Data management

Session 01

AGENDA

- **Prerequisites & technicalities**
  - Setting up a Git identity
  - Gitlab/Github accounts
  - Howto: Issues on Gitlab, The handbook's repository, Readthedocs
- **Session 01**
  - What is a DataLad dataset?
  - YODA principles for dataset organization
- **Hands-on 01:** Data in a DataLad dataset

GIT IDENTITY

- Git: free & open source version control software
- Git is already installed on the cluster
- Git identity: The name and e-mail address associated with what you "save".
- Configuration with `git config` command in a terminal:

```
$ git config --global user.name "Adina Wagner"
$ git config --global user.email adina.wagner@example.com
```

- **Hands-on**: Log into `brainbfast` and configure your Git identity, if it isn't set up yet.

GITHUB & GITLAB

- Two different web-based Git repository managers with similar features. Both are used to host Git repositories and to ease collaboration.

GitHub

- Github.com: Most popular, proprietary, extensive functionality on free plans
- Core concepts: Repositories, organizations.

GitLab

- Similar to GitHub, but is open source. The FZJ hosts many different GitLab instances.
- JuGit (jugit.fz-juelich.de): The GitLab instance we recommend.
- Core concepts: Groups, subgroups, projects.

HANDBOOK REPOSITORIES

- The DataLad Handbook: User-oriented, introductory course on DataLad and the basis for the data management course.
- Source code on
  - Github (github.com/datalad-handbook/book) and
  - Gitlab (jugit.fz-jeulich.de/inm7/training/datalad-handbook)
- **File issues** if you have questions or requests!
- Contribute by **pull requesting** changes, additions, and fixes!

FILING ISSUES ON GITLAB

- File issues if you have DataLad-related or course-related questions in the repository hosted on **Gitlab**
- **Hands-on**: File an issue right now!
    - go to jugit.fz-juelich.de
    - find the handbook project
    - file an issue with any content

READTHEDOCS

- The book is rendered with Sphinx and hosted on Readthedocs.org
- Readthedocs supports HTML, eReader, and PDF formats
- Rendered version: handbook.datalad.org
- There is an additional **INM-7 specific** version with additional sections on internal workflows
- **Hands-on**: Access public and INM-7-specific versions of the handbook in HTML and PDF format

DATALAD DATASETS

DataLad datasets are DataLad's core data structure. Datasets have many features:

Version controlled content, regardless of size
: Relying on the tools Git and Git-annex working in the background.

Provenance tracking
: Record and find out how data came into existence (including the software environment), and reproduce entire analyses.

