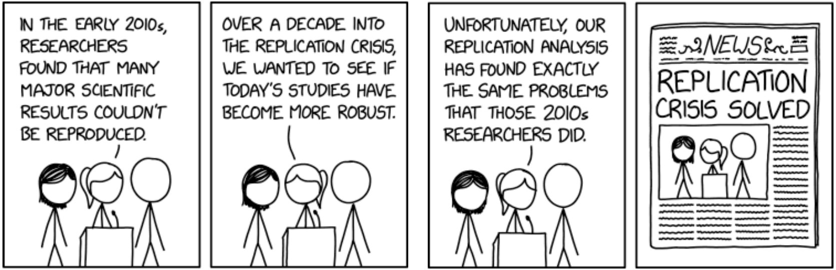
Practical tools for reproducible experimental analyses

Charlie J. Paxman (GANIL)

EURO-LABS ATS: Collaborative Software, Feb 2026



xkcd #3117

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L. A. Barba (2018)[1]

Repeatable	Same team, same setup
Replicable	Diff. team, same setup
Reproducible	Diff. team, diff. setup

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[1] *Terminologies for Reproducible Research*, arXiv, `https://doi.org/10.48550/arXiv.1802.03311`

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X. Chen *et al.* (2019)[2]

Repeat	Same team, setup, lab
Reproduce	Diff. team, setup, lab
Rerun	Variation, same lab
Replicate	Same setup, different lab
Reuse	New independent discovery

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[2] *Open is not enough*, Nature Phys. **15**, 113–119 (2019). `https://doi.org/10.1038/s41567-018-0342-2`

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- What we're talking about...

‘The Turing Way’[2]	
Reproducible	Same analysis, same data
Replicable	Same analysis, diff data
Robust	Diff analysis, same data
Generalisable	Diff analysis, diff data

Finally ran out of "R" words...

---

[2] `https://book.the-turing-way.org/reproducible-research/overview/overview-definitions/` (Accessed 28/01/2026)

What is Reproducibility?

For our purposes, we care about **computational reproducibility**:

Computational Reproducibility

"[computational] reproducibility is obtaining consistent results using the **same input data; computational steps, methods, and code;** and conditions of analysis." [3]

- Can be performed by a different person, different machine, at a different time

⇒ Without relying on personal knowledge of the process!

- Collaboration: share your analysis with a colleague without version conflicts
- Future-proofing: store your analysis for yourself in 1 month, 6 months, 5 years...

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[3] Nation. Acad. Sci. Eng. Med. (2019). *Reproducibility and Replicability in Science.* `https://doi.org/10.17226/3531.`

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Every physics researcher is an amateur software engineer → mistakes are inevitable!

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Simplest (and most convincing?) reason: **laptops break!**

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If an analysis is self-contained and reproducible, then it can be easily passed from person to person and machine to machine

Why bother with reproducible analyses?

Minor programming mistakes

*"Analysis of a 2019 randomised controlled trial showed a treatment benefit for patients with chronic obstructive pulmonary disease (COPD). The intervention was a three-month self-management program delivered by COPD-specialised nurses; the control group was usual care. ... **Ten months later the paper was retracted.** The authors had detected a programming mistake in the analysis of the data set. The group assignment (treatment versus control) was **coded in the format of "1, 2" and was converted to a binary type of "0, 1"**, but the assignment was made incorrectly and flipped the two study groups. Thus, **the correct result reversed the main finding.**"* [4]

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[4] S. Schwab and L. Held, *Statistical Programming: Small Mistakes, Big Impacts*, Significance **18** 3 (2021). `https://doi.org/10.1111/1740-9713.01522`

Why bother with reproducible analyses?

