DATA MANAGEMENT FOR OPEN & REPRODUCIBLE SCIENCE

Adina Wagner
@AdinaKrik

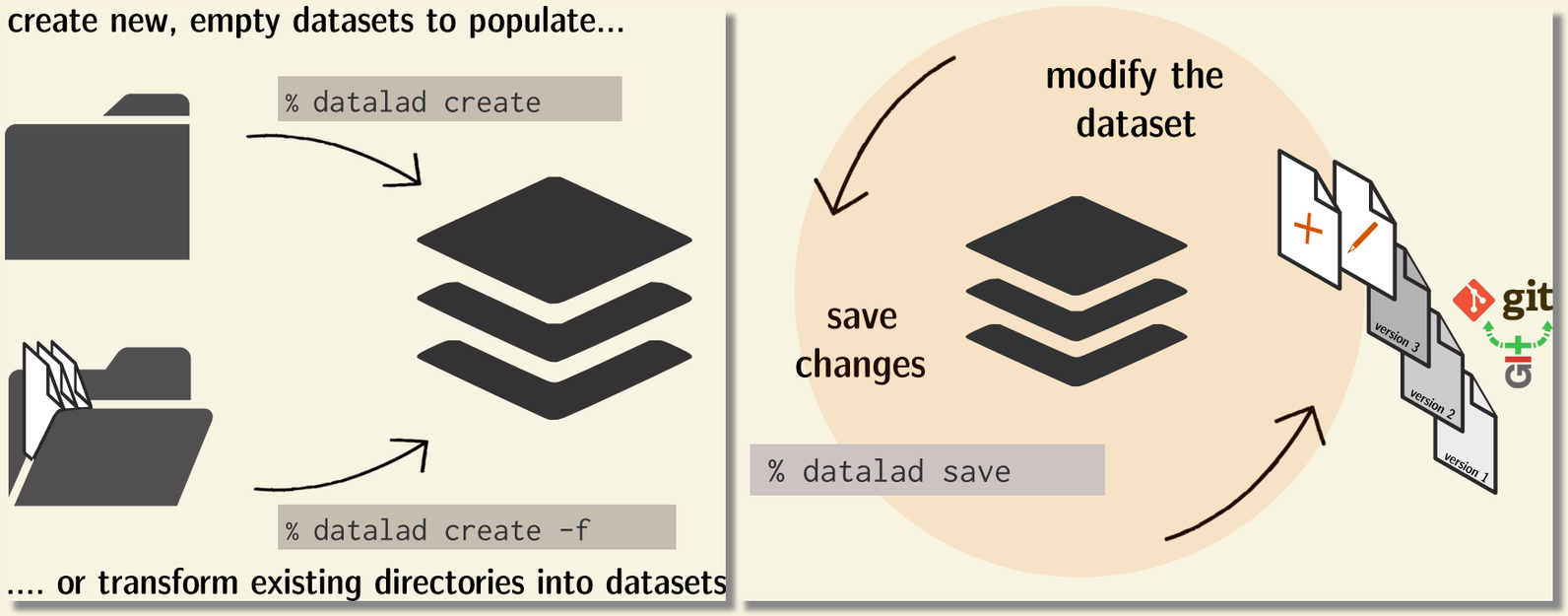
Psychoinformatics lab,
Institute of Neuroscience and Medicine, Brain & Behavior (INM-7)
Research Center Jülich
ReproNim/INCF fellow

Slides: DOI 10.5281/zenodo.5702023 (Scan the QR code)
Sources: github.com/datalad-handbook/course

- A command-line tool, available for all major operating systems (Linux, macOS/OSX, Windows), free & open source
- Build on top of Git and Git-annex
- **Main features:**
  Version control for arbitrarily large content
  version control data and software alongside to code!
  Transport logistics for sharing and obtaining data
  consume and collaborate on data (analyses) like software
  Computationally reproducible data analysis
  Track and share provenance of all digital objects
- Completely domain-agnostic

VERSION CONTROL

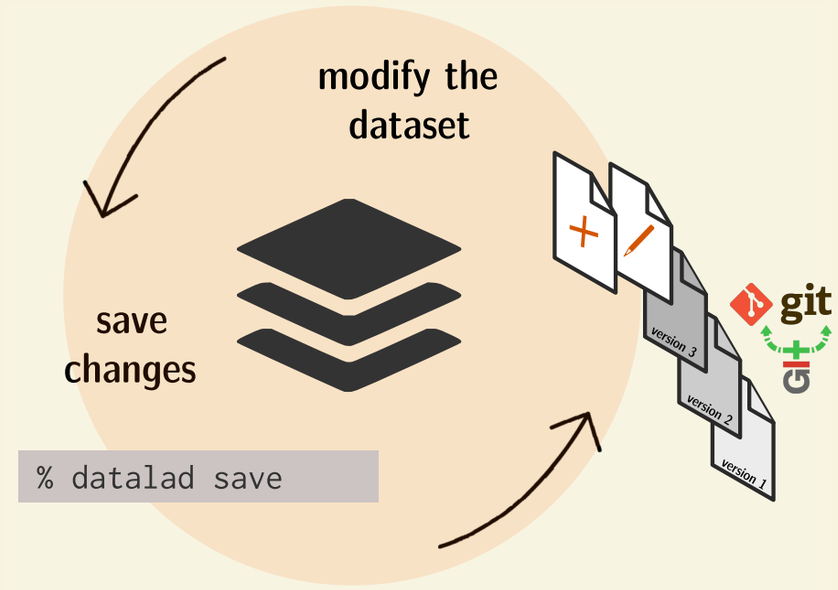
- DataLad knows two things: Datasets and files



- A DataLad dataset is a **Git repository**:
  - keep track of changes
  - revert changes or go back to previous states
  - collect and share digital provenance