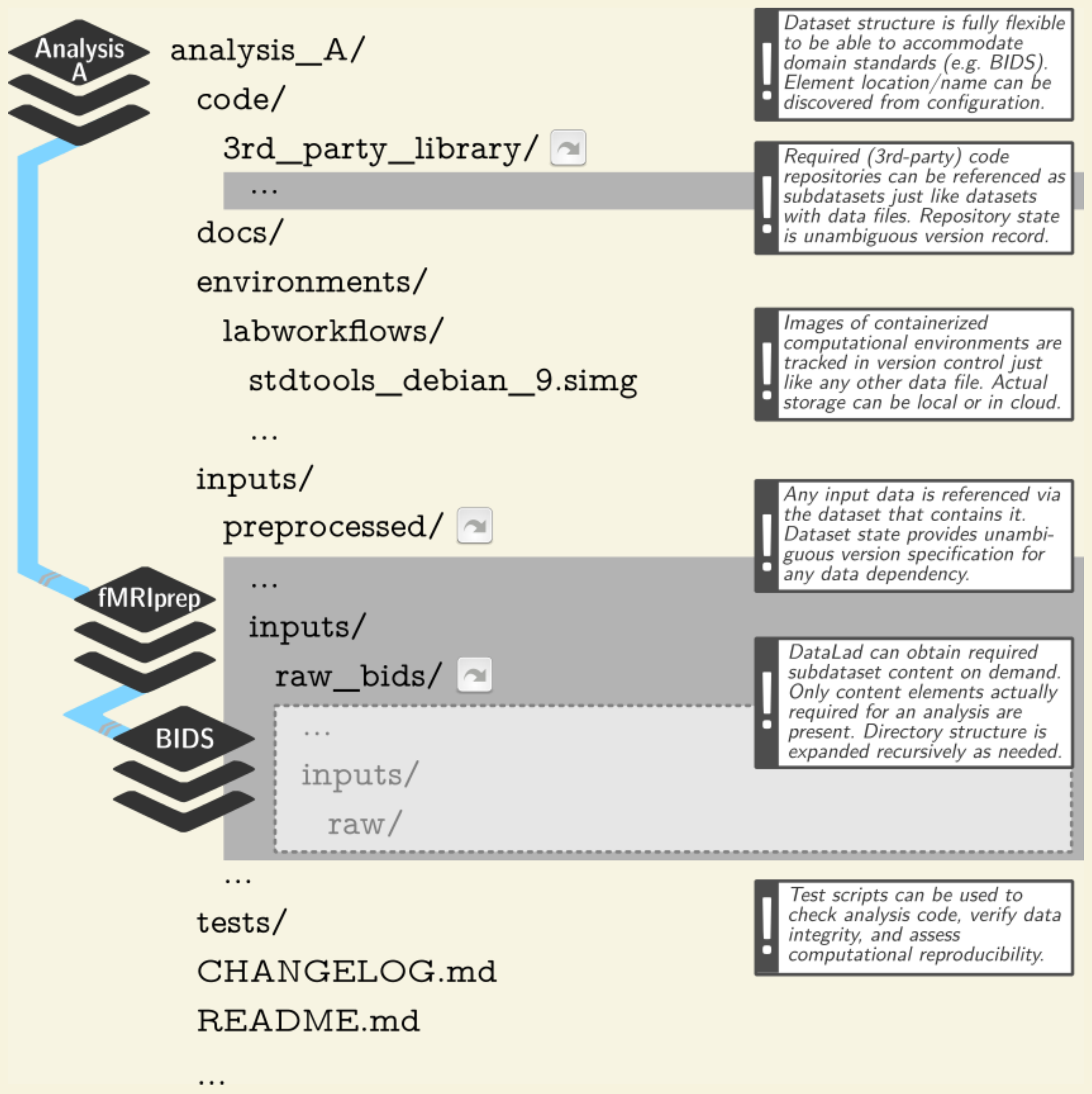
Easy collaboration
: Install others' datasets, share datasets, publish datasets with third-party services.

Staying up to date
: Datasets can know their copies or origins. This allows to **update** datasets from their sources with a single command.

Modularity & Nesting
: Individual datasets are independent, versioned components that can be *nested* as *subdatasets* in *superdatasets*. Subdatasets have a stand-alone version history, and their *version state* is recorded in the superdataset.

DATALAD DATASETS

DataLad datasets look like any other directory on your computer, and subdatasets look like subdirectories. DataLad, Git-annex, and Git work in the background (e.g., `.datalad/`, `.git/`, ...).



Analysis A
analysis_A/
code/
3rd_party_library/
...
docs/
environments/
labworkflows/
stdtools_debian_9.simg
...
inputs/
preprocessed/
fMRIprep
...
inputs/
raw_bids/
BIDS
...
inputs/
raw/
...
tests/
CHANGELOG.md
README.md
...
Dataset structure is fully flexible to be able to accommodate domain standards (e.g. BIDS). Element location/name can be discovered from configuration.
Required (3rd-party) code repositories can be referenced as subdatasets just like datasets with data files. Repository state is unambiguous version record.
Images of containerized computational environments are tracked in version control just like any other data file. Actual storage can be local or in cloud.
Any input data is referenced via the dataset that contains it. Dataset state provides unambiguous version specification for any data dependency.
DataLad can obtain required subdataset content on demand. Only content elements actually required for an analysis are present. Directory structure is expanded recursively as needed.
Test scripts can be used to check analysis code, verify data integrity, and assess computational reproducibility.

