Universität Münster

CIT

# DataLad – A users view

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# Part I

# Basics and concepts

# Motivation

## Why even bother?

Computational analysis and computers are ubiquitous in science.

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  - easy typesetting, plotting, access to papers
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- What to do?

# FAIR?[1]

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- **F**indable ⇒ (Machine readable) Metadata? (Domain specific) Index or Search?

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⇒ How do we implement this?

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# Provenance and Reproducibility

## As a road to FAIRness

You could...

... link data to final paper...
... link previous data to final results...
... give your data a DOI or similar...
... license your code...
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... to...

- ... enable others to use your data.
- ... build trust in your data.
- ... make it more findable.
- ... aid for yourself and later projects.

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Software-wise:

- (version controlled) Open-Source Software
- fixed software stack (e.g. one compiler, one `python` version...)
- use tools to make your life easier: `make`, `just`, `snakemake`...

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- *Track transformations* $\rightarrow$ *version controlled?*

# DataLad – to the rescue

## What is DataLad?

In their words:

DataLad is a free and open source distributed data management system that keeps track of your data, creates structure, ensures reproducibility, supports collaboration, and integrates with widely used data infrastructure.[2]

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- Tracks data transformations
- Reproducible
- Version control via git
- Data back-end git-annex
- distribute data

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- help with metadata and labelling
- data is read-only by default, conscious unlock needed

# Installation

- current version: 1.1.0 (7.5.2024)
- written in `python`
- use package `datalad-installer` to search for the easiest way to install it on your system
- relies on `git` and `git-annex`, which need to be installed
- for Linux: `git` and `python` are everywhere, `git-annex` can be installed easily on mayor distros, otherwise compile yourself with GHC

# Basic usage

Kind of git...

```
$ datalad create <path> // git init <path>
$ datalad save -m "message" <path> // git add <path> && git commit -m
"message"
$ datalad clone <url> // git clone <url>
$ datalad status // git status
$ datalad siblings // git remote -v
```

+ all git commands that you know and love :)

# Basic usage

...plus some extras

```
$ datalad create-sibling-[github/gitlab/gitea/ria/...] // automatically set up a new siblings of the given type
$ datalad unlock <path> // unlock given file to alter it
$ datalad install <url> // clone-like
$ datalad get <path> // get a file from a remote location
$ datalad run <cmd> // run command and commit changes to the dataset
$ datalad rerun <commit-id> // rerun the command belonging to a certain commit
$ datalad gooey // GUI
$ datalad copy-file <src> <dest> // copy a file from one repo to another and note where to find this file
```

This is not exhaustive! Look at the documentation!

# Code-Along I

# Basics

# What have we seen?

- How to make a dataset
- What is tracked in a dataset
- How to bind another dataset in the first one
- What `datalad run` and `datalad rerun` does
- placeholder files $\neq$ content files
  - content in `.git/annex`-directory
  - `git-annex` keeps track of where the contents are (local and remote)

# Part II
# Cluster Usage

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- push data to websites and other servers ⇒ easily make independent backups

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## Pros and Cons

- Pros:
  - provenance & data versioning on cluster
  - reproducible workflow
  - easier distributed computing
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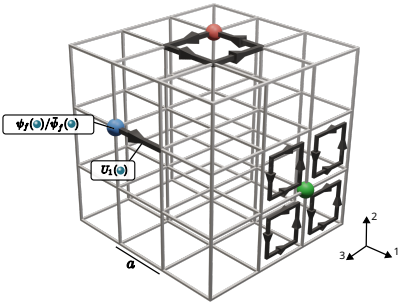
$\Rightarrow$ Need to find a workaround for that in our workflow

# Intermezzo: Technical side of Lattice QCD

How does this map to my own research?

