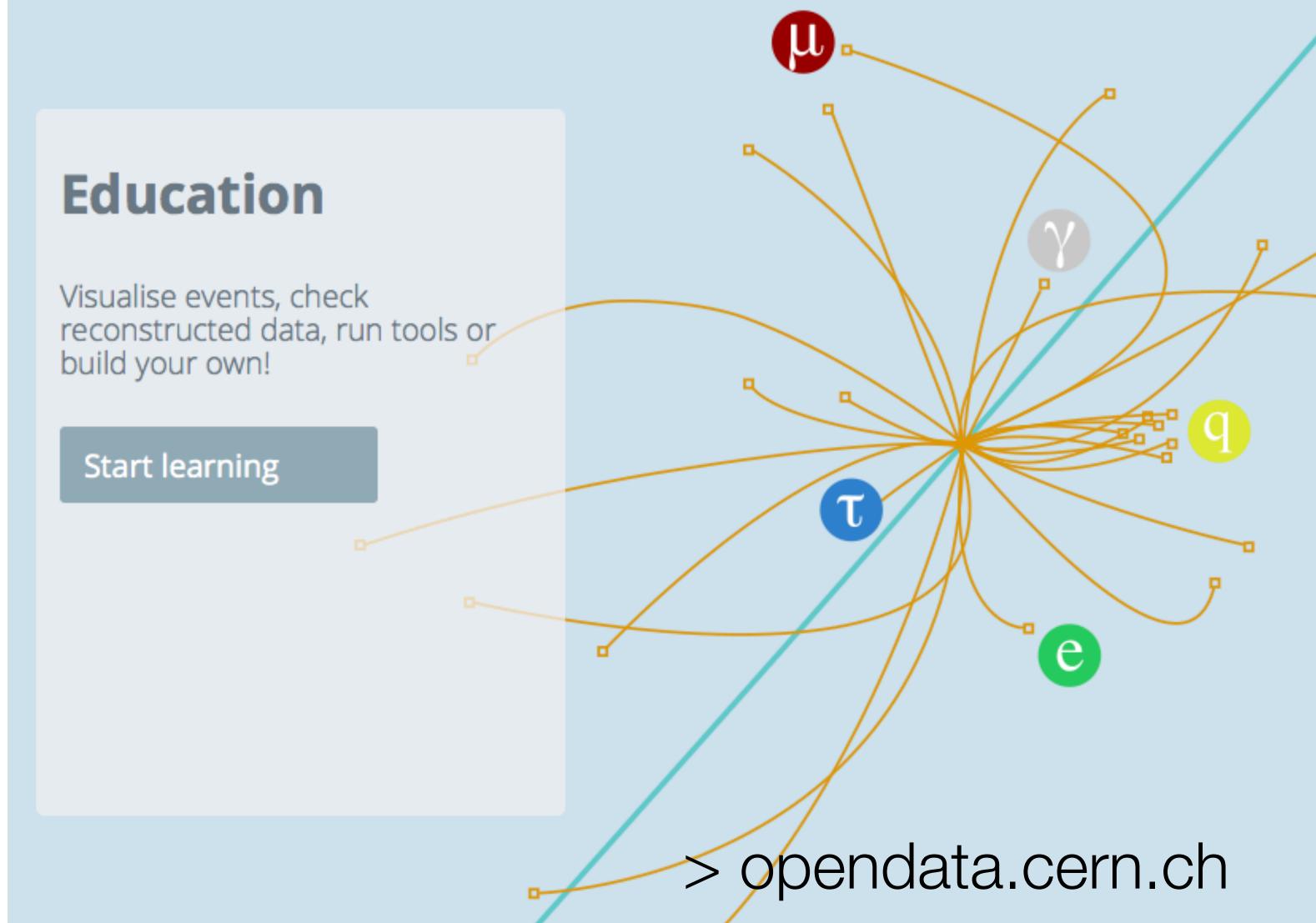
# First requirements

- Link articles and data/software, enable data discovery
- Incentivize open data and code sharing (data/software citation)

