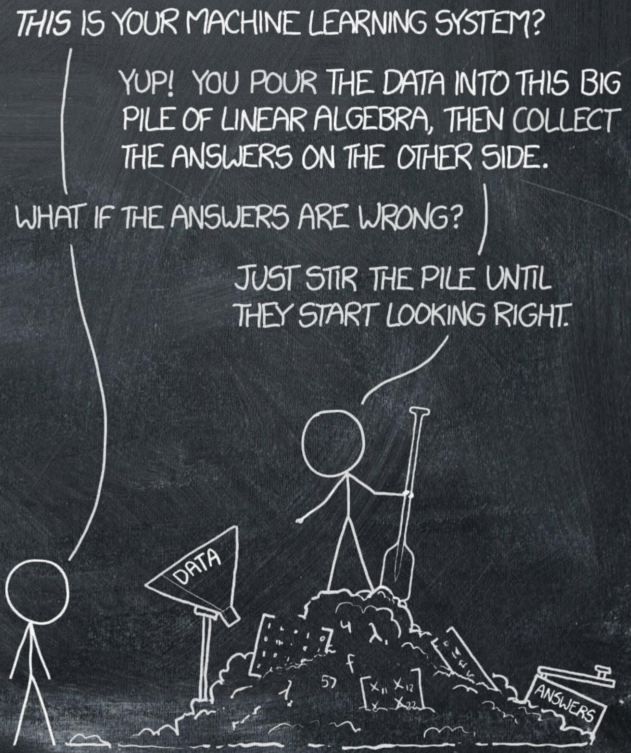
A desperate guide to data analysis workflow improvements

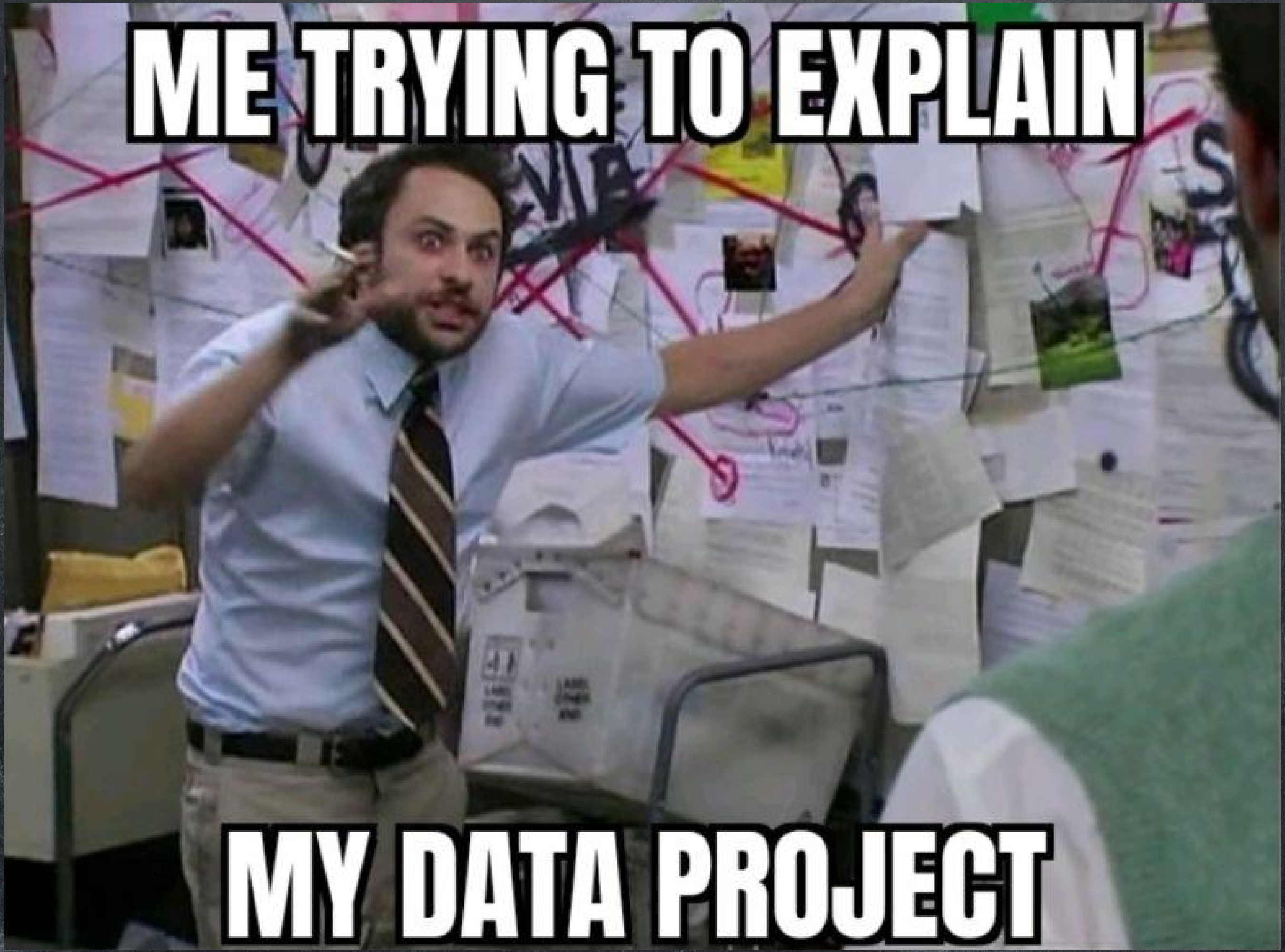
Peter Regner

“Reproducible Data Analysis”
Data Science @ BOKU initiative

2024-02-29
BOKU Wien


THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

https://xkcd.com/1838/


ME TRYING TO EXPLAIN
MY DATA PROJECT

Our goal: reproducibility!

...but in practice:

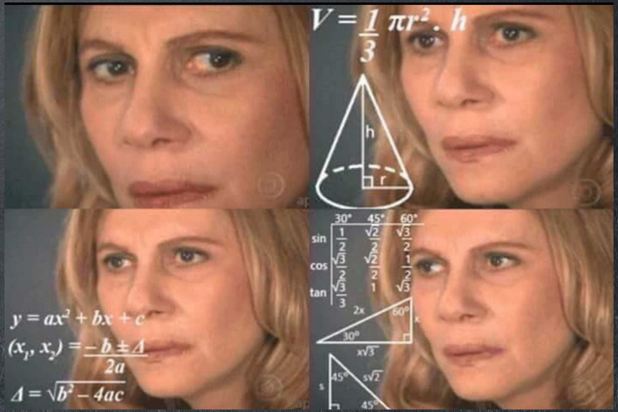
nobody re-runs it or it is broken

irreproducibility by hardware demands

irreproducibility by obscurity

traceability

comprehensibility



some users might be interested mostly in results

Make things more usable - for yourself and others!

Reproducibility in practice: How easily can somebody use the thing later?

Think about your target audience to set priorities!

Do they want to…

- re-run all your scripts?
- run the code as piece of software?
- use the code and adapt it?
- use the computation results only?
- understand what and how we did it?

7 Steps towards more use-able data analysis projects

Gamification: count every ✓, if you follow the guideline already!

