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Example: Astronaut Analysis

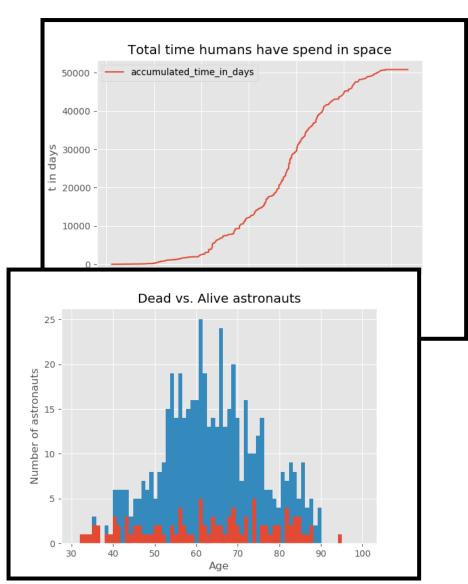


Astronauts Analysis is a data publication consisting of:

- Data set
- Analysis script written in Python using pandas and matplotlib
- Result plots

Scenario:

- I created it on my own as part of my job.
- I want to make its <u>reuse as easy as possible</u> and make it available under an open source license.



Make your code reusable



- Step 1: Put your code under version control
- Step 2: Make sure that your code is in a sharable state
- Step 3: Add essential documentation
- Step 4: Add a license
- Step 5: Release your code

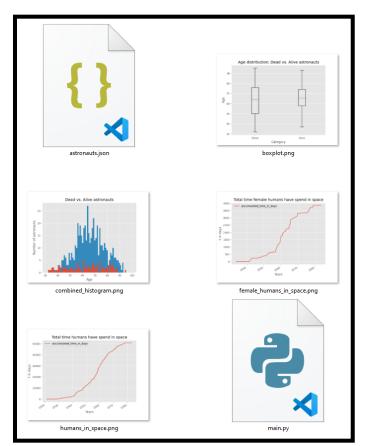
Essential aspects which you should try to already address for "internal" software!

Step 1: Put Your Code Under Version Control

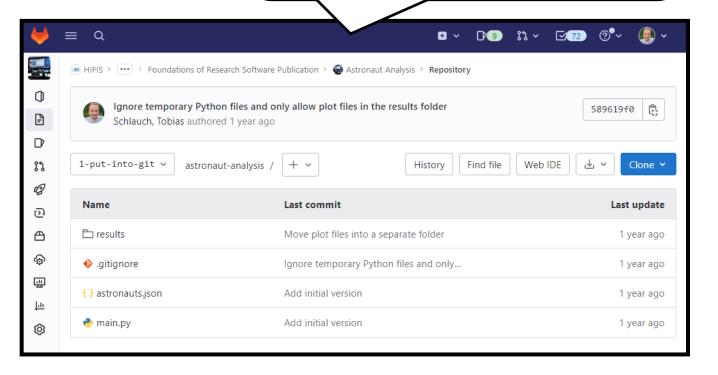
Where Should I Store My Code?

Minimum: Use a local Git repository + backup

Recommended: Use a code collaboration platform







Step 1: Put Your Code Under Version Control What Belongs in the Repository?



- Everything to make a usable version of your code such as:
 - Source code, documentation, build scripts, test cases, configuration files, input data, ...
- Avoid adding generated files such as:
 - Third-party libraries, generated binaries, ...
- How to handle large (data) files?
 - Available could be <u>git-lfs</u>, <u>git-annex</u>, <u>Datalad</u> or your research data management publication repository

Please note:

- Details depend on the "product" that you manage in the Git repository
- **.gitignore files** helps you to control what goes into your repository. See also https://gitignore.io/ for templates.

Step 2: Make Sure That Your Code Is in a Sharable State General Hints



- Make sure others can run your code:
 - No dependencies on internal resources (servers, storage, licensed software, ...)
 - No absolute paths
 - Clearly state dependencies + provide required build / installation scripts (e.g.: <u>pip-tools</u>, <u>poetry</u>) => crucial aspect of reproducibility
- Organize files in a suitable directory structure (e.g.: <u>Python Application</u> <u>Layouts</u>, <u>Good Data Practices</u>)
- Do not share sensitive data such as passwords, user accounts, SSH keys, internal IP addresses, etc. (e.g.: <u>gitleaks</u>)
- Orientate on standards of your domain / community

Step 2: Make Sure That Your Code Is in a Sharable State Improve Your Code Style and Structure



- Strive for understandable code:
 - Apply a code style consistency is more important than convenience (e.g.: <u>PEP8</u>)
 - Use a consistent and light code layout
 - Structure your code in suitable "building blocks" such as functions
 - Use specific and appropriate names for all artifacts
 - Provide sufficient level of code comments
- Read code of others for inspiration
- Try to do pair programming and reviews (even if it is with your rubber duck)

Step 2: Make Sure That Your Code Is in a Sharable State Think About Testing and Automation



- Small tests are done easily but already show effect:
 - Code linters and checkers help to find poor code snippets and help to enforce coding styles (e.g.: <u>flake8</u>, <u>black</u>)
 - Automated tests work as an executable documentation (e.g.: <u>pytest</u>)
- Tests offer a good starting point for your automation efforts!