- Build further connections early in the research process → towards a network of research objects
  - That enable collaborators to understand the research context
  - That can be searched for (internally) to accelerate research processes
  - Preservation







#### ABOUT SEARCH EDUCATION RESEARCH

## Research

Get the genuine working environments, virtual machines and datasets to start your research

Start analysing

# Impact

### The Washington Post

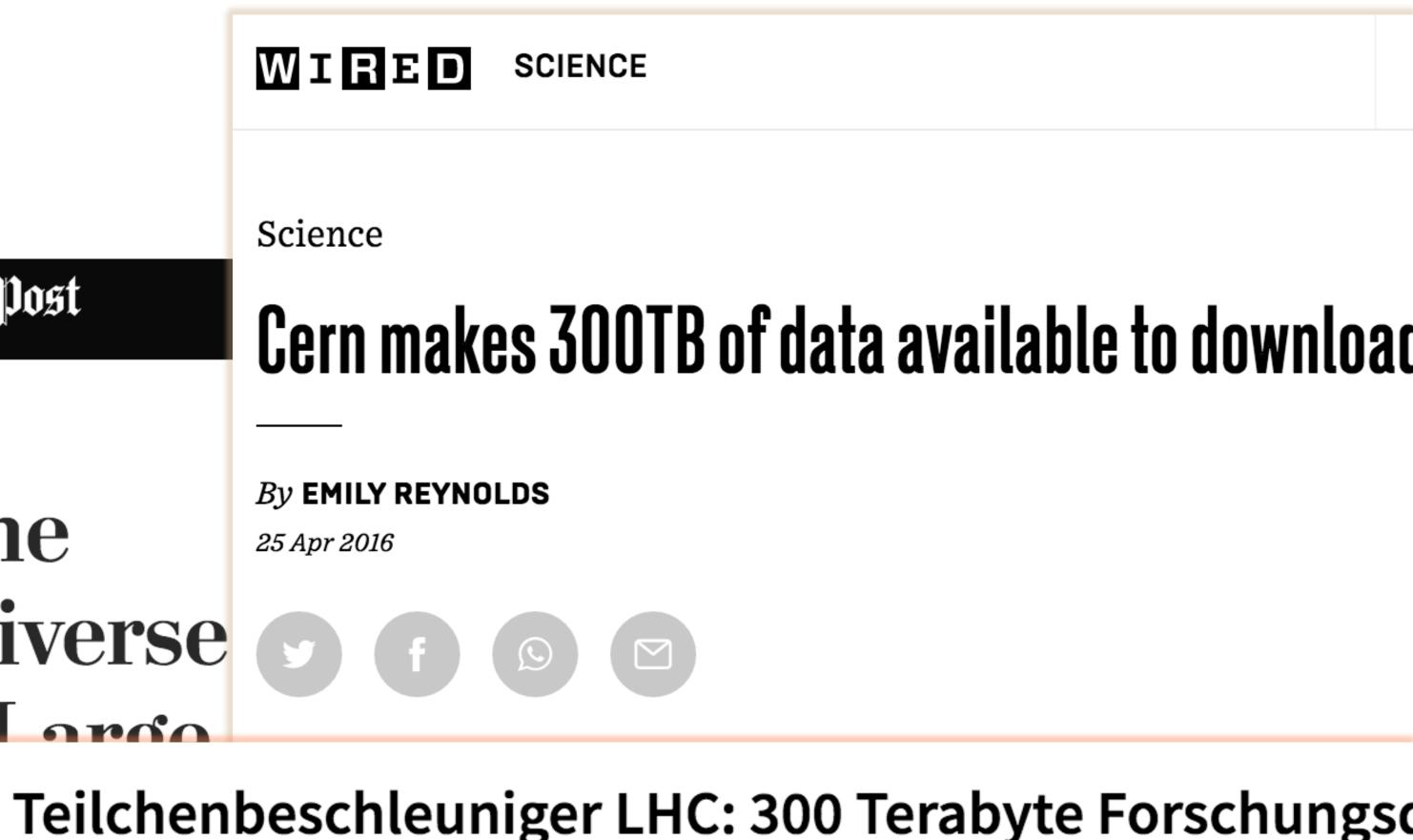
**Speaking of Science** 

## **Open sourcing the** 25 Apr 2016 secrets of the universe huge amount of I and Hadron Collider freigegeben now online

By Sarah Kaplan April 26 🔽







heise online 26.04.2016 11:34 Uhr – Martin Holland







#### Aad, Georges et al. **Q** Browse all

#### Kernel And Antiparties Anti

Measurement of the dependence of transverse energy production at large pseudorapidity on the hardscattering kinematics of protonproton collisions at  $\sqrt{s} = 2.76$ TeV with ATLAS

Aad, Georges, Abbott, Brad, Abdallah, Jalal, Abdinov, Ovsat, Aben, Rosemarie, Abolins, Maris, AbouZeid, Ossama, Abramowicz, Halina , Abreu, Henso, Abreu, Ricardo ATLAS