(1) Publish your result data sets ✓

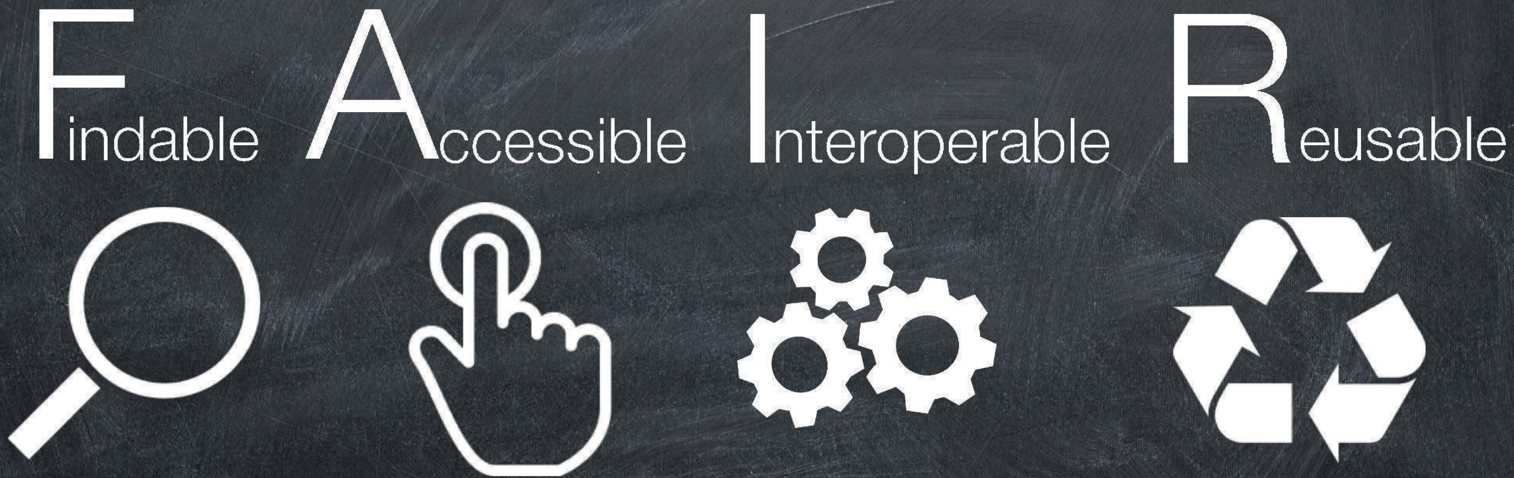
Wicherts, J. M., Bakker, M., & Molenaar, D. (2011). **Willingness to Share Research Data Is Related to the Strength of the Evidence and the Quality of Reporting of Statistical Results**. In R. E. Tractenberg (Ed.), PLoS ONE (Vol. 6, Issue 11, p. e26828). Public Library of Science (PLoS). https://doi.org/10.1371/journal.pone.0026828

Willingness to Share Research Data

is related to

Strength of the Evidence

(1) Publish your result data sets: in a fair way!



Findable Accessible Interoperable Reusable

https://www.go-fair.org/fair-principles/
https://doi.org/10.1038/sdata.2016.18

by SangyaPundir under CC-BY-SA 4.0

(1) Publish your result data sets: how?

✓ Use an open license if possible! (Allows others to publish your results as input data!)

✓ Label and document the fields of your result data set properly

✓ A CSV or NetCDF file on Zenodo is already pretty good

✗ tables in the PDF of the supplementary material

✗ non-open or non-standard file formats like *.gdx (GAMS)

✗ units for quantities not documented

More data providers: Dataverse, FigShare, AUSSDA, Dryad, Mendeley Data, DataHub, DANS, EUDat, ...

(2) Publish your Code ✓

- use an open license, e.g. MIT license or CC-BY ✓ (unless you need GPL libraries)
- For maintained projects: Use GIT / Github ✓
- Include a README file ✓
  - What does it do? (summary & link to article) ✓
  - Requirements: hardware & software ✓
  - How to run / use the thing ✓

(3) Use reproducible virtual environments ✓

Virtual environments (e.g. Conda) allow you to:

- Multiple versions of a library on one machine
- Pretty portable (Windows, Linux, Mac OS)
- Easier to use than Docker

...and to export all used libraries & precise versions!

Alternatives to conda: renv, pipenv, ...

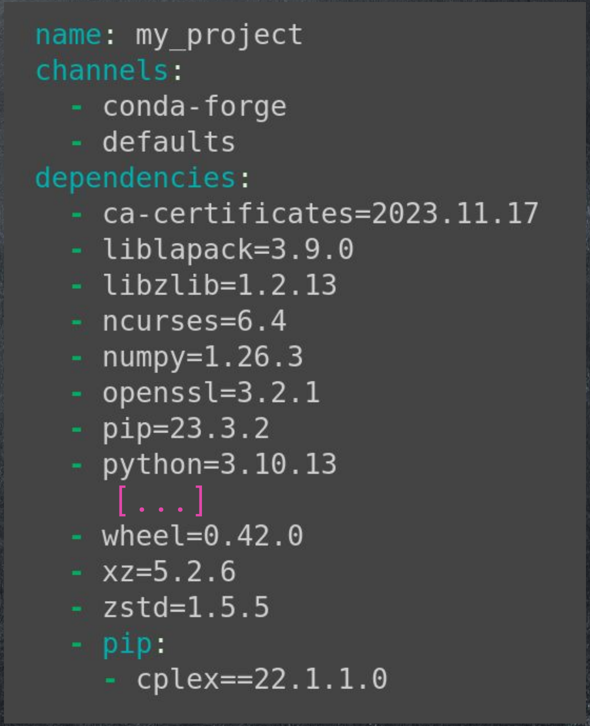
Export all used dependencies using conda: ✓

```
conda env export --no-builds | grep -v "^prefix: " > env.yml
```

Use micromamba - conda is too slow! ✓

https://mamba.readthedocs.io/en/latest/installation/micromamba-installation.html

env.yml:



```
name: my_project
channels:
   - conda-forge
   - defaults
dependencies:
   - ca-certificates=2023.11.17
   - liblapack=3.9.0
   - libzlib=1.2.13
   - ncurses=6.4
   - numpy=1.26.3
   - openssl=3.2.1
   - pip=23.3.2
   - python=3.10.13
       [...]
   - wheel=0.42.0
   - xz=5.2.6
   - zstd=1.5.5
   - pip:
     - cplex==22.1.1.0
```

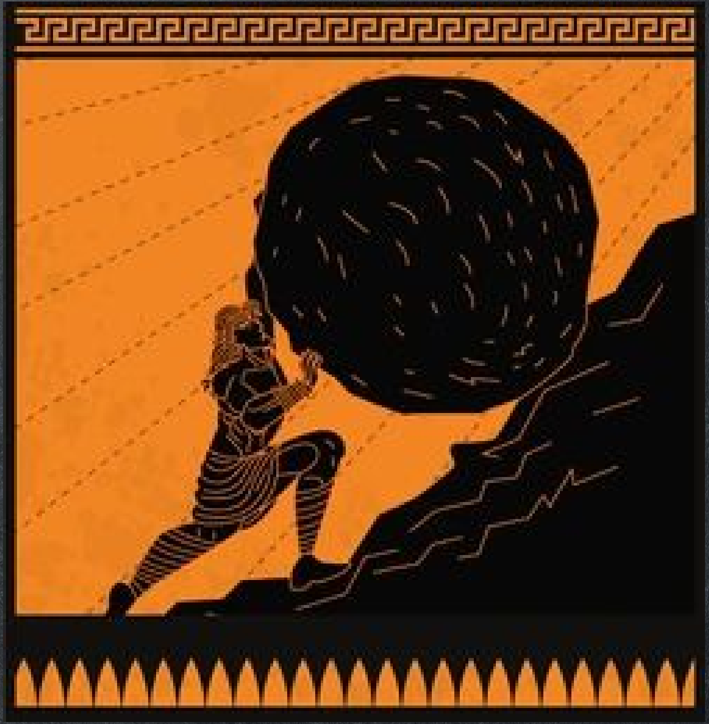
(4) Automate everything

Manual steps are...