VERSION CONTROL: DATA

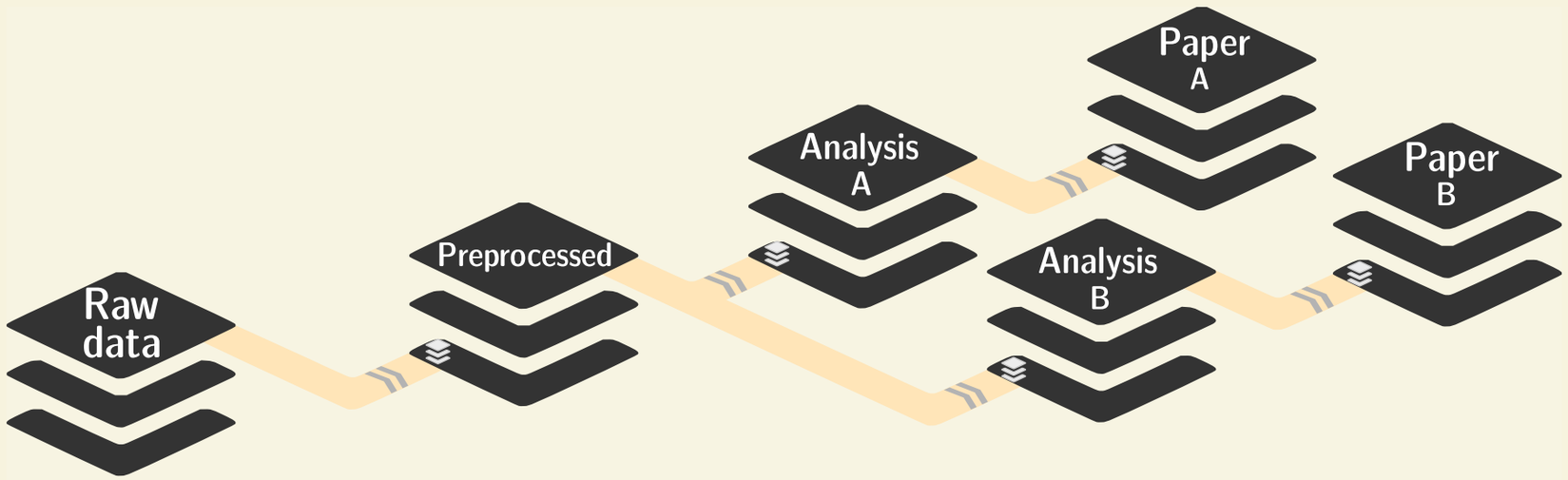
- Datasets have an optional annex for (large or sensitive) data (or text/code).
- Identity (hash) and location information is put into Git, rather than file content. The annex, and transport to and from it is managed with **git-annex** (git-annex.branchable.com)
  → decentralized version control for files of any size.
- DataLad works towards wrapping Git and git-annex into a non-complex core-API (helpful for data management novices).



- Flexibility and commands of Git and git-annex are preserved (useful for experienced Git/git-annex users).

VERSION CONTROL: NESTING

- Link datasets as "dependencies":



Nest modular datasets to create a linked hierarchy of datasets, and enable recursive operations throughout the hierarchy

  - hierarchies of datasets in super-/sub-dataset relationships
- ✓ Scalability

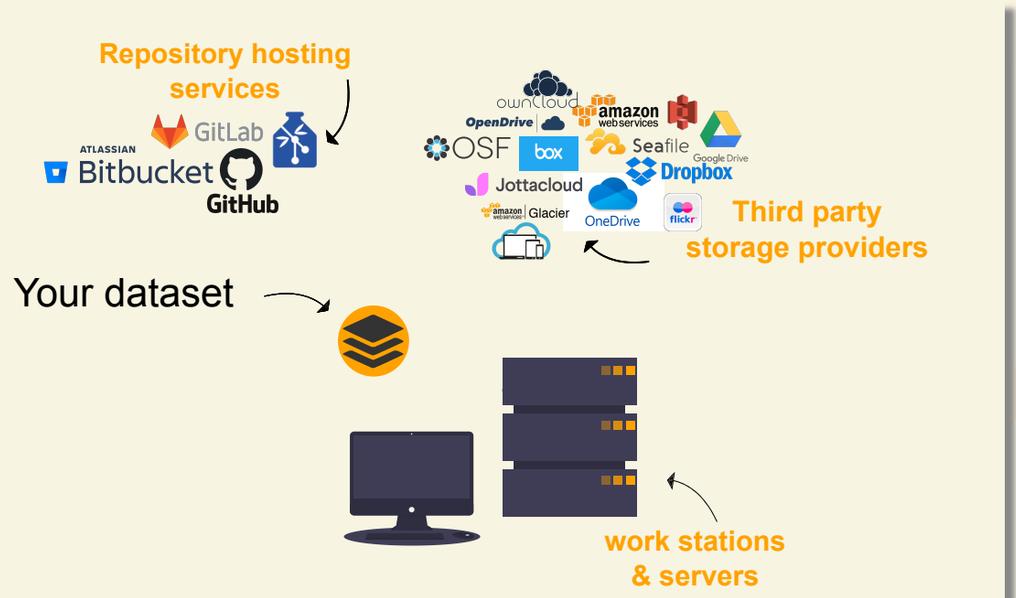
```
adina@bulk1 in /ds/hcp/super on git:master❱ datalad status --annex -r
15530572 annex'd files (77.9 TB recorded total size)
nothing to save, working tree clean
```