Step 3: Add DocumentationGeneral Hints



Mind your target groups:

- Typical perspectives: Users, contributors
- **Users:** Installation / usage instructions, tutorials, support channels, ...
- Contributors: Contribution guidelines, technical overview, ...

Think about adding typical documentation files such as:

• README (project front page), CONTRIBUTING (contributions guidelines), CODE_OF_CONDUCT (communication rules), LICENSE (license information), CHANGELOG (major changes), CITATION (citation metadata)

Please note:

- Markdown or another markup language is quite often used to write documentation
- Usually, you will need additional documentation, for example, in a docs directory (e.g.: Sphinx, MkDocs)

Recommendations from the workshop "Foundations of Research Software Publication"



- Step 1: Put your code under version control
- Step 2: Make sure that your code is in a sharable state



- Step 3: Add essential documentation
- Step 4: Add a license
- Step 5: Make your code citable
- Step 6: Release your code

Goal - Provide a citable release



"The data set and the analysis code has been published separately [1]."

References:

[1] Schlauch, T. (2024). Astronaut Analysis (2024-03-20) [Data set]. Zenodo. https://doi.org/10.5072/zenodo.402763

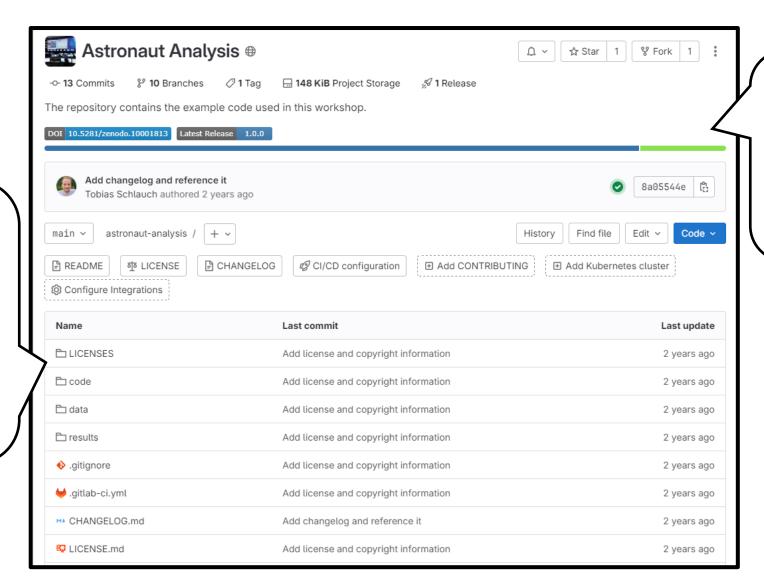
See also: <u>Software Citation Principles</u>

- ✓ Source code repository: We keep the repository in our own GitLab instance.
- ✓ Release versioning style: We use <u>calendar versioning</u>.
- ✓ Git tag style: Tags have the name of the release version number.
- ✓ Release package format: The release package is a "snapshot" of the repository content.
- ✓ Citation metadata: Part of the source code repository in the Citation File Format.
- ✓ Publication repository: We only use Zenodo to publish/archive our releases.

Astronaut Analysis Release



License information for code, data, results properly annotated via REUSE



Release
1.0.0 marked
as Git tag in
the repository

Astronaut Analysis Release

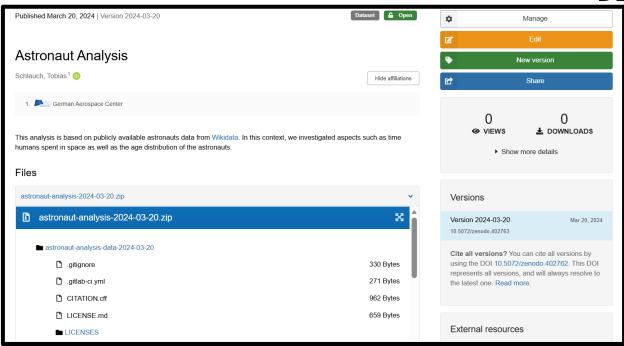


DOI 10.5072/zenodo.402763

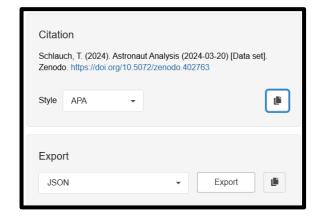
cff-version: 1.2.0 title: Astronaut Analysis message: >-If you use this analysis, please cite it using the metadata from this file. type: dataset authors: - given-names: Tobias family-names: Schlauch email: tobias.schlauch@dlr.de affiliation: German Aerospace Center (DLR) orcid: 'https://orcid.org/0000-0001-8760-8913' identifiers: - type: doi value: 10.5072/zenodo.402762 description: Conceptual DOI



- Citation metadata in Citation File Format
- DOI via Zenodo







Summary



- Step 1: Put your code under version control
- Step 2: Make sure that your code is in a sharable state



- Step 3: Add essential documentation
- Step 4: Add a license
- Step 5: Release your code



Impressum



- Content created based on DLR/HIFIS training "Foundations of Research Software Publication" and example project "Astronaut Analysis"
 - https://codebase.helmholtz.cloud/hifis/software/education/hifis-workshops/foundations-of-research-software-publication/workshop-materials
 - https://codebase.helmholtz.cloud/hifis/software/education/hifis-workshops/foundations-ofresearch-software-publication/astronaut-analysis

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