- error prone
- time consuming
- not documented

Every command or click should be stored in a way, such that it can be executed again!

Be realistic! You will do things over and over again...



But you can automate all steps!

Please don't take this too literally!

(4) Automate everything

Goal: a single executable script ✓

- download of input data
- preprocessing
- computation
- write results to files
- create figures

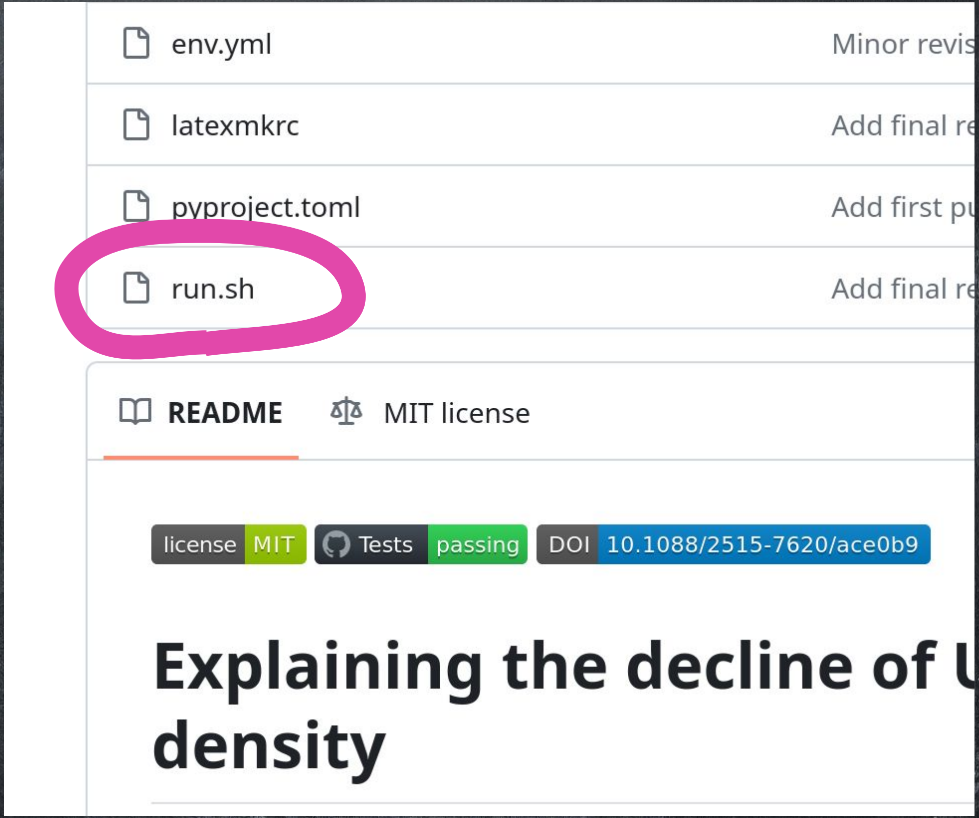
article

LaTeX

or

quarto

how to & links in bonus slides



env.yml	Minor revis
latexmkrc	Add final re
pyproject.toml	Add first pu
run.sh	Add final re

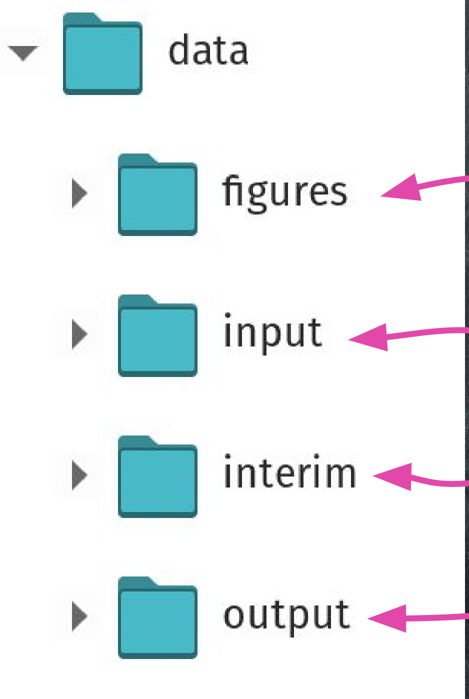
README MIT license

license MIT | Tests passing | DOI 10.1088/2515-7620/ace0b9

Explaining the decline of U density

https://github.com/inwe-boku/windpower-decomposition-usa

(5) Use a good folder structure ✓



ideally PDF files, directly used by LaTeX

raw input files, not modified after download

large files, less important interim results

results to be published

(5) Use a good folder structure

your project

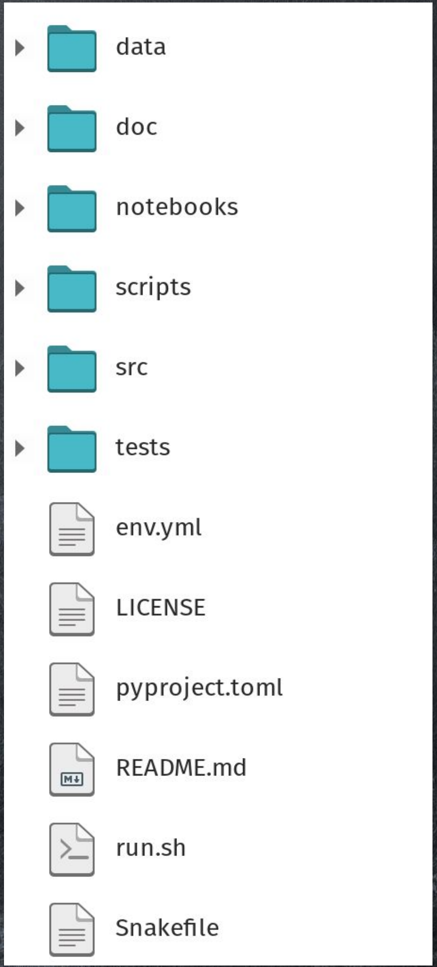
Follow common conventions!