Phys.Lett. B756 (2016) 10-28, 2016

http://dx.doi.org/10.17182/hepdata.71318

DOI

View paper in Inspire

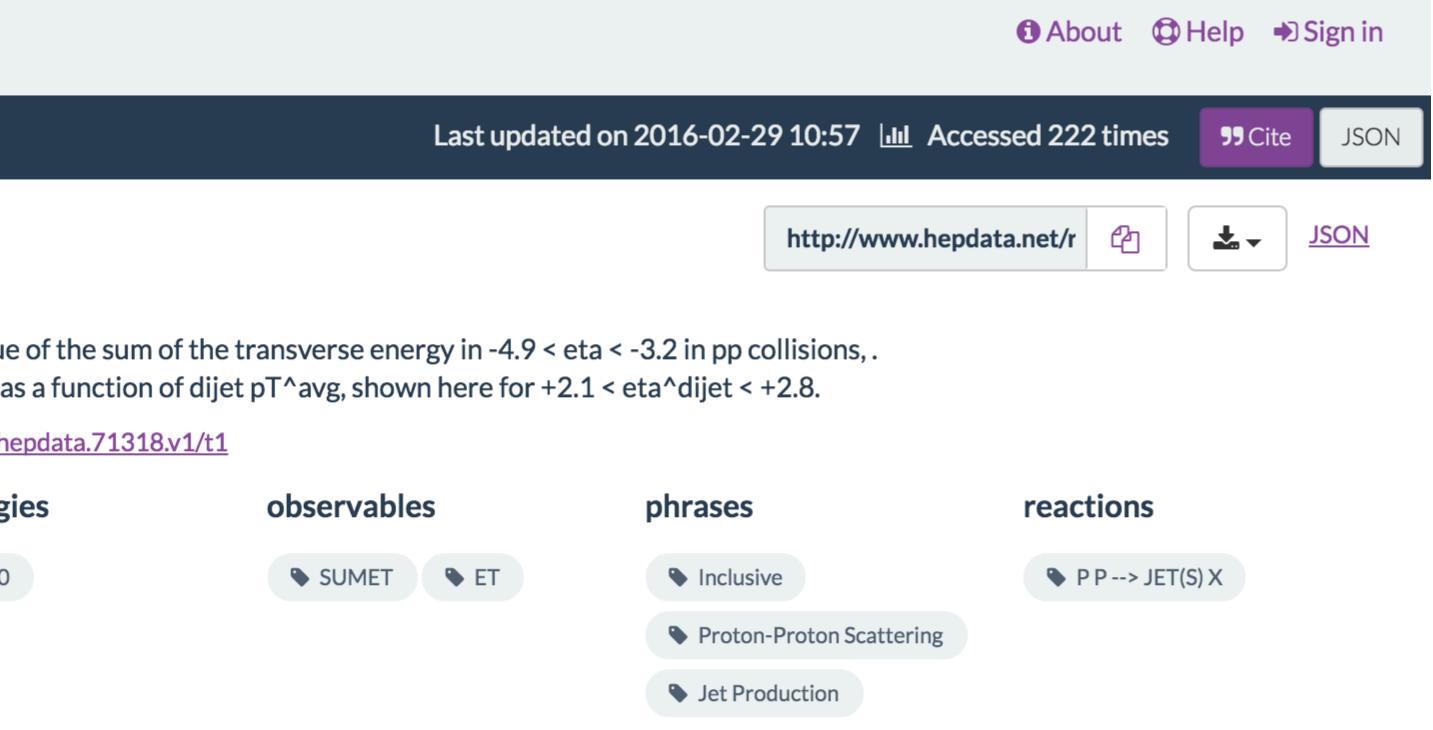
View old HepData

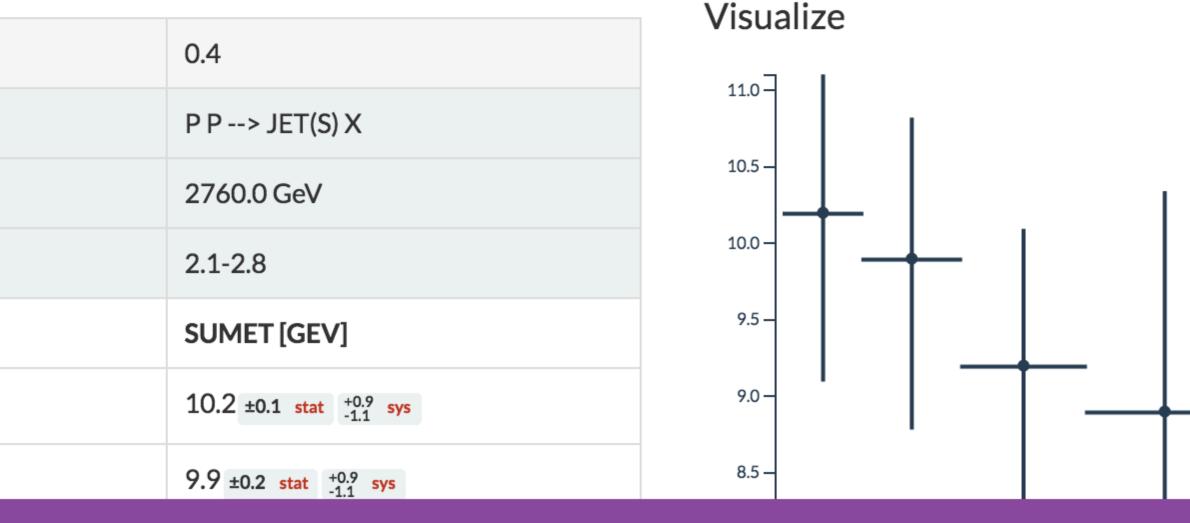
#### Abstract (data abstract)

CERN-LHC. The relationship between jet production in the central region and the underlying-event activity in a pseudorapidityseparated region is studied in 4.0  $pb^{-1}$  of  $\sqrt{s} = 2.76$  TeV pp collision data recorded with the ATLAS detector at the LHC. The underlying

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collisions, <sumet>.</sumet>		63.10 - 79.40		

Copyright ~1975-Present HEPData, funded by STFC, UK, developed and hosted at CERN, supported by IPPP Durham. Terms of Use.





