# Curating and Publishing Big Datasets Using CU Boulder High Performance Computing Infrastructure

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#### View the slides



https://github.com/ResearchComputing/rmacc\_2025



#### Introduction

- No two people on any campus will agree on what "Data" actually is
- Publication of research datasets is now a requirement of most funding agencies and journals
- Just publishing datasets in repositories isn't enough to make research reproducible or replicable
- Data curation is the process of ensuring that datasets are findable, accessible, and usable
- Big data creates added challenges for curating and publishing data





#### What is Research Data?

- 3D models and printable files
- Accreditation reports
- Archival university papers
- Artistry and performance materials
- Audio
- Books
- Computer code & scripts
- Conference proceedings
- Course catalogs
- Datasets
- Designs & blueprints
- Digital journals
- Dissertations
- Documentation
- GIS files
- Grant proposals
- "Grey" literature
- Historical documents
- Images
- Interviews
- Journals
- Lab notebooks

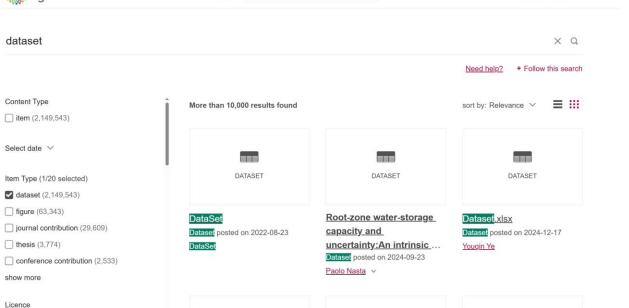
- Learning materials
- Lecture transcriptions
- Maps
- Methodologies & Workflows
- •MOOCs
- Newsletters
- Oral History
- Physical artifacts and specimens
- Point clouds
- Posters
- Presentations
- Seismic recordings
- Software
- Spreadsheets / CSV files
- Surveys
- Technical reports
- Teaching tools designed by faculty
- Theses
- Transcripts
- Video
- Visualizations
- Websites
- •\Mbita papare

# What is a Repository?

- A digital space used for publishing, sharing, and preserving works
- Repositories include articles, reports, slide decks, theses, data, and more
- There are general, domain-specific, national, and institutional
- Content may be openly accessible immediately, embargoed to a future date, or only accessible to certain users
- Gained popularity as many journals and funders now require data to be shared when articles are published







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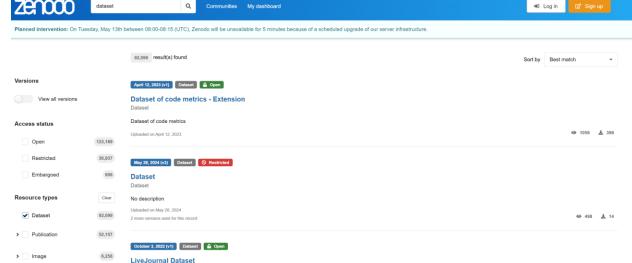
#### **NPDN National Data Repository**

The NPDN National Data Repository (NDR) is a database that collects diagnostic data from NPDN diagnostic laboratories throughout the USA and its territories. It provides the plant diagnostic community with information on whether a pest or pathogen is new, emerging, re-emerging, or increasing in any given area. NPDN diagnosticians upload diagnostic data to maintain the NDR with the most current information. New data is added every day.

The NDR is managed by the NPDN IT Center.

As intentional or accidental disclosure of some pest occurrence data can have trade implications and can put state regulators in a difficult situation, data in the NDR is not of public access. Before accessing the NDR for the first time, NPDN users take a short training to understand these data confidentiality concerns and agree to terms of use that prohibit any data disclosure. They are asked to review and agree to this data use policy once a year.

In order to better serve the plant health community, NPDN wants to make non-sensitive diagnostic data available to a broader audience. Non-NPDN parties can request pest diagnostic data using the data request form. NDR users can also use the data request form to request permission to share data.



# oTrPAC The Molecular Map of Exercise

Welcome to the data repository for the Molecular Transducers of Physical Activity Consortium; a national research initiative that aims to generate a molecular map of the effects of exercise and training.