- no spaces in file names ✓
- file names in lower case or ALL_CAPS ✓
- avoid CamelCase for files and folders ✓

auto-create from templates

COOKIECUTTER ✓

https://github.com/cookiecutter/cookiecutter



data
doc
notebooks
scripts
src
tests
env.yml
LICENSE
pyproject.toml
README.md
run.sh
Snakefile

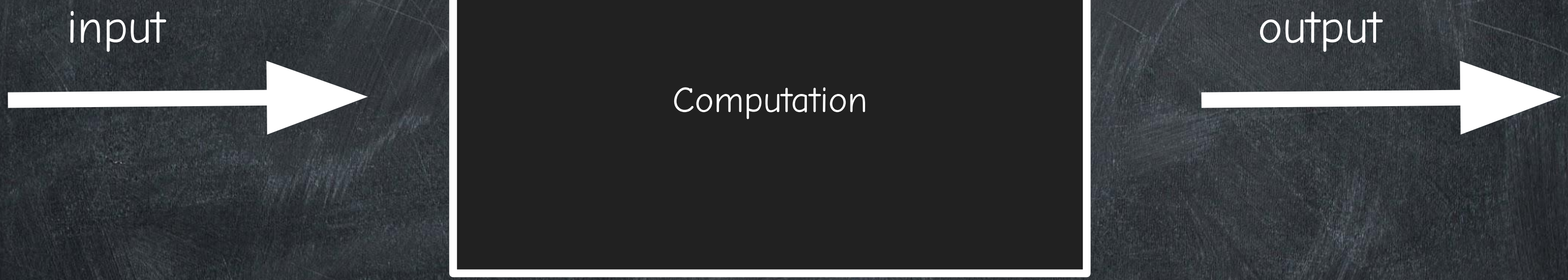
Literature:

[1] G. Wilson, J. Bryan, K. Cranston, J. Kitzes, L. Nederbragt, and T. K. Teal, “**Good enough practices in scientific computing,**” PLOS Computational Biology, vol. 13, no. 6, p. e1005510, Jun. 2017, doi: 10.1371/journal.pcbi.1005510.

[2] W. S. Noble, “**A Quick Guide to Organizing Computational Biology Projects,**” PLOS Computational Biology, vol. 5, no. 7, p. e1000424, Jul. 2009, doi: 10.1371/journal.pcbi.1000424.

[3] “**Cookiecutter Data Science.**” https://drivendata.github.io/cookiecutter-data-science/