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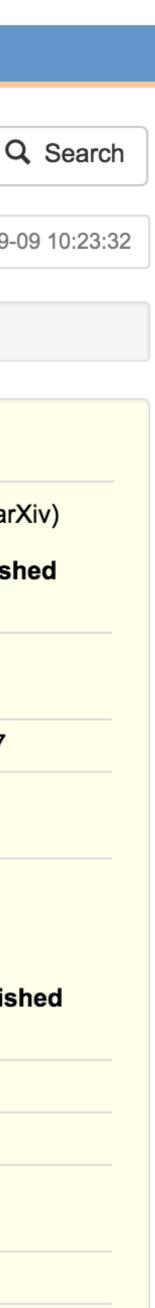


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	/iew Profile	Manage Profile Manage	Publications Help
P	ERSONAL INFOR	MATION	PUBLICATIONS AND OUTPUT
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	Name	Kyle S. Cranmer	1. Data from figure 1 from: Search for glu
	Current Institution	New York U.	leptons, jets and missing transverse m $pp$ collisions at $\sqrt{s} = 7$ TeV 2. Data from figure 1 from: Search for glu
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	Identifiers	BAI: K.S.Cranmer.1 INSPIRE: INSPIRE-00074922	
		ORCID: 0000-0002-5769-7094	Co-Authors
	Period 5	ARXIV: cranmer_k_1	B.Mellado.1 (13) W.Quayle.1 (11) C.T.Potter 1 (9)

Welcome to INSPIRE, the High Energy Physics information system. Please direct questions, comments or concerns to feedback@inspirehep.net.

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# Barriers to practicing reproducible research

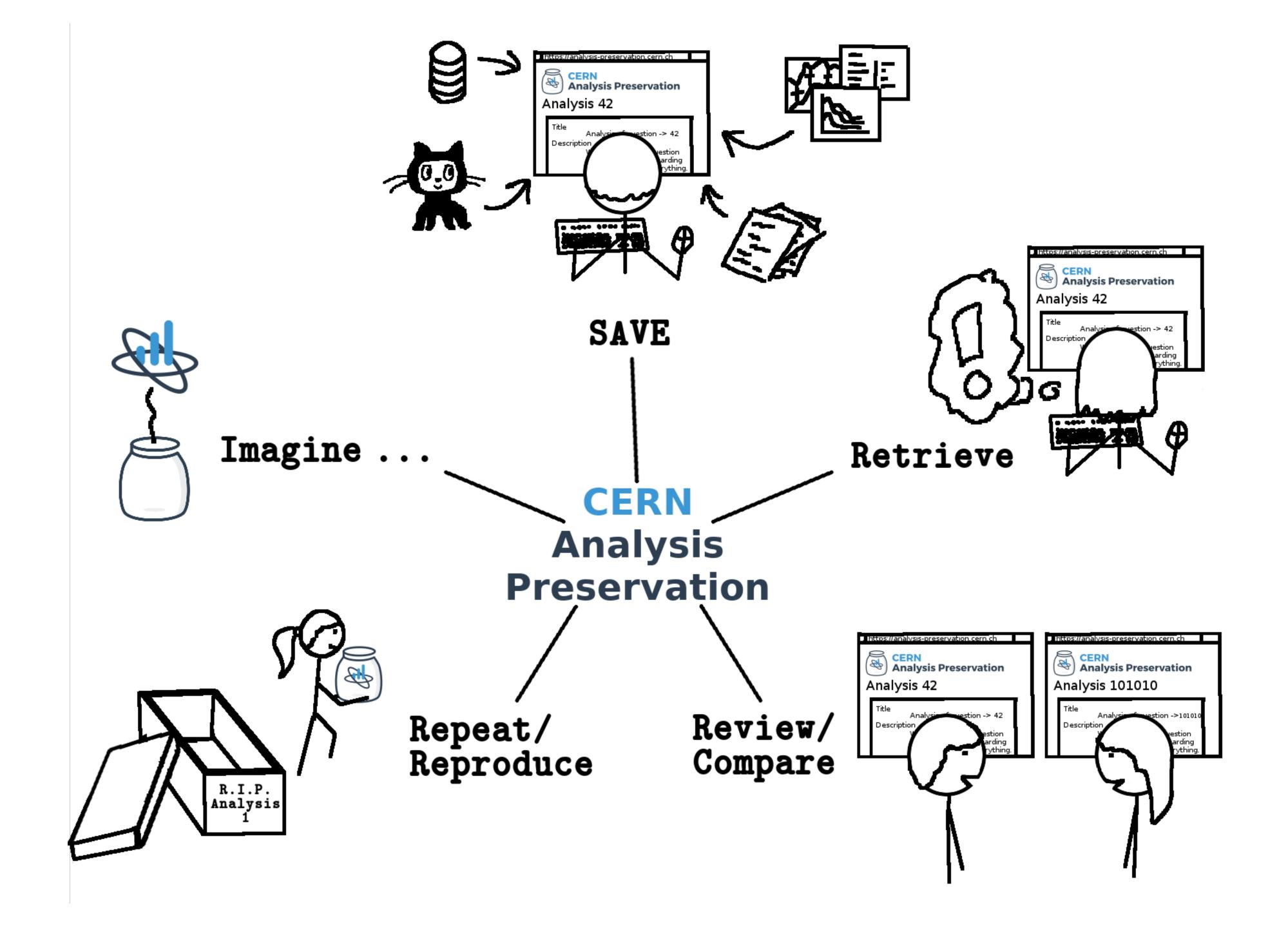
"We find that code, data, and ideas are each regarded differently in terms of how they are revealed and that guidance from scientific norms varies with pervasiveness of computation in the field.