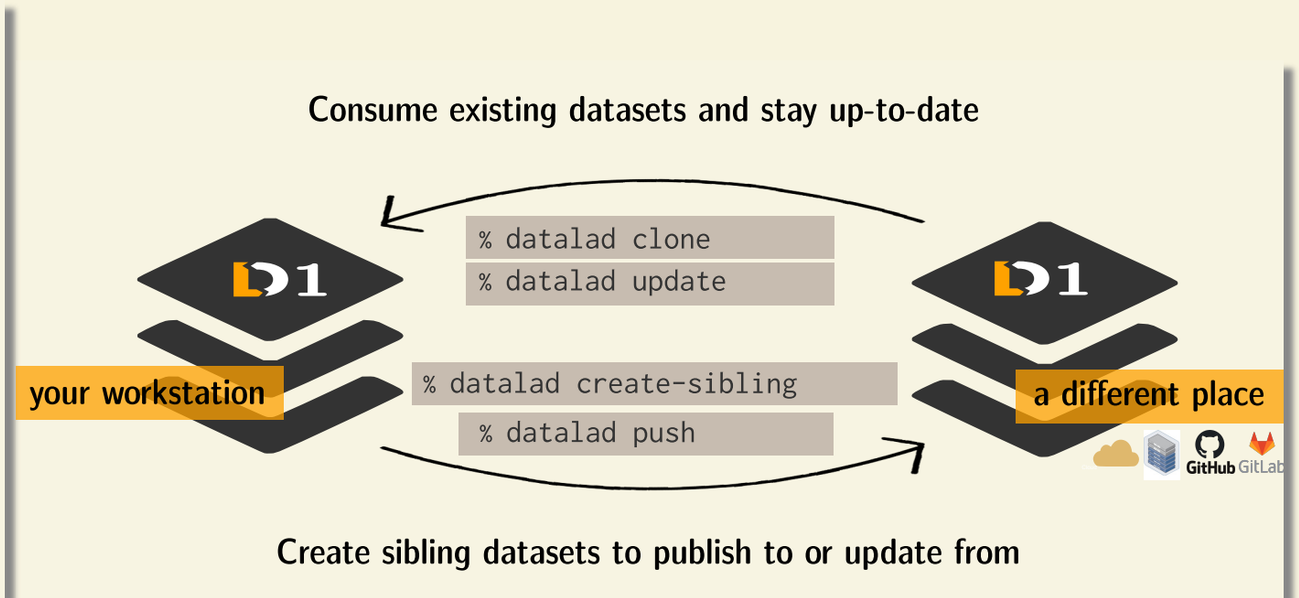
(github.com/datalad-datasets/human-connectome-project-openaccess)

- ✓ Modularizes research components for transparency, reuse, and access management

TRANSPORT LOGISTICS

- Share datasets easily
- Datasets can be "cloned", "pushed", and "updated" from and to local paths, remote hosting services, cloud services, ...





TRANSPORT LOGISTICS

- Disk-space aware workflows: Cloned datasets are lean:

```
$ datalad clone git@github.com:datalad-datasets/machinelearning-books.git
install(ok): /tmp/machinelearning-books (dataset)
$ cd machinelearning-books && du -sh
348K    .
```

```
$ ls
A.Shashua-Introduction_to_Machine_Learning.pdf
B.Efron_T.Hastie-Computer_Age_Statistical_Inference.pdf
C.E.Rasmussen_C.K.I.Williams-Gaussian_Processes_for_Machine_Learning.pdf
D.Barber-Bayesian_Reasoning_and_Machine_Learning.pdf
[...]
```

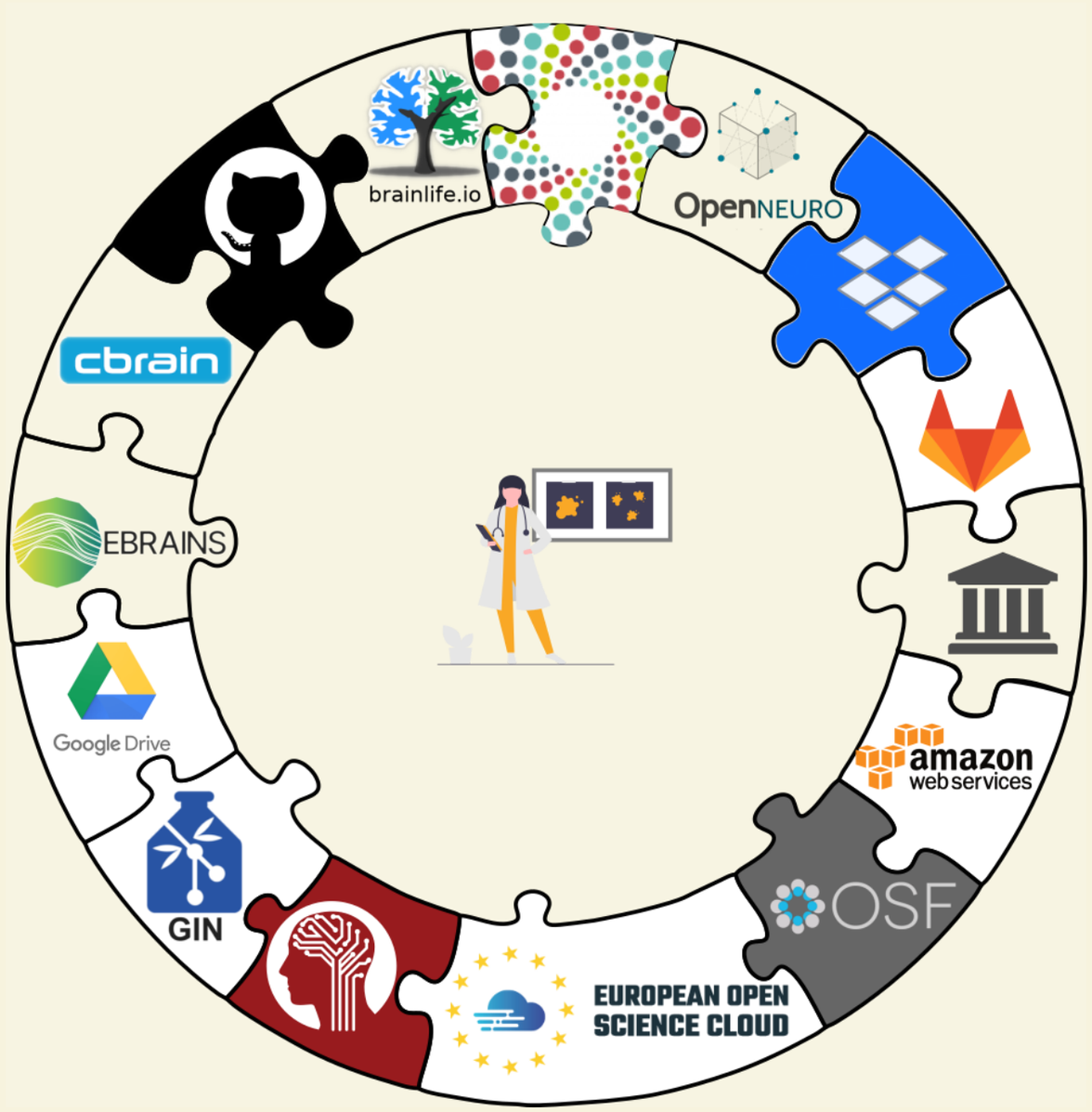
  - file contents are retrieved & dropped on demand on up to per-file granularity:

```
$ datalad get A.Shashua-Introduction_to_Machine_Learning.pdf
get(ok): /tmp/machinelearning-books/A.Shashua-Introduction_to_Machine_Learning.pdf (file) [from web...]
```

```
$ datalad drop A.Shashua-Introduction_to_Machine_Learning.pdf
drop(ok): /tmp/machinelearning-books/A.Shashua-Introduction_to_Machine_Learning.pdf (file) [checking https
```