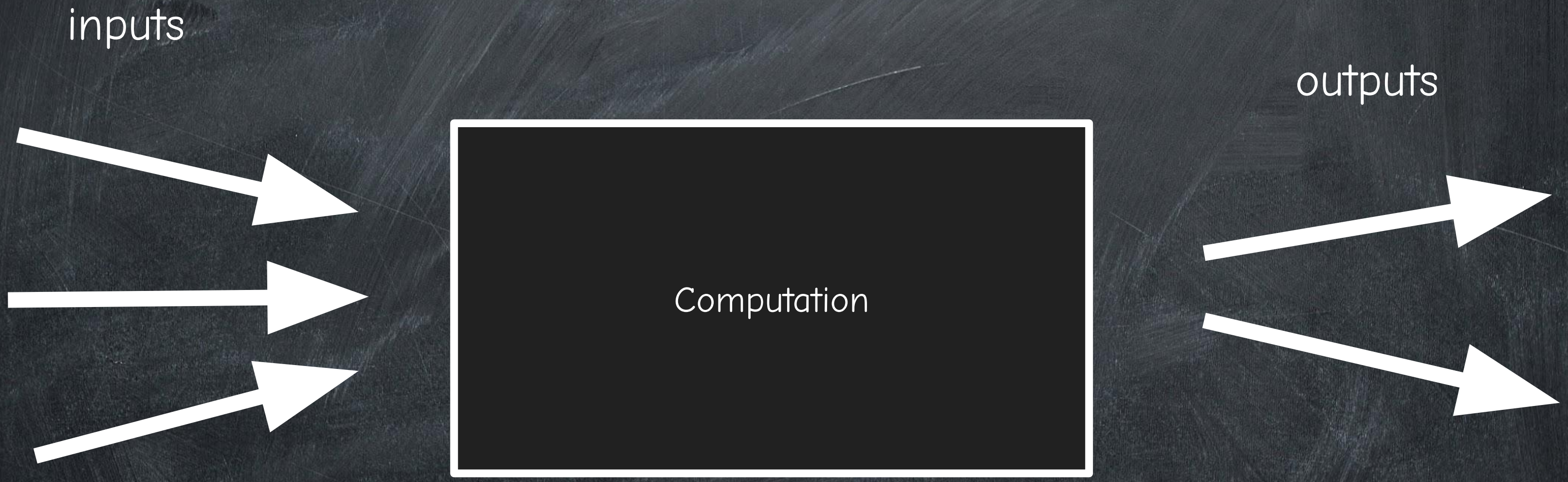
Organize your computation pipeline



input

Computation

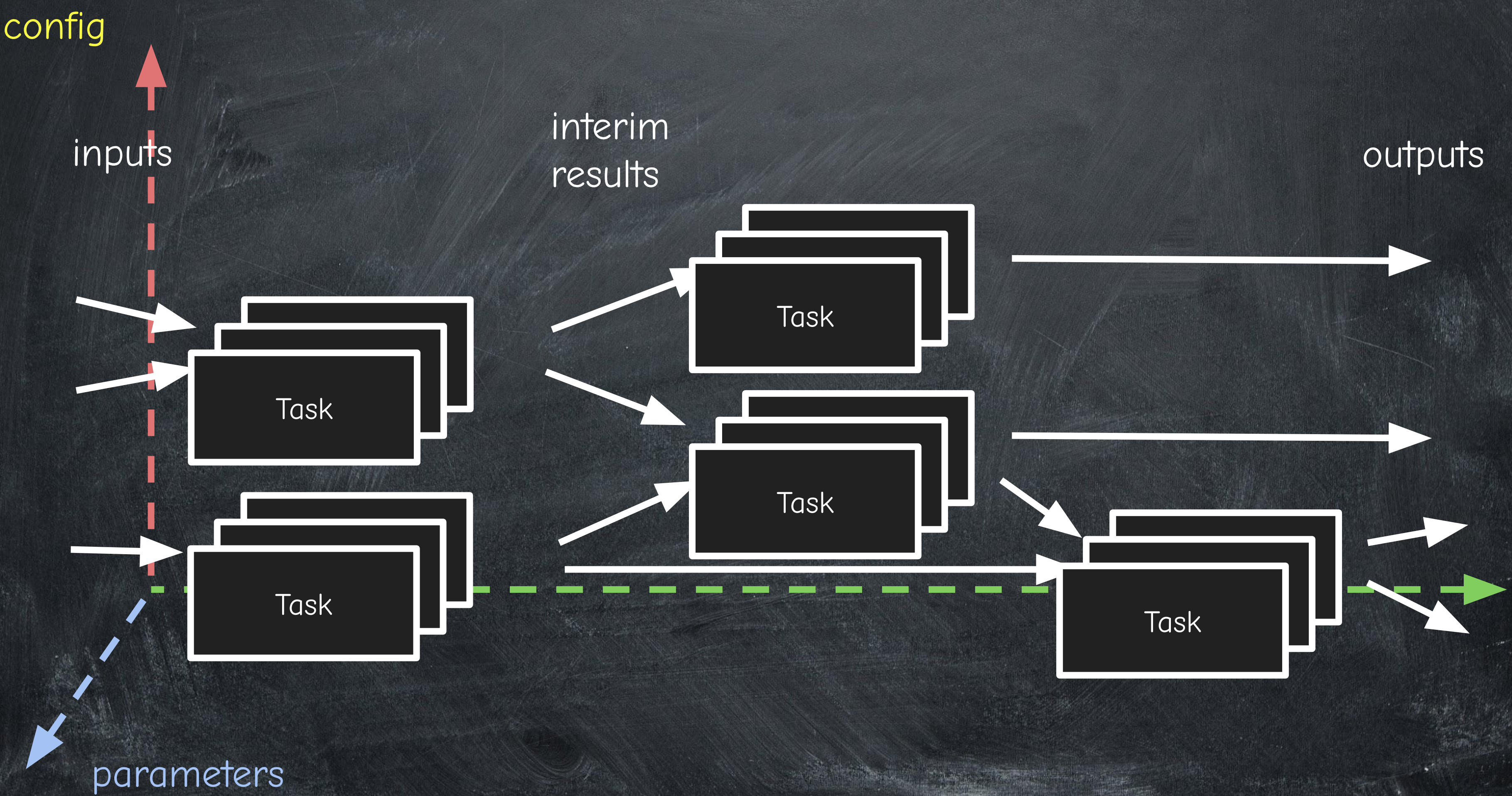
output



inputs

Computation

outputs


config
inputs
interim results
outputs
Task
Task
Task
Task
Task
parameters

(6) Use a pipeline tool ✓

- Caching / incremental builds
  → skip tasks if nothing changed (inputs, code, config, parameters)

- Parametrizing tasks
  → specify (multi dimensional) parameter spaces via ranges or lists

- Run tasks in parallel
  → on different CPUs or on different nodes on a cluster (e.g. VSC)

Ruffus Rabix KNIME Analytics Platform Fission Workflows Polynote Gwf

Dask Sushi Stpipe ActivePapers Workflow Patterns Initiative

Reflow Pydra Common Workflow Language

OpenMOLE DSL Mario Remake Anduril Yet Another Workflow Language Workflow Patterns Library Redun

pyperator Zeppelin Flyte Arvados

TaskGraph Factual's Drake SciLuigi Pentaho Kettle Makeflow Argo Balsam noWorkflow

Sake Adage Joblib Antha

LinkedPipes ETL Swift Just Snakemake

pyppl Cadence Drake R package Nextflow Clusterjob Pinball

ecFlow Zenaton VisTrails Seqtools Bistro Ophidia

Compss Substation Consecution

Mistral Workflow Description Language

Cosmos Signac

BioMake Moa Luigi Domino Quilt OpenGE

NiPype Dagster Bioshake Digdag Ruigi

d6tflow Ketrew Toil

Pathomx Clubber Cluster Flow Pegasus PipEngine ResearchObject.org

Kepler Hamilton Kestra

SoS ActionChain Martian Dbt Orchest Apache Iravata Workflow 4 Ever workflow research object model pypyr AWE

Workflow 4 Ever Initiative Conan2

Watchdog Sundial Galaxy Targets Reprozip SciPipe

DataJoint doit

Dockerflow Yap Shake Parsl Tibanna Wallaroo Mara Drake

QsubsecBinder Porcupine Wings

HyperLoom Cromwell

lakeFS APE Scons Longbow Spiff MetaFlow Dataform Bpipe

BazelCompi FlowHub

Couler BioQueue Rubra

Nessie Stolos Steppy Yabi ZenML SmartPipeline

Ploomber Suro DVC Yapp

StreamPipes RedPoint Notebooks

omega|ml DataOps Platform AiiDA OpenMOLE Ray

Rain Fireworks Briefly Kedro NextflowWorkbench Kronos WorldMake Polyaxon Guix Workflow Language

Qdo Loom Popper Kiba ETL Prodmodel

Reana CDS PyFlow Flex Maestro Temporal

Piper StreamFlow Arteria Gc3pie Flowr

Chipster Covalent Pachyderm Make DataLad Dagr

Butler Scoop Cloudgene Workflow Language Anvi'o

https://github.com/pditommaso/awesome-pipeline

Cuneiform Taverna Prefect Rmake Gradle Dray

HPC Grid Runner MD Studio

(7) Keep old versions of your data ✓

Re-running computations might be difficult or take long time... Keep old versions!

It would be nice to...

- know how artefacts (figures, output files, ...) were generated
  → record Git hash / code, all inputs, parameters, conda environment, config, ...
- delete large files later when disk space is an issue
- compare between different versions of data

Git alone is not enough to fulfill these requirements!

Note that Git offers more features:

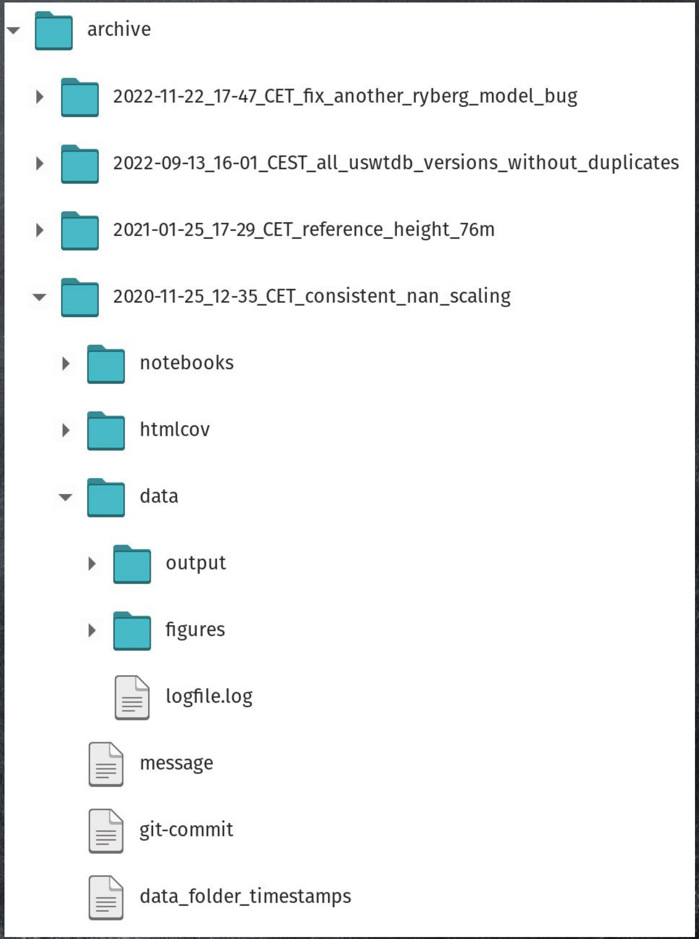
- Sync to other machines / collaboration with others
- Publish the repository - but data is not always publishable due to licence issues

Tools for large data: DVC, GIT-LFS, git-annex, DataLad, ...

My poor-man data versioning

`run.sh` script:

- runs the computation
- creates a Git tag
- copies outputs to an archive folder



```
archive
    2022-11-22_17-47_CET_fix_another_ryberg_model_bug
    2022-09-13_16-01_CEST_all_uswtdb_versions_without_duplicates
    2021-01-25_17-29_CET_reference_height_76m
    2020-11-25_12-35_CET_consistent_nan_scaling
        notebooks
        htmlcov
        data
            output
            figures
            logfile.log
        message
        git-commit
        data_folder_timestamps
```

Open issues:

- How to sync data between machines? Use Unison?
- How to collaborate with others using the same data?
- How to sync figures to Overleaf without Git?

https://github.com/inwe-boku/windpower-decomposition-usa/blob/main/run.sh

Cookies for all of you!