The largest barriers to sharing are time involved in preparation of work and the legal Intellectual Property framework scientists face." [6]

# Moving upstream

In the research lifecycle





# Considerations for service providers

- Future purpose: reuse, reproducibility, preservation
- What are the components of an analysis (where are they stored now)
- How much do these components vary within the collaboration
- How is quality defined
- What are the dependencies (software, methods)
- Versioning
- Linking
- Size (10-15TB per analysis)









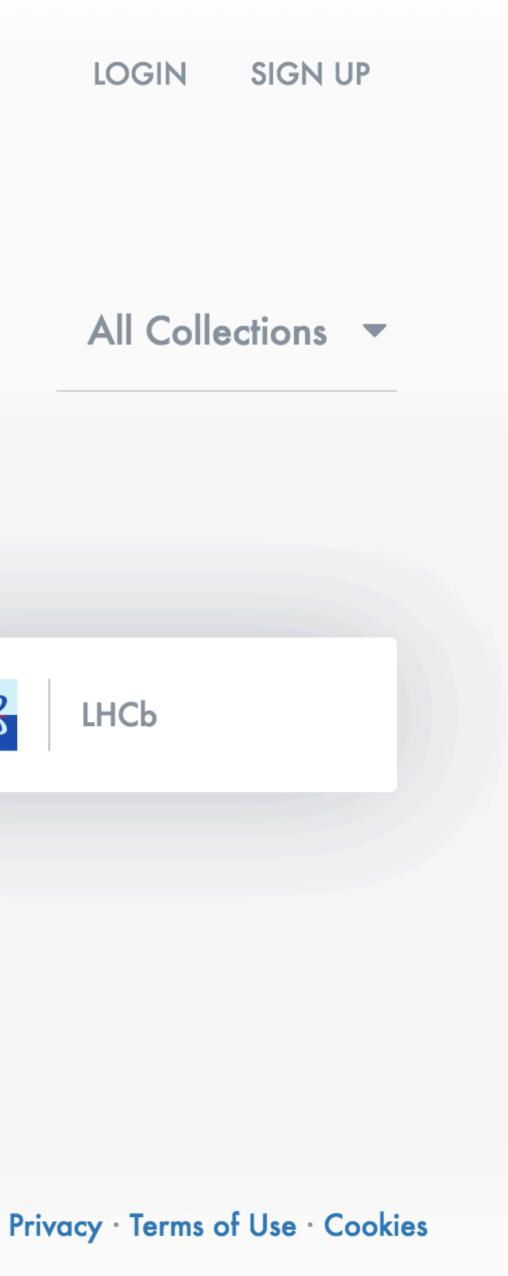
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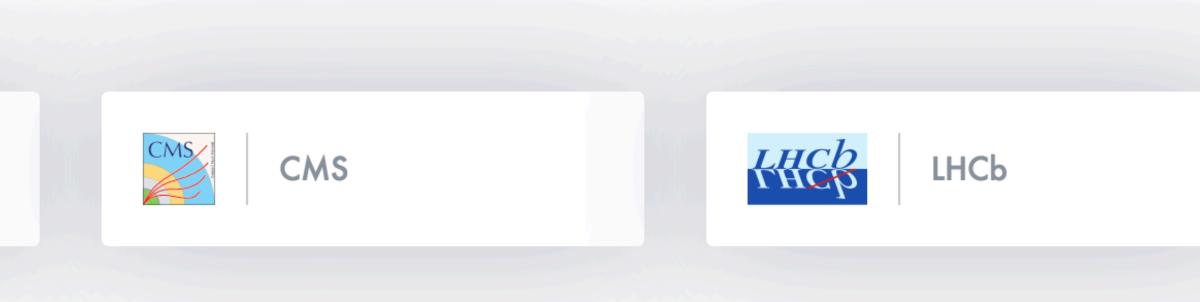
ATLAS