DATA DOWNLOAD

**VIDEO TUTORIALS** 

**EXPLORE DATA** 

**PUBLICATIONS** 

Join our monthly open office event to learn more

## Institutional Repositories (IRs)

- For work created by those affiliated with the institution
- Usually run by libraries
- Can be general (include articles, etc.) or data-specific
- Data is usually associated with a published academic article
- Repositories may allow for self-deposit and instant publication or require data to be curated



#### **CU Scholar** UNIVERSITY LIBRARIES

HOME ABOUT HELP CONTACT

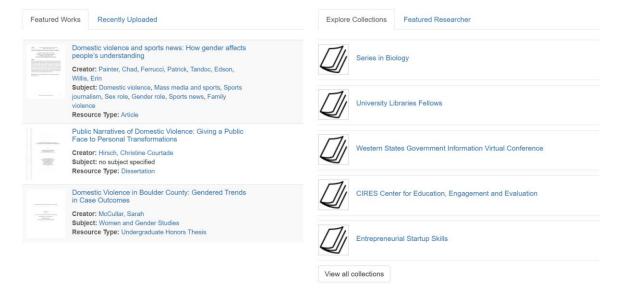
Search CU Scholar

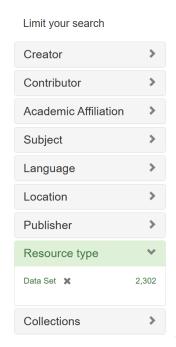
Enter search terms or select 'Go' to browse

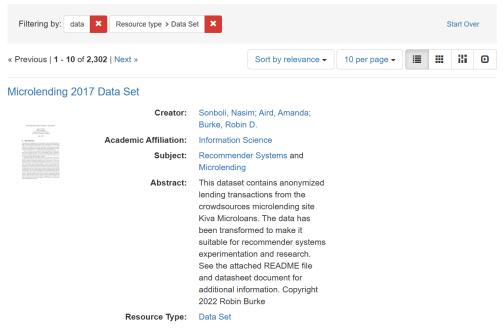
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Terms of Use







#### Data used for 2001-2020 spotted knapweed research

Seastedt, Timothy R Creator: Academic Affiliation: Institute of Arctic & Alpine Research Abstract: Data documentation required for submission of manuscript, "Biological control of spotted knapweed (Centaurea stoebe) in Colorado: A 20-year perspective" Resource Type: Data Set

#### Data sets associated with "Sediment Production in French Alpine Rivers"



Creator: Pitlick, John Academic Affiliation: Geography

> Annual Sediment Yield and Subject:

> > Sediment Transport

Abstract: This repository stores two data

sets associated with the manuscript titled "Sediment Production in French Alpine Rivers". The first file,