Everything we have seen today in a cookiecutter template:

- folder structure
- code snippet for including results in LaTeX
- Script for building a zip file for arXiv.org
- run.sh script
- Snakemake file
- README.md, .gitignore, LICENSE, …
- …

→ https://github.com/inwe-boku/cookiecutter-data-research

Reproduce all the things!

Download slides:

https://bit.ly/desperate-guide

peter.regner@boku.ac.at

https://github.com/inwe-boku/

https://refuel.world/

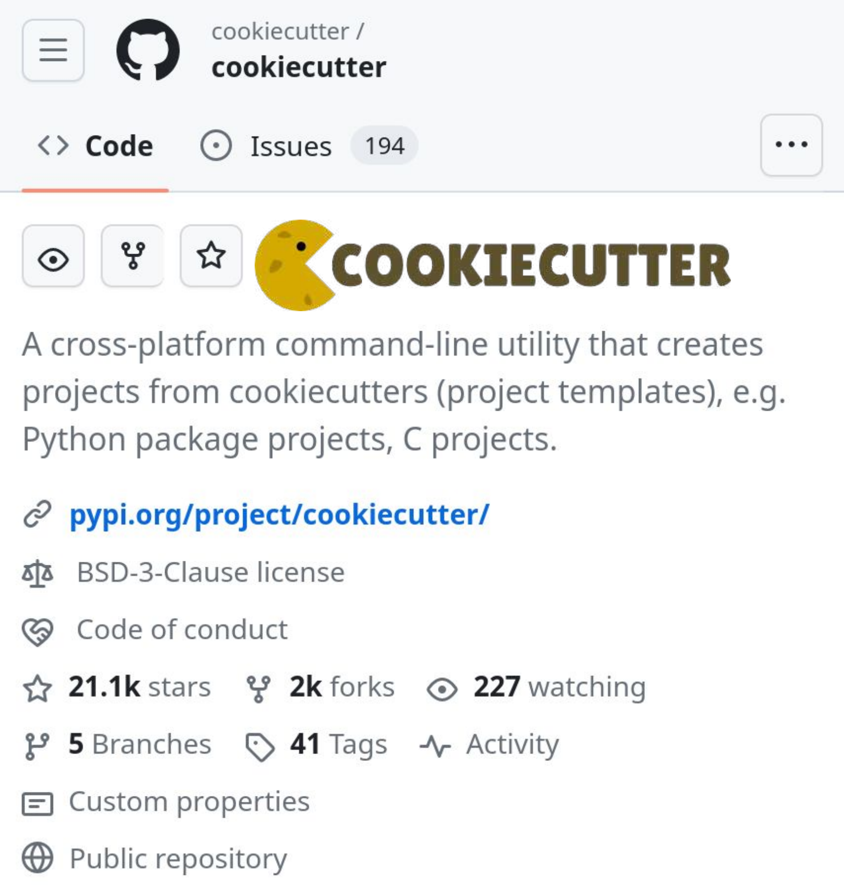
We gratefully acknowledge support from the European Research Council ("reFUEL" ERC-2017-STG 758149).

Automate project creation ✓

Create a new folder from a template:

- folder structure
- LICENSE file
- .gitignore file
- code snippets
- ...

https://github.com/cookiecutter/cookiecutter



cookiecutter / **cookiecutter**

A cross-platform command-line utility that creates projects from cookiecutters (project templates), e.g. Python package projects, C projects.

pypi.org/project/cookiecutter/

BSD-3-Clause license

Code of conduct

21.1k stars **2k** forks **227** watching

5 Branches **41** Tags Activity

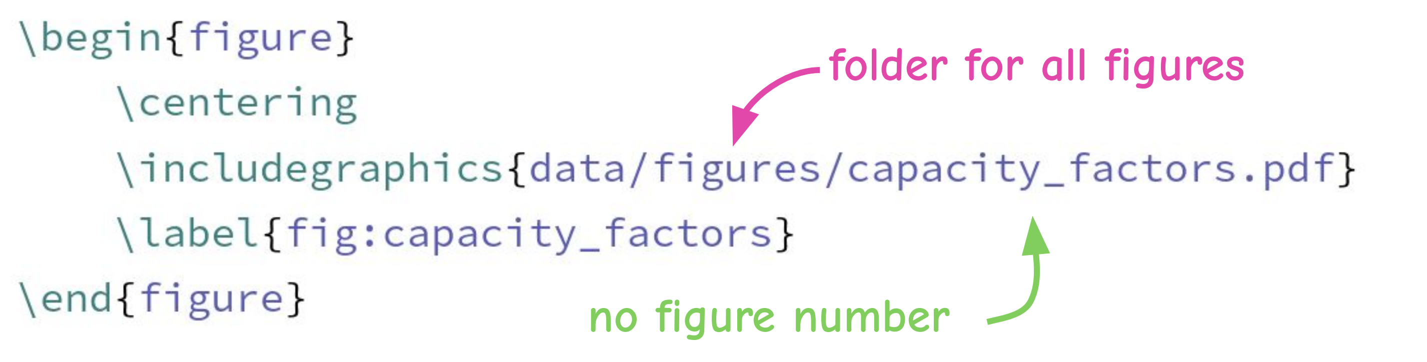
Custom properties

Public repository

Include figures in LaTex documents ✓

MS Word: use linked images

Latex:



```
\begin{figure}
    \centering
    \includegraphics{data/figures/capacity_factors.pdf}
    \label{fig:capacity_factors}
\end{figure}
```

folder for all figures

no figure number

Overleaf: use GIT, Github or dropbox to sync figures - premium only... :-/

https://www.overleaf.com/learn/how-to/Dropbox_Synchronization https://www.overleaf.com/learn/how-to/Git_Integration_and_GitHub_Synchronization

Include results in LaTex documents ✓

Turns out to be surprisingly difficult! 😱

```
result_values = {}

meaning_of_life = 42
result_values['meaning_of_life'] = f'{meaning_of_life:d}'

gravity_ms2 = 9.80665
result_values['gravity'] = f'{gravity_ms2:.2f}', 'm/s^2'

write_result_values(result_values)
```

script writes results to a file with custom LaTeX commands

```
\newcommand{\meaning_of_life}{42}
\newcommand{\gravity}{\qty{9.81}{m/s^2}}
```

auto-generated LaTeX commands

More details and other Solutions like Knitr:
https://tex.stackexchange.com/a/711627/8964

Do more good things

- Write good code
  - Don't do no magic numbers ✓
  - No absolute file paths ✓
  - No unnecessary Abbrev. ✓
  - Follow code conventions (e.g. pep8) ✓
- Write unit / functional tests ✓

  Automatically check if things are behaving as expected!
- Use a code linter (e.g. as GIT hook) ✓

  Tools to automatically check code for errors and style violations, for Python: flake8, black (auto-formatter),
- Use Continuous integration ✓