- non-perturbative description of the strong interaction
- Discretize space-time on a 4D-lattice
- Solve high dim. integrals with Monte-Carlo techniques
- usually done in three steps (generation $\rightarrow$ calculation $\rightarrow$ analysis)
- generation and calculation steps are highly computationally expensive $\Rightarrow$ prime candidate for HPC




©Jan Neuendorf

# My daily workflow

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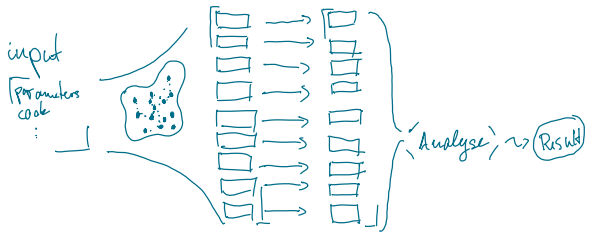
- Calculate basic observables on Monte-Carlo samples
- Analyse in `python`
- include statistics
- Look at results



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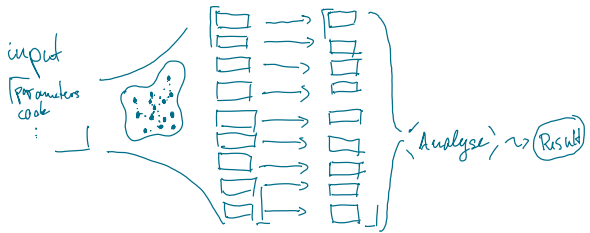


- How do we track this?

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## provenance data and content

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- How do we do this with the tools at hand?

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## ria-stores

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$\Rightarrow$ let's take this as our content-storage!

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- take care of parallel workflows:
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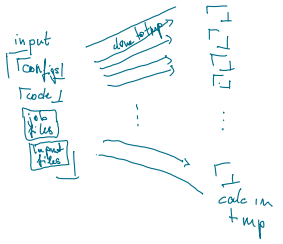


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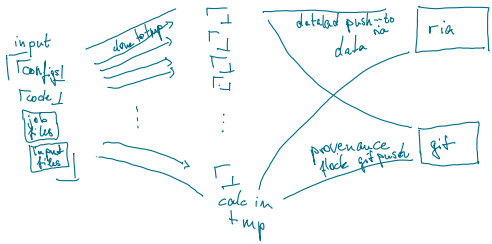


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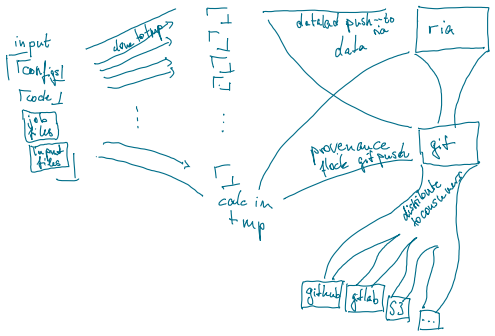


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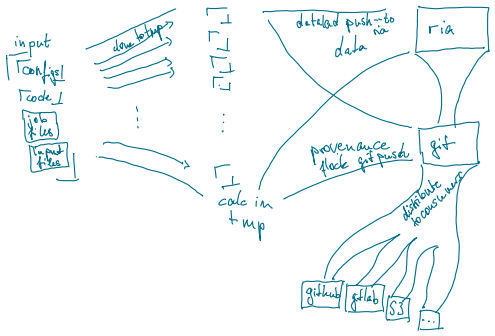


- Careful, in the end you have your data twice... please delete your data once you are done.

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# Code-Along II

# Cluster setup

# Conclusions

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## Take-home messages

- DataLad can help us to make our research more reproducible
- this in turn helps to adhere to the FAIR principles
- takes more time, but its time well invested
- setup for analysis fairly easy
- setup on cluster more complicated, but worth your time

# Additional content and further reading

The datalad Website:
`https://www.datalad.org/`
The handbook:
`https://handbook.datalad.org/`
The cheat-sheet:
`https://handbook.datalad.org/en/latest/basics/101-136-cheatsheet.html`
The FAIR principles:
`https://www.go-fair.org/fair-principles/`
The documentation of git-annex:
`https://git-annex.branchable.com/`