INTEROPERABILITY

- DataLad is built to maximize interoperability and use with hosting and storage technology



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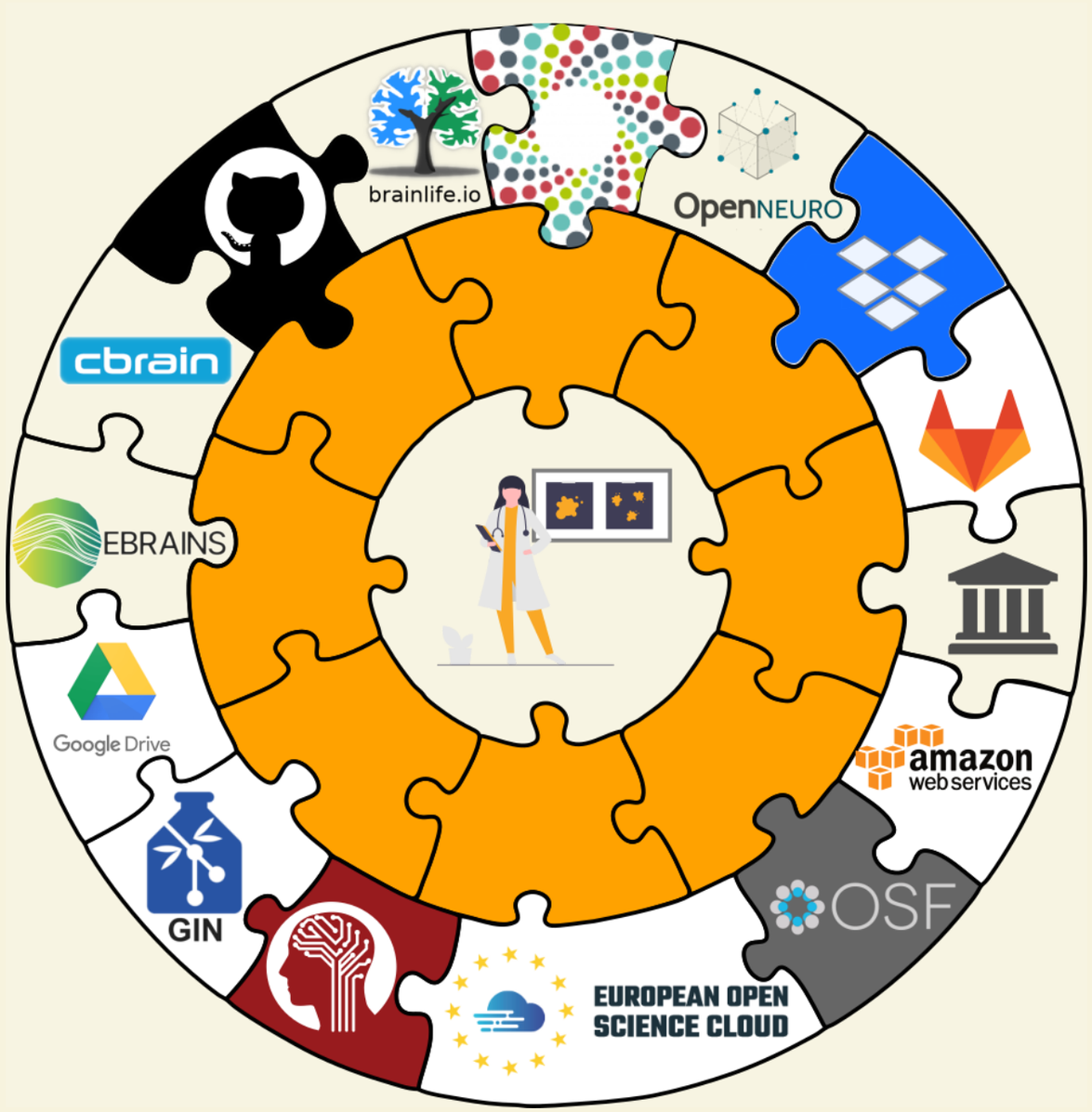
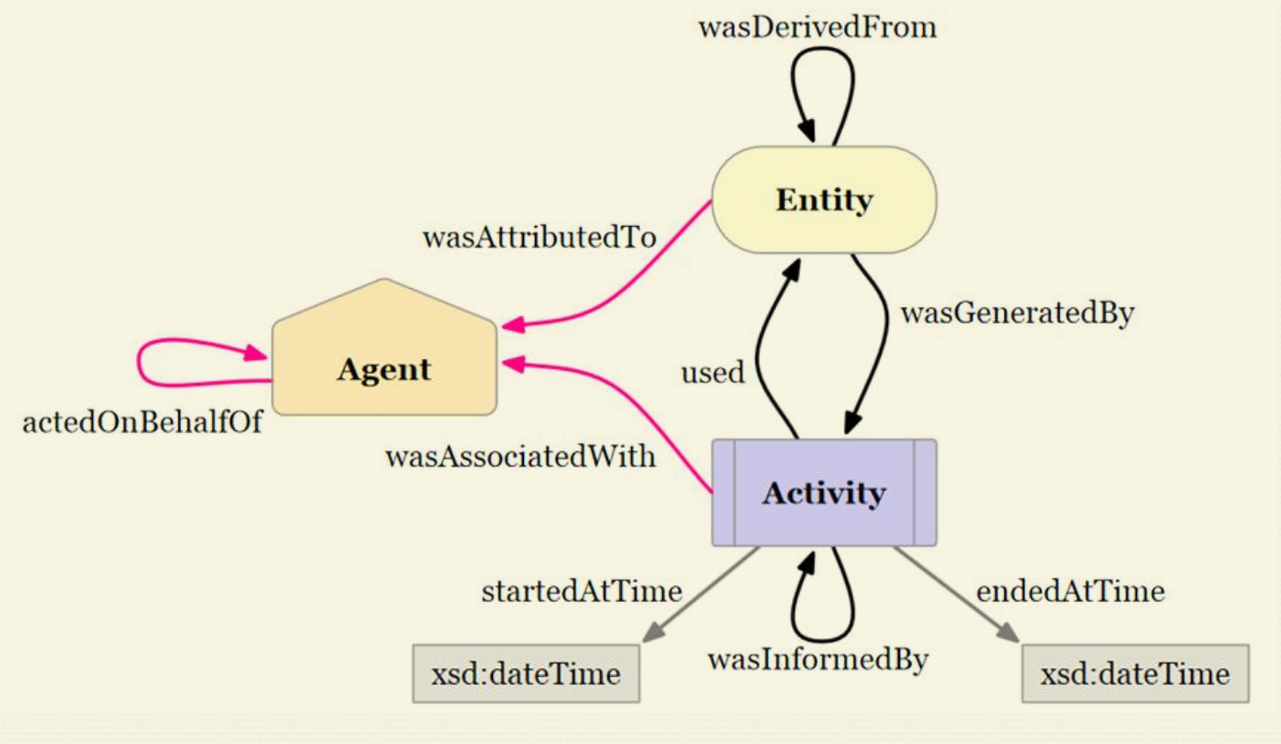