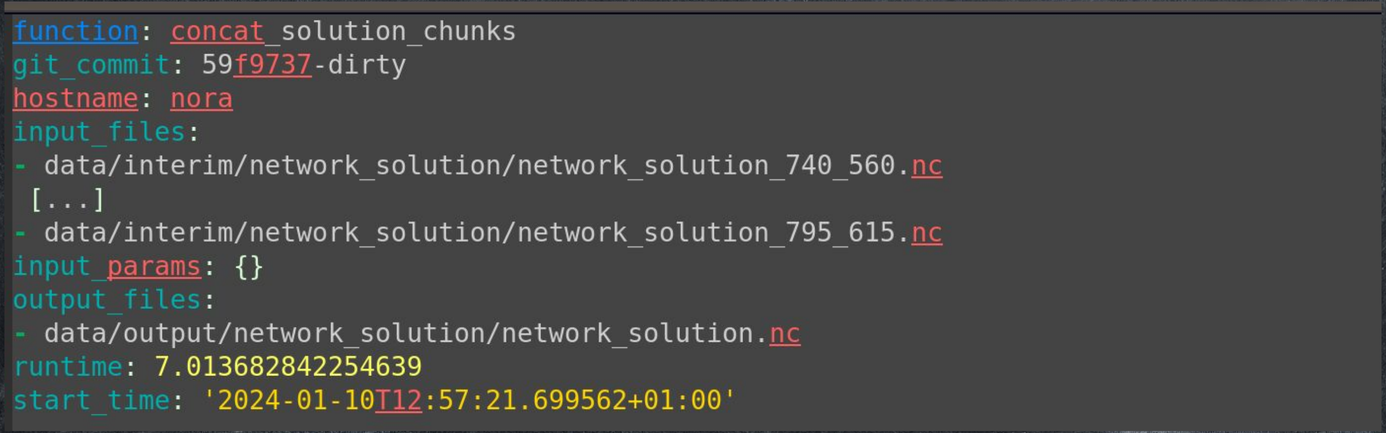
  Run tests, code linter or computations automatically, e.g. via Github Actions
- Do code review ✓

  A great way to improve quality and spread knowledge in your team!

Tracking additional computation information

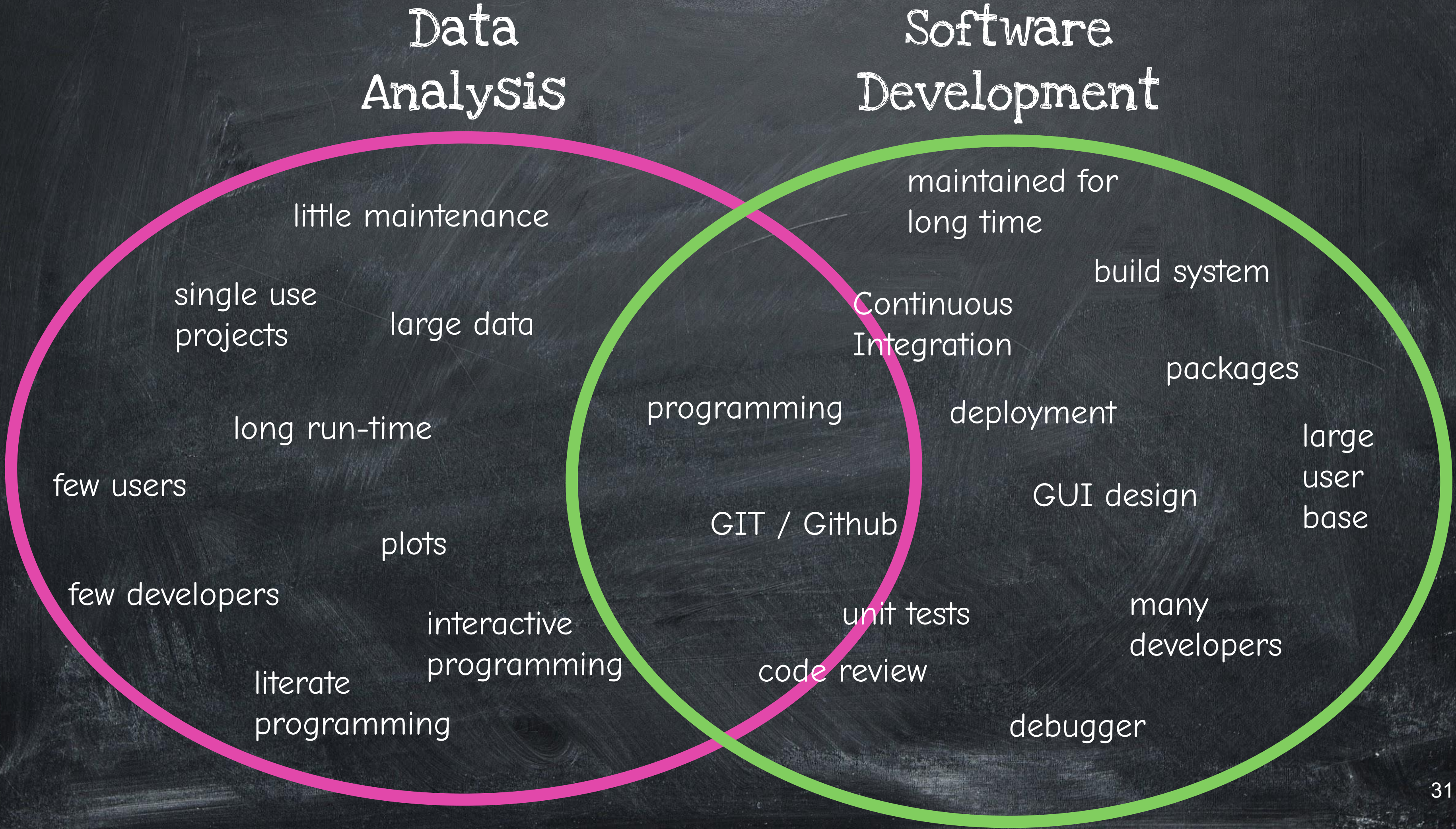
```
@task
def my_fancy_func(some_param, inputs, outputs):
    # do something here
    ...
```

The `@task` decorator creates a file with metaparameters for each output:



```
function: concat_solution_chunks
git_commit: 59f9737-dirty
hostname: nora
input_files:
- data/interim/network_solution/network_solution_740_560.nc
 [...]
- data/interim/network_solution/network_solution_795_615.nc
input_params: {}
output_files:
- data/output/network_solution/network_solution.nc
runtime: 7.013682842254639
start_time: '2024-01-10T12:57:21.699562+01:00'
```

Link to source: https://github.com/inwe-boku/cookiecutter-data-research/blob/main/%7B%7B%20cookiecutter.repo_name%20%7D%7D/src/task.py