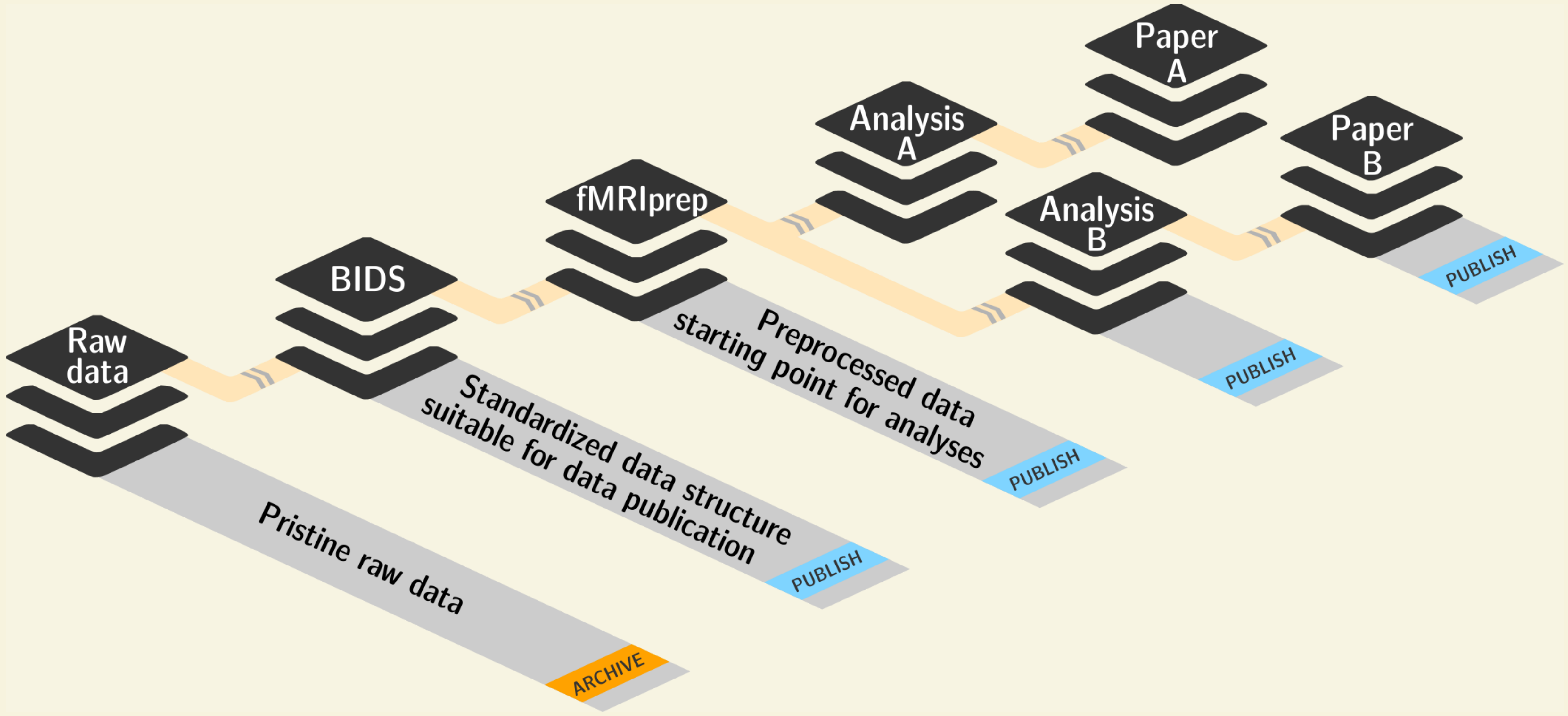
You can **create & populate** a dataset from scratch, or **install** existing datasets from collaborators or open sources.

DATALAD DATASETS FOR DATA ANALYSIS

- A DataLad dataset can have *any* structure, and use as many or few features of a dataset as required.
- However, for **data analyses** it is beneficial to make use of DataLad features and structure datasets according to the **YODA principles**:

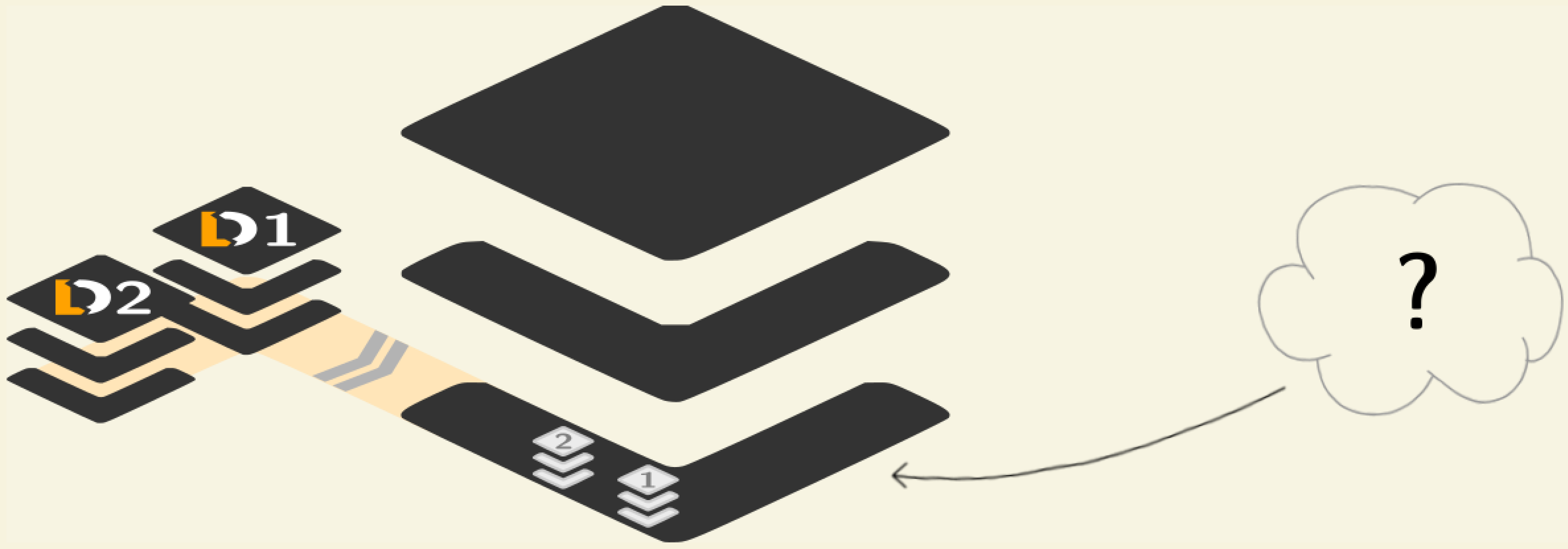
P1: One thing, one dataset
P2: Record where you got it from, and where it is now
P3: Record what you did to it, and with what

P1: ONE THING, ONE DATASET



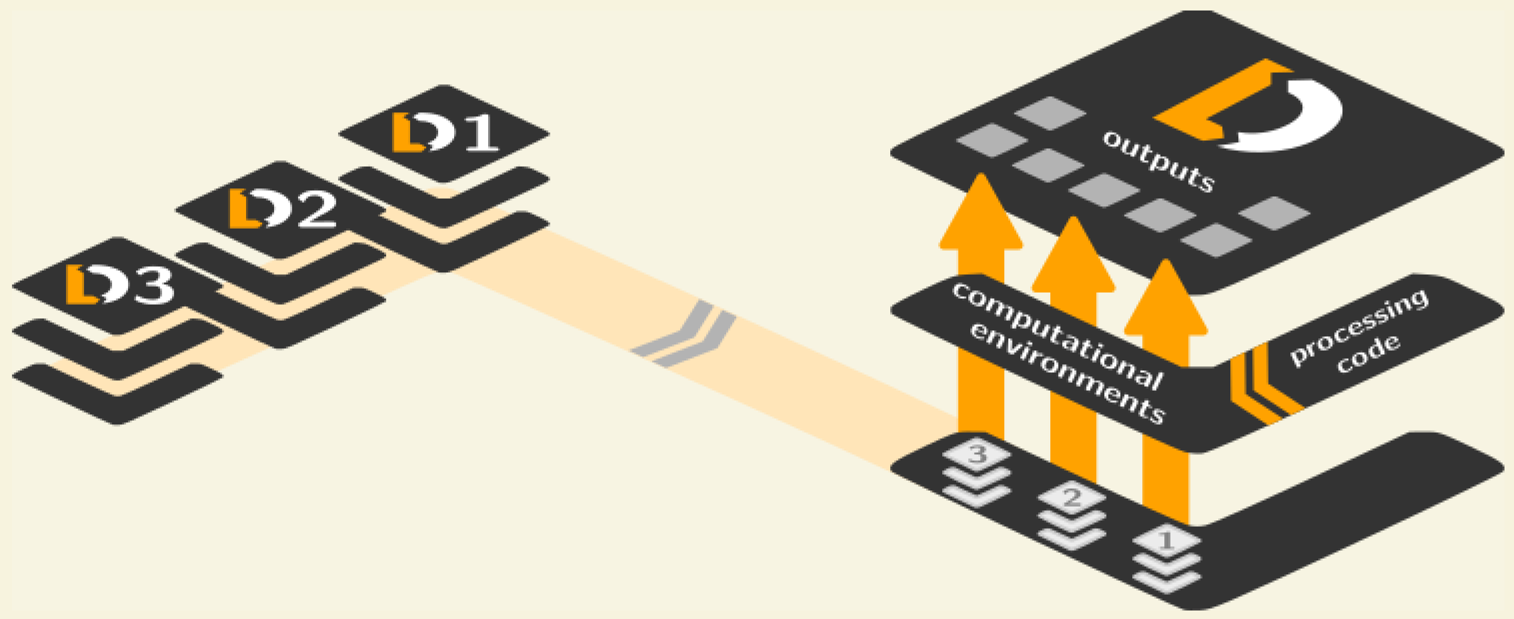
- Bundle all components of one analysis into one superdataset.
- Whenever a particular collection of files could anyhow be useful in more than one context (e.g. data), put them in their own dataset, and install it as a subdataset.
- Keep everything clean and modular: Within an analysis, separate code, data, output, execution environments.