PROVENANCE CAPTURE

- Datasets can capture dataset **transformations** and their **cause** in order to track the entire evolution and lineage of files in datasets



- "How did this file came to be?", "What steps were undertaken to transform the raw data into the published result?", "Can you recompute this for me?"

PROVENANCE CAPTURE

- **Basic provenance**: DataLad can capture arbitrary dataset transformations (e.g., from computing analysis results) and record the cause of such a change

```
$ datalad run -m "Perform eye movement event detection"\
  --input 'raw_data/*.tsv.gz' --output 'sub-*' \
  bash code/compute_all.sh

-- Git commit -- Michael Hanke < ... @gmail.com>; Fri Sep 21 22:00:47 2019
    [DATALAD RUNCMD] Perform eye movement event detection
    === Do not change lines below ===
    {
     "cmd": "bash code/compute_all.sh",
     "dsid": "d2b4b72a-7c13-11e7-9f1f-a0369f7c647e",
     "exit": 0,
     "inputs": ["raw_data/*.tsv.gz"],
     "outputs": ["sub-*"],
     "pwd": "."
    }
    ^^^ Do not change lines above ^^^
---
 sub-01/sub-01_task-movie_run-1_events.png | 2 +-
 sub-01/sub-01_task-movie_run-1_events.tsv | 2 +-
...
```

PROVENANCE CAPTURE

- **Computational provenance**: Datasets can track **software containers**, and perform and record computations inside it:

```
$ datalad containers-run -n neuroimaging-container \
  --input 'mri/*_bold.nii --output 'sub-*/LC_timeseries_run-*.csv' \
  "bash -c 'for sub in sub-*; do for run in run-1 ... run-8;
     do python3 code/extract_lc_timeseries.py \$sub \$run; done; done'"

-- Git commit -- Michael Hanke < ... @gmail.com>; Fri Jul 6 11:02:28 2019
    [DATALAD RUNCMD] singularity exec --bind {pwd} .datalad/e...
    === Do not change lines below ===
    {
     "cmd": "singularity exec --bind {pwd} .datalad/environments/nilearn.simg bash..",
     "dsid": "92ea1faa-632a-11e8-af29-a0369f7c647e",
     "inputs": [
      "mri/*.bold.nii.gz",
      ".datalad/environments/nilearn.simg"
     ],
     "outputs": ["sub-*/LC_timeseries_run-*.csv"],
     ...
    }
    ^^^ Do not change lines above ^^^
---
 sub-01/LC_timeseries_run-1.csv | 1 +
...
```