Data Analysis

Software Development

little maintenance

single use projects

large data

long run-time

few users

plots

few developers

interactive programming

literate programming

programming

GIT / Github

unit tests

code review

maintained for long time

build system

Continuous Integration

packages

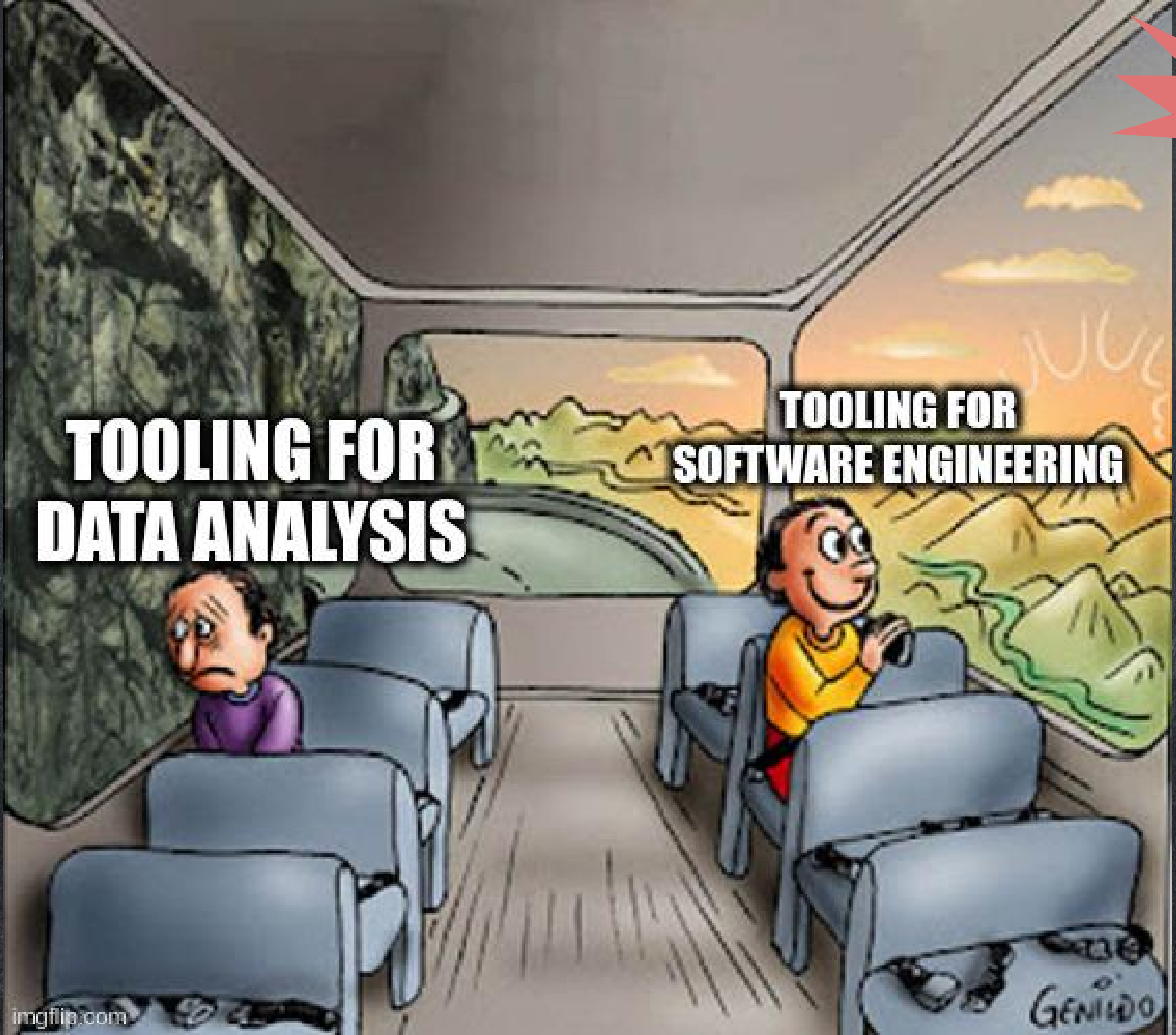
deployment

large user base

GUI design

many developers

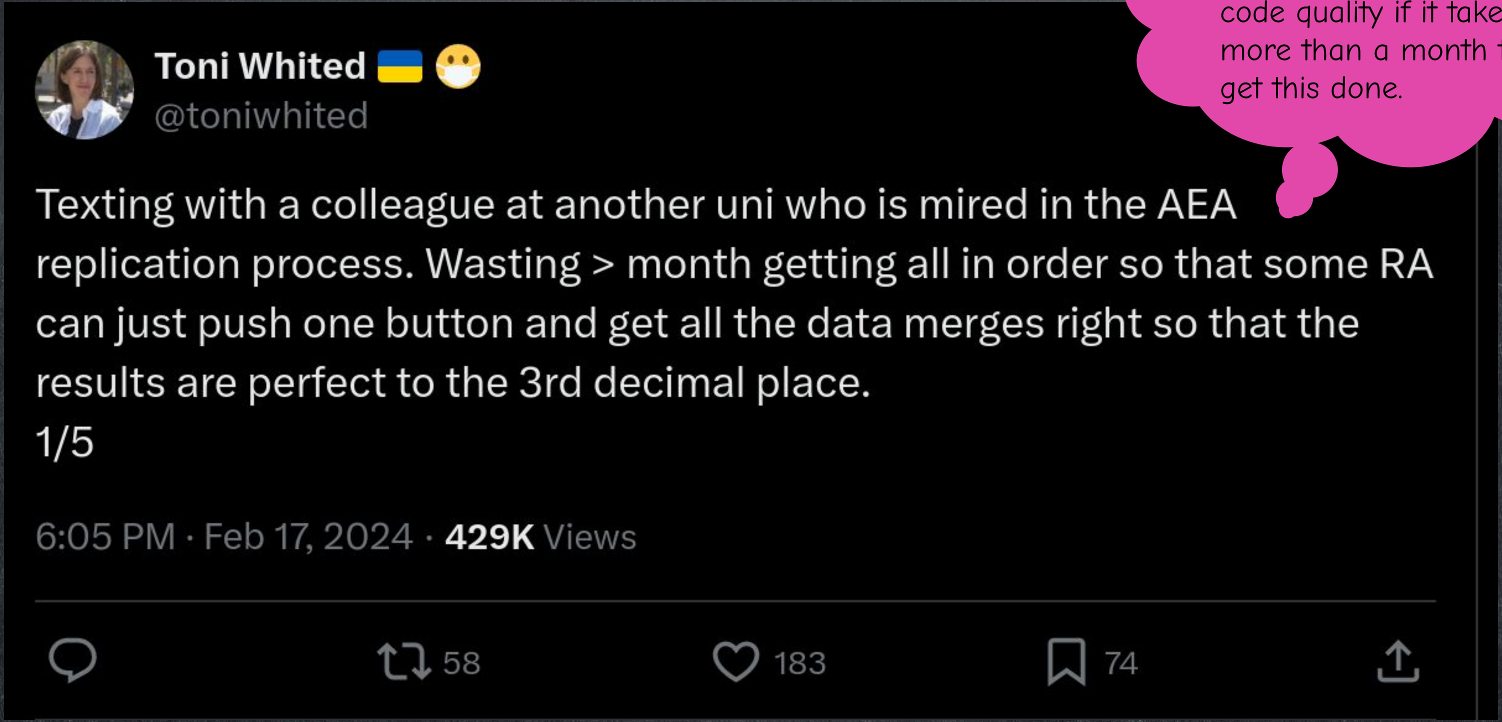
debugger



opinionated!

Reproducibility is a hot topic…

It should not be the only priority, but I'd be a bit skeptical about code quality if it takes more than a month to get this done.



Toni Whited 🇺🇦 😷
@toniwhited

Texting with a colleague at another uni who is mired in the AEA replication process. Wasting > month getting all in order so that some RA can just push one button and get all the data merges right so that the results are perfect to the 3rd decimal place.
1/5

6:05 PM · Feb 17, 2024 · **429K** Views

https://twitter.com/toniwhited/status/1758900448596291953