Ecrins Site Data.xlsx,is an Excel workbook listing data for the 16

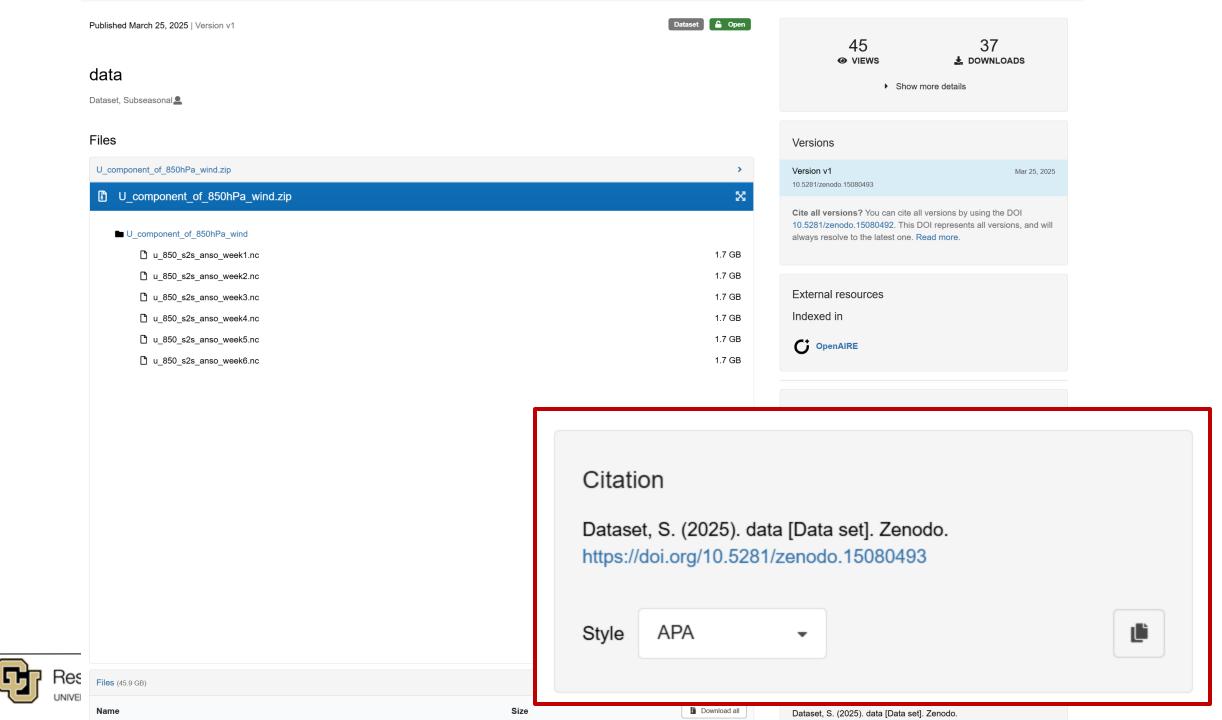




#### **Data Curation**

- The process of ensuring that data is FAIR:
  - Findable
  - Accessible
  - Interoperable
  - Reusable
- Why do we need to do this?





## Data Curation Network's CURATE(D) Steps

- Check files/code and read documentation
- Understand the data (or try to)
- Request missing information or changes
- Augment metadata for findability
- Transform file formats for reuse
- Evaluate for FAIRness
- Document all curation activities throughout the process





#### When we use HPC resources for data curation

- The data requires specific software or code that can only be run using HPC resources
- The data <u>is</u> specific software/code that can only be run using HPC resources

## Example

- Curator cannot open/run files on their computer
- Files are uploaded to a HPC server and tested
- Oh no! They don't work:
  - Scripts have hardcoded paths (researcher updates scripts)
  - Specific libraries are required (researcher adds documentation)
  - A different version of the software is required (researcher adds documentation)





## **Publishing Data**

- The data has been curated and is ready to be published
  - The data is ready to be reused
  - The documentation is complete
  - There's accurate metadata (authors, etc.)
  - A DOI has been issued
- Problems
  - The dataset is too big for the institutional repository
  - The dataset requires HPC resources to be used





# Framework for big data publishing at CU Boulder

1. Landing page

2. Storage infrastructure

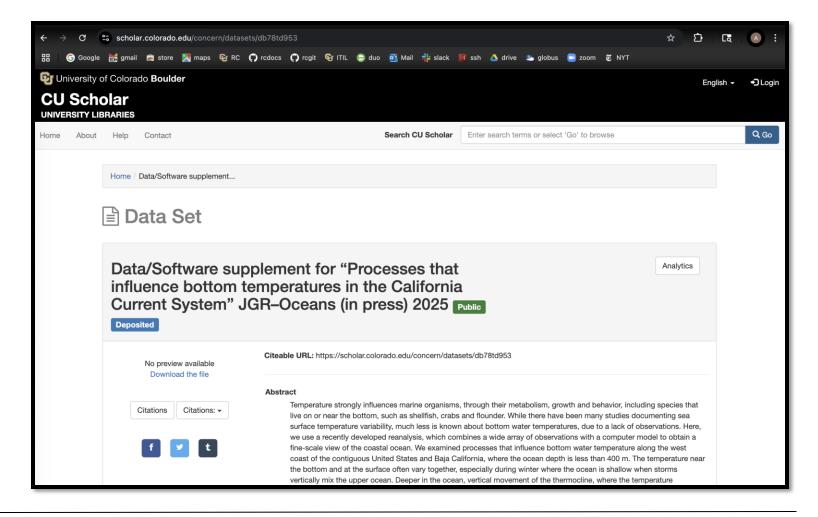
3. Data transfer



# **Landing Page**

CU Libraries host on CU Institutional repository:

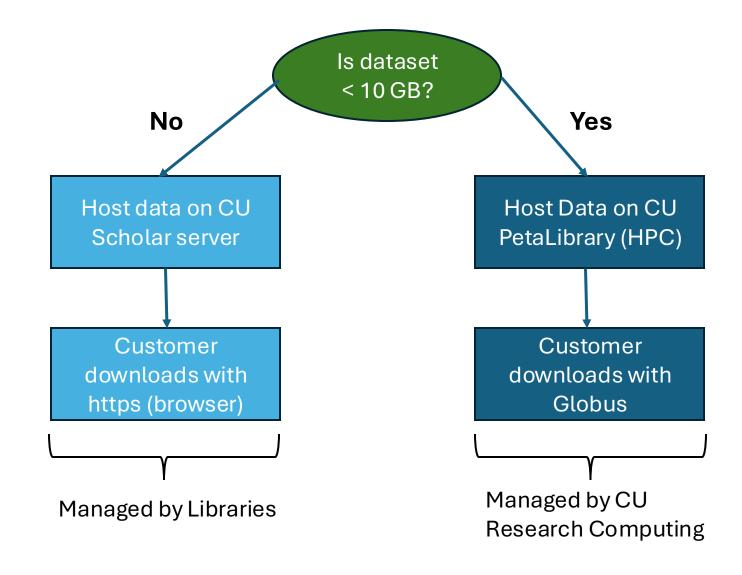
https://scholar.colorado.edu







# Storage Infrastructure

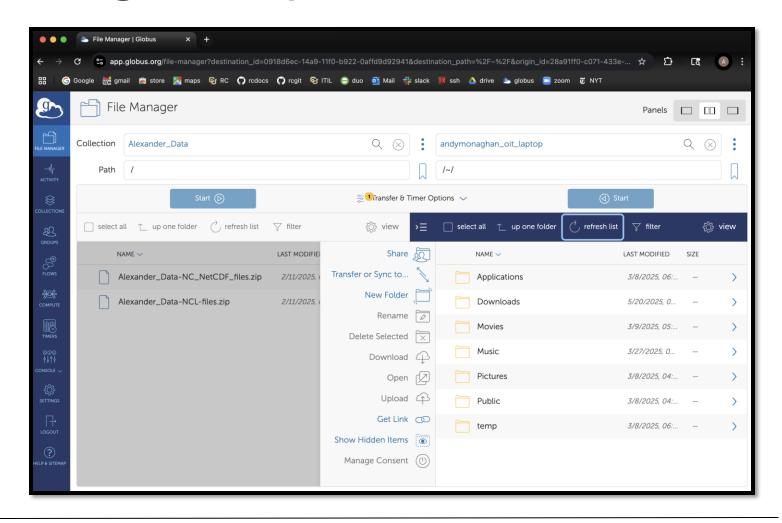






# Data Transfer for "big data" publications

- Uses Globus
  - GridFTP transfer protocol
  - Fast, stable, fault tolerant
  - Anyone can use Globus
  - Guidance provided on CU Scholar landing page







#### Costs

Is there a cost for publishing large datasets at CU Boulder?

- If size < 500 GB: No</li>
- If size > 500 GB: Yes (\$450/TB)

If the data is related to a student's thesis or dissertation we'll talk with them to see what we can do (this hasn't happened yet)



## How to get started:

• Email <u>cuscholaradmin@colorado.edu</u>

We can advise on data curation, assist with data upload, etc.

• Reach out to the libraries/IR administrators at your institution





#### **Future**

- How can we expand use of HPC resources to provide increased access to datasets?
- Emulation
- Virtual access
- Containers