PROVENANCE CAPTURE

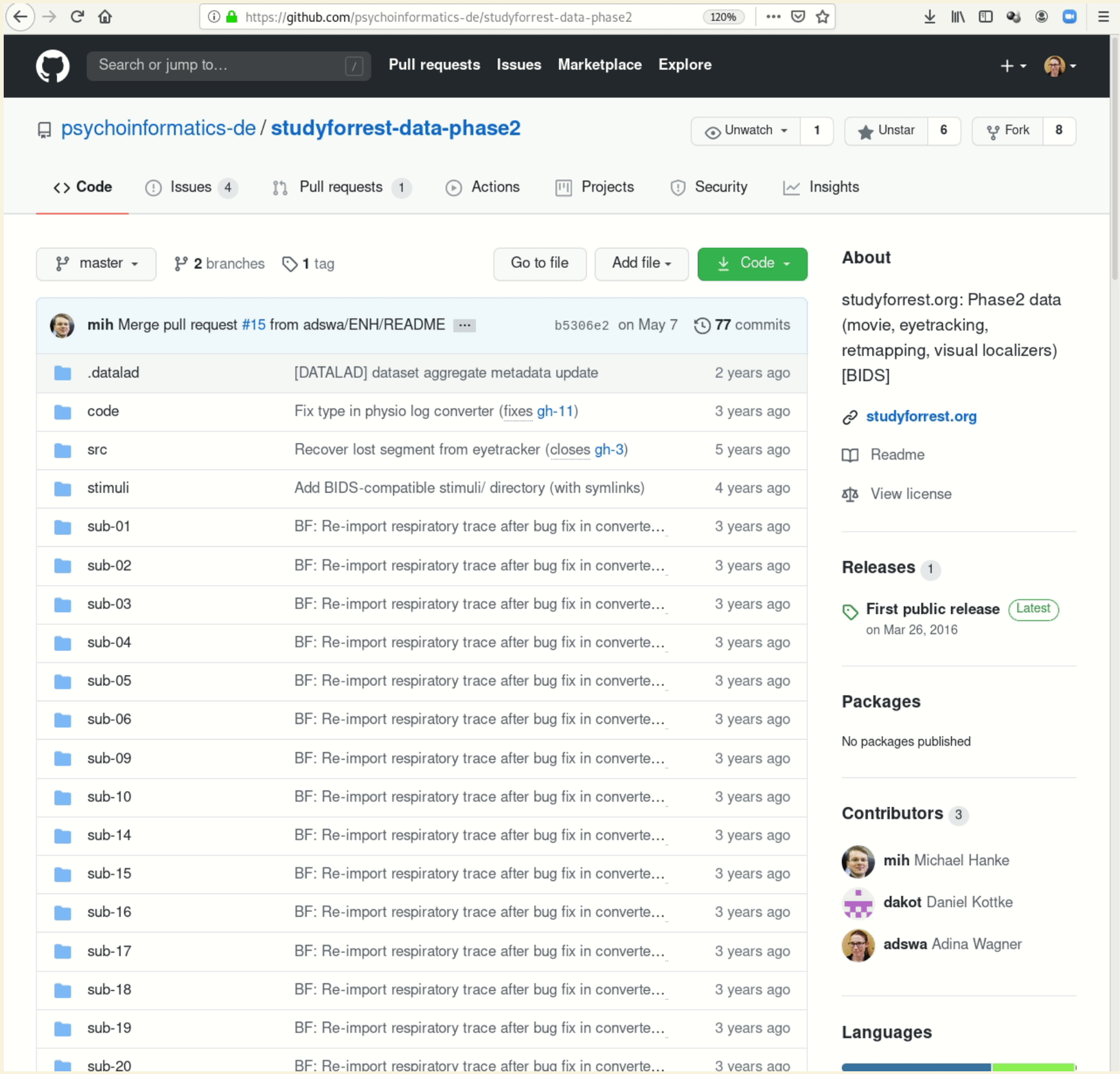
- All recorded transformations can be re-computed automatically

```
$ datalad rerun eee1356bb7e8f921174e404c6df6aadcc1f158f0
[INFO] == Command start (output follows) =====
[INFO] == Command exit (modification check follows) =====
add(ok): sub-01/LC_timeseries_run-1.csv (file)
...
save(ok): . (dataset)
action summary:
  add (ok: 45)
  save (notneeded: 45, ok: 1)
  unlock (notneeded: 45)
...
```

  - Aid with the reproducibility of a result and verify it (via content hash)
  - Use complete capture and automatic re-computation as alternative to storage and transport