© 2015 CERN Analysis Preservation











# A loooong form

Submission form with autocomplete functionality (based on connections made to existing databases within the collaboration) WARNING: This is just a DEMO. Data saved is NOT backed-up at the moment and might be lost during any system upgrade

**Basic Information** 

Please provide some informatio

**Analysis Numb** 

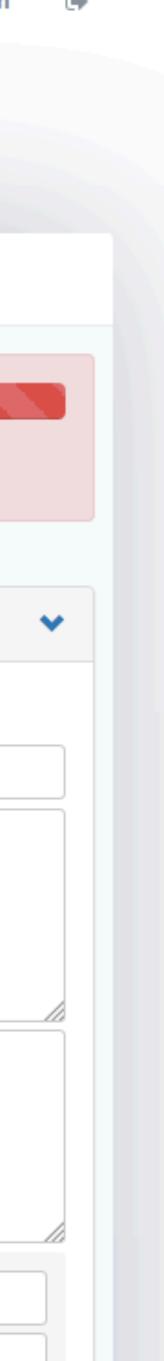
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# Detailed physics metadata

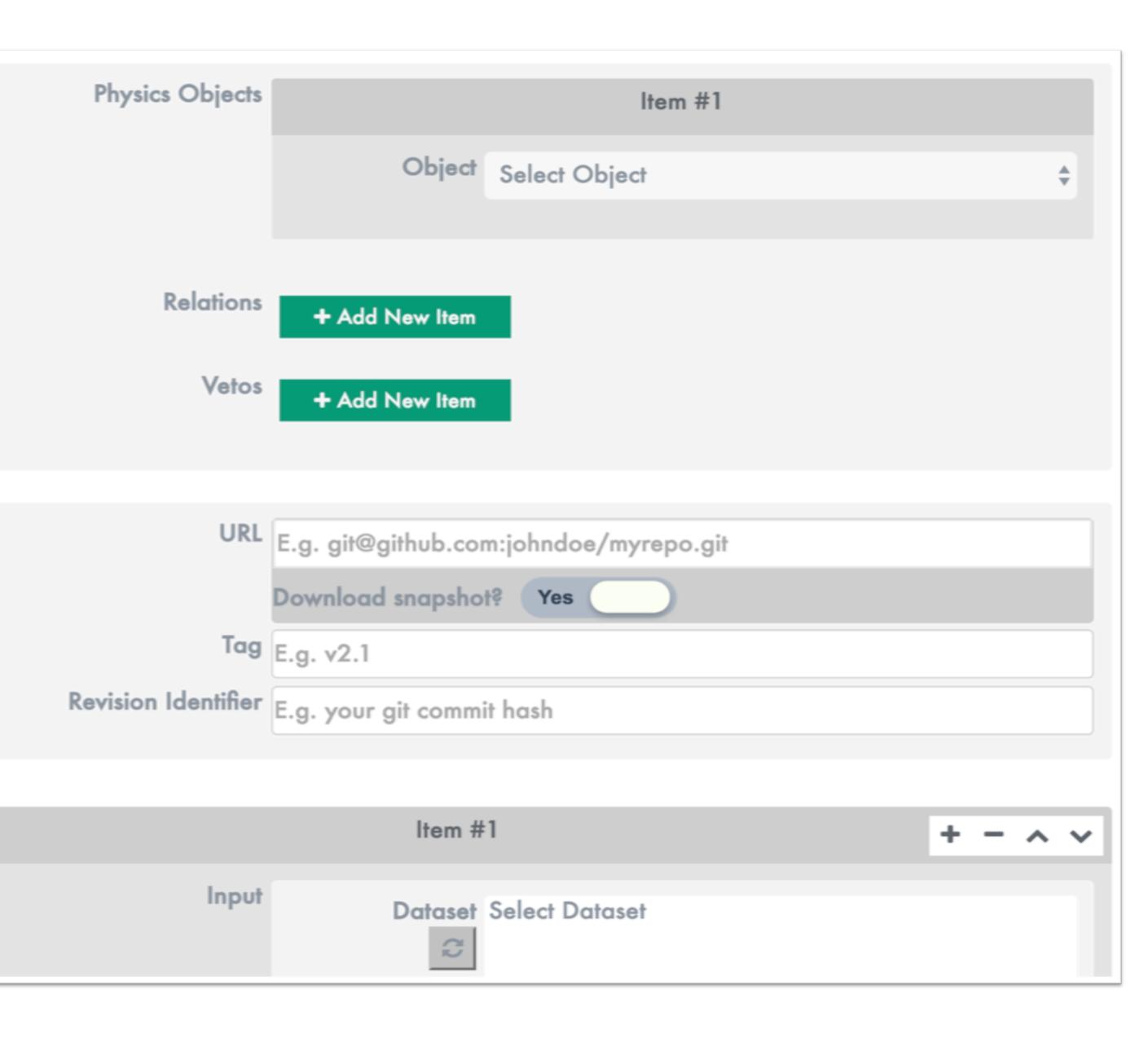
Access via APIs to internal databases provides key information – CAP connects it

Further information, such as OS, analysis software and related internal discussions, presentations and publications

Detailed physics information (e.g. final state particles, cuts and vetos) for future reuse **Event Selection** 

User Code Base

Processing





# Reproducibility 1<sup>st</sup> lessons learnt

- Challenge of granularity, complexity, dependencies
- Solutions available to do data/software publishing, linking and data citation