P2: RECORD WHERE YOU GOT IT FROM, AND WHERE IT IS NOW



- Link individual datasets to declare data-dependencies (e.g. as subdatasets).
- Record data's orgin with appropriate commands, for example to record access URLs for individual files obtained from (unstructured) sources "in the cloud".
- Keep a dataset self-contained with relative paths in scripts to subdatasets or files.
- Share and publish datasets to collaborate.

P3: RECORD WHAT YOU DID TO IT, AND WITH WHAT



- Collect and store provenance of all contents of a dataset that you create (more on this in later sessions).

HANDS-ON EXCERSISE

Objective: How would you get data into a dataset?

- Use github.com/datalad/example-dicom-functional as test data. Download branch `1block` as a **ZIP archive**.
- Log into `brainbfast`, get the data on `brainbfast`, and try to get this data into a DataLad dataset with a sensible structure suitable for data analysis.
- This excersise is meant for **exploration**:
    - use `datalad --help`, the handbook, or the documentation at docs.datalad.org to find out about available commands to solve this task,
    - use tools of your choice to download/extract data,
    - try to set up an appropriate dataset structure.

HANDS-ON SOLUTION

- transform the zip folder into a DataLad dataset:

```
$ cd example_dicom_functional_block
$ datalad create -f
[INFO   ] Creating a new annex repo at [...]/example-dicom-functional-1block
create(ok): [...]example-dicom-functional-1block (dataset)

$ datalad save -m "add dicoms from functional acquisition" .
add(ok): LICENSE (file)
add(ok): dicoms/MR.1.3.46.670589.11.38317.5.0.4476.2014042516045740754 (file) [...]
```

- create a dataset for a data analysis (independent from the data directory)

```
$ cd ../
$ datalad create -c yoda myanalysis
[INFO   ] Creating a new annex repo at [...]/myanalysis
[INFO   ] Running procedure cfg_yoda
[INFO   ] == Command start (output follows) =====
[INFO   ] == Command exit (modification check follows) =====
create(ok): [...]/myanalysis (dataset)
```

- create a data directory and install the dicom dataset as a subdataset

```
$ cd myanalysis
$ mkdir data
$ datalad install -d . -s ../example_dicom_functional_1block data/dicoms
[INFO   ] Cloning ../example-dicom-functional-1block into '[...]/myanalysis/data/dicoms'
install(ok): data/dicoms (dataset)
action summary:
  add (ok: 2)
  install (ok: 1)
  save (ok: 1)
```

Hands-on: Explore this dataset

FURTHER READING

You will find the topics of this session in more detail in the following chapters of the handbook:

- **The basics on datasets:**
  - Chapter DataLad Datasets in the handbook.
- **Best practices for data analyses in datasets (YODA):**
  - The section YODA principles in the handbook.
- **A preview into automatically reproducible analyses in datasets:**
  - Usecase "An automatically reproducible neuroimaging analysis of public data" in the handbook.

OUTLINE: WHAT COMES NEXT?

- DataLad is installed on the cluster, try it out further, and ask questions on GitLab.
- Sessions will start with open question time about a past excersise, and end with an excersise for the upcoming session.
- Upcoming topics: Reproducible analysis, collaboration, INM-7 specific workflows on data retrieval & JSC.
- **Which date is suitable?** > Doodle poll <

QUESTIONS?