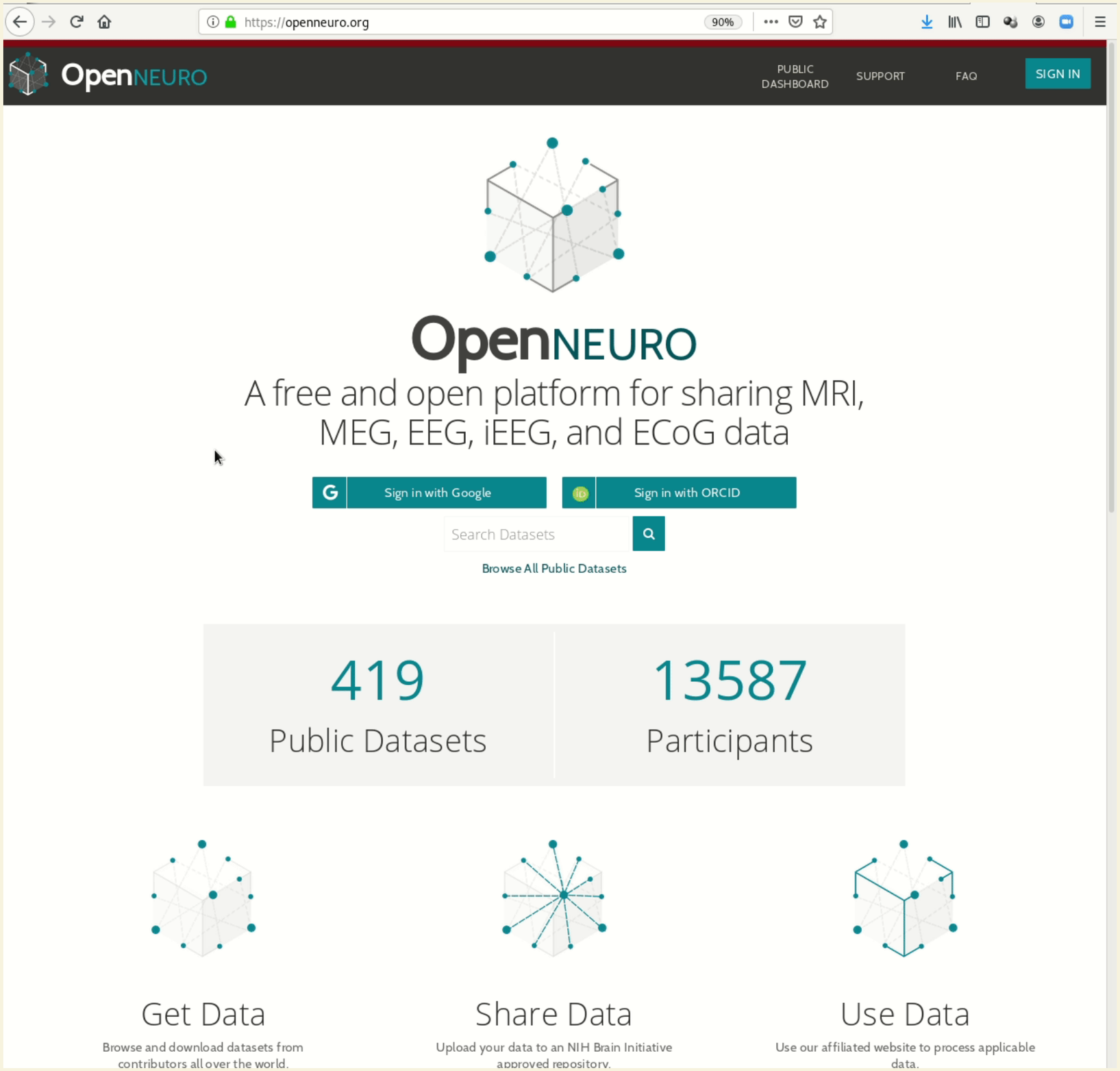
EXAMPLES OF WHAT DATALAD CAN BE USED FOR:

- **Publish or consume datasets** via GitHub, GitLab, OSF, or similar services



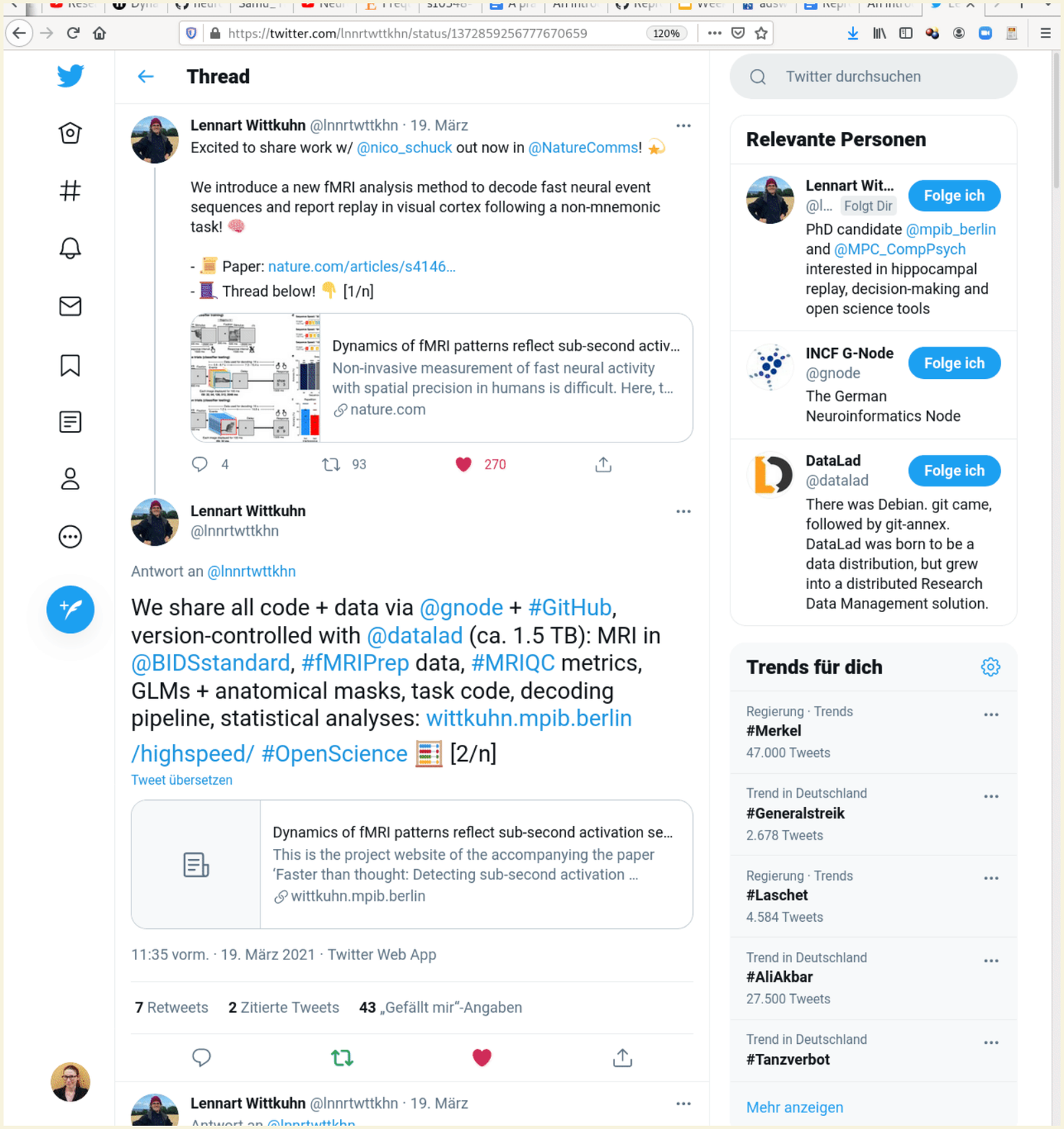
EXAMPLES OF WHAT DATALAD CAN BE USED FOR:

- Behind-the-scenes **infrastructure component for data transport and versioning**



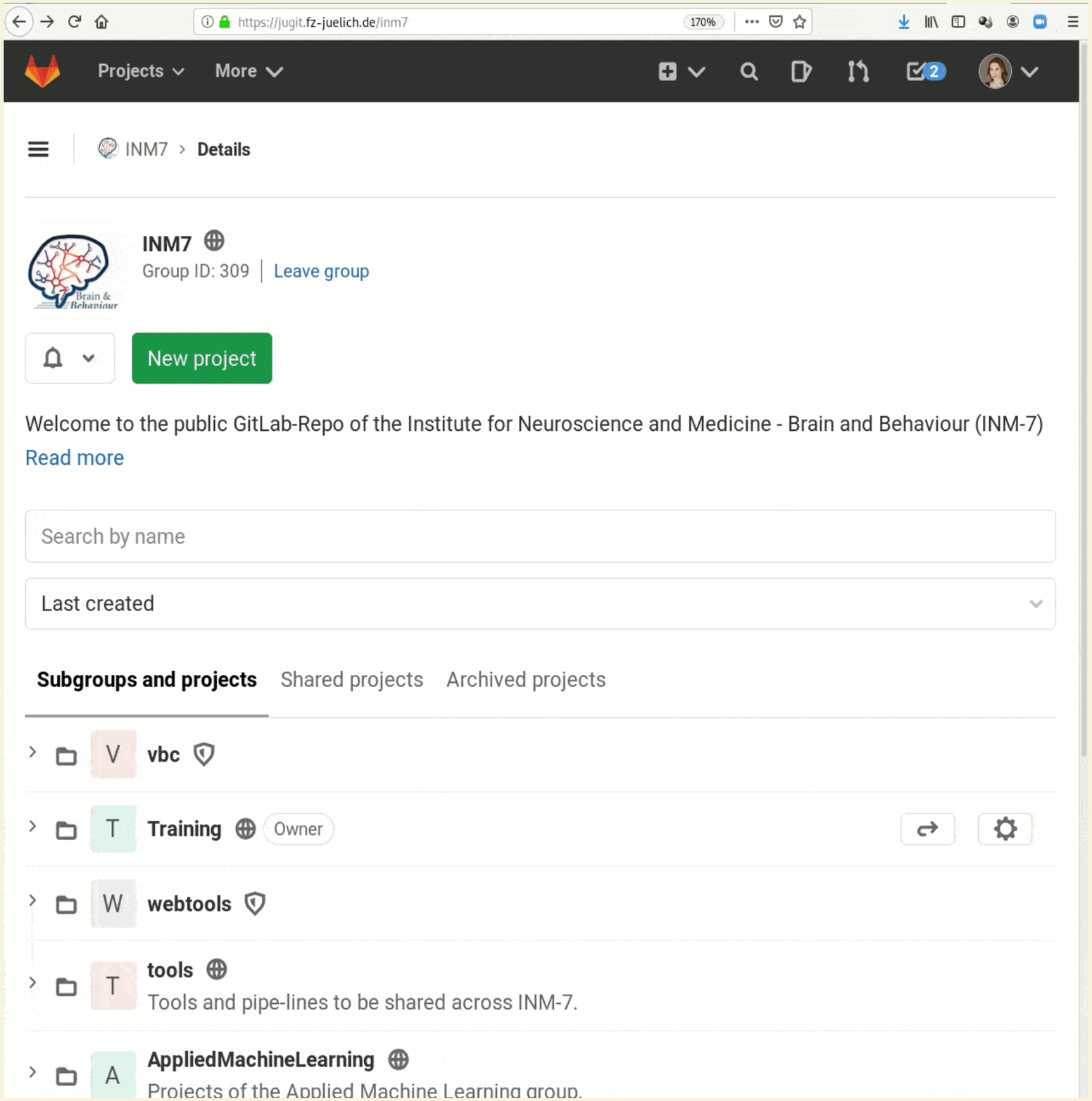
EXAMPLES OF WHAT DATALAD CAN BE USED FOR:

- **Creating and sharing reproducible, open science:** Sharing data, software, code, and provenance



EXAMPLES OF WHAT DATALAD CAN BE USED FOR:

- **Central data management** and archival system



EXAMPLES OF WHAT DATALAD CAN BE USED FOR:

- **Reproducible computation** at the largest scale

FAIRly big: A framework for computationally reproducible processing of large-scale data (doi.org/10.1101/2021.10.12.464122)

FURTHER INFORMATION

- User documentation & tutorials: handbook.datalad.org
- Source code, issue tracker: github.com/datalad/datalad
- Technical docs: docs.datalad.org
- Video tutorials: www.youtube.com/datalad
- User support: DataLad Matrix Channel
- "DataLad Office Hour" (weekly): DataLad Office Hour Matrix Channel
- DataLad Paper: doi.org/10.21105/joss.03262

Use it on Hilbert:

```
module load datalad
```

Install it on your own hardware: handbook.datalad.org/r.html?install

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DataLad software

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- Joey Hess (git-annex)
- Kyle Meyer
- Benjamin Poldrack
- *32 additional contributors*

DataLad handbook

- Adina Wagner
- *41 additional contributors*

Collaborators

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cbrain

brainlife.io

THANKS!