  - Applicable to other disciplines as well
- Moving upstream to enable reproducible research without "too much extra work"
- Role of docker, VMs?

# Thanks to

CERN IT J. Delgado, J. Kunčar, T. Smith, T. Šimko ALICE M. Gheata, M. Zimmermann ATLAS K. Cranmer, L. Heinrich, LHCb S. Amerio, M. Bettler, B. Couturier, T. Head, A. Trisovic, A. Ustyuzhanin CERN CernVM J. Blomer CERN EOS L. Mascetti DASPOS M. Hildreth, C. Vardeman, G. Watts **DPHEP** F. Berghaus, J. Shiers **THOR Project** 



- CERN SIS A. Dani, R. Dasler, P. Fokianos, P. Herterich, E. Maguire, A. Mattmann, L. Rueda

CMS A. Calderon, A. Huffman, K. Lassila-Perini, T. McCauley, A. Rao, A. Rodriguez Marrero

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[2]Key Components in Data Publishing: DOI: 10.1007/s00799-016-0178-2

[3] http://opendata.cern.ch/

[4] www.hepdata.net

[5] www.inspirehep.net

4773-10. Available at SSRN: http://ssrn.com/abstract=1550193



# [6] Stodden, Victoria, The Scientific Method in Practice: Reproducibility in the Computational Sciences (February 9, 2010). MIT Sloan Research Paper No.