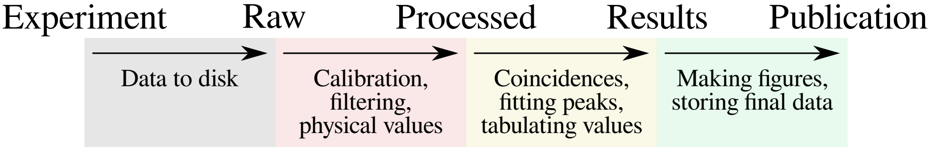
Variance with software and OS version

"Using a set of ***30 anatomical T1-weighted 3T MRI scans****, we investigated the effects of data processing variables such as* ***FreeSurfer version*** *(v4.3.1, v4.5.0, and v5.0.0), workstation (Macintosh and Hewlett-Packard), and Macintosh operating system version* ***(OSX 10.5 and OSX 10.6)****. Significant differences were revealed between FreeSurfer version v5.0.0 and the two earlier versions.* ***These differences were on average 8.8 ± 6.6% (range 1.3-64.0%) (volume) and 2.8 ± 1.3% (1.1-7.7%) (cortical thickness).*** *About a factor two smaller differences were detected between Macintosh and Hewlett-Packard workstations and between OSX 10.5 and OSX 10.6.* ***The observed differences are similar in magnitude as effect sizes reported in accuracy evaluations and neurodegenerative studies.****"* [5]

---

[5] E. H. B. M. Gronenschild *et al.*, *The Effects of FreeSurfer Version, Workstation Type, and Macintosh Operating System Version on Anatomical Volume and Cortical Thickness Measurements*, PLOS ONE **7** 6 (2012). `https://doi.org/10.1371/journal.pone.0038234`

Which stages of the research process?



Experiment Raw Processed Results Publication

Data to disk

Calibration, filtering, physical values

Coincidences, fitting peaks, tabulating values

Making figures, storing final data

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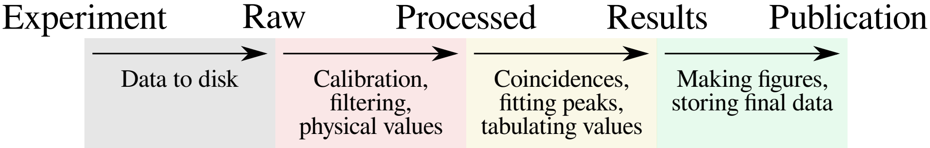

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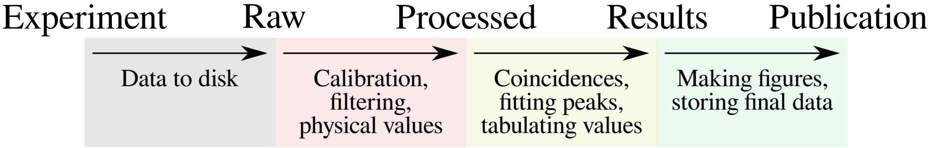

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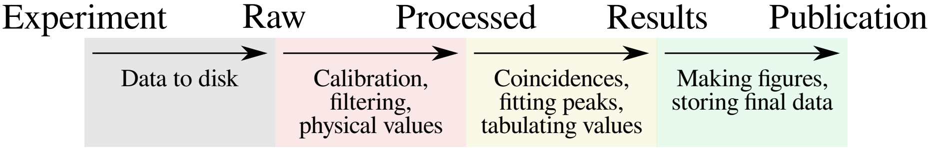

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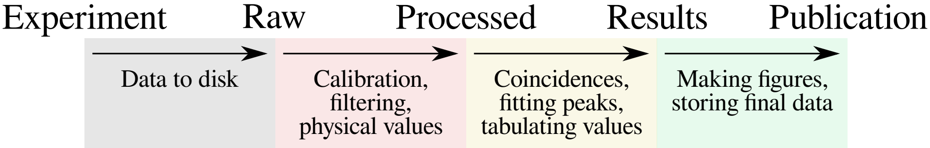

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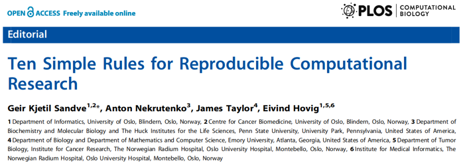
- However, the rest of the process is up to you!
- But how? Again, a few of different "5 simple steps..."



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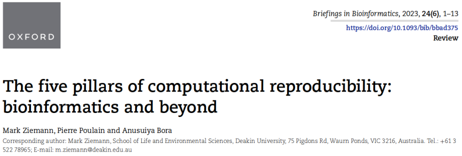
PLOS | COMPUTATIONAL BIOLOGY

Editorial

Ten Simple Rules for Reproducible Computational Research

Geir Kjetil Sandve[1,2*], Anton Nekrutenko[3], James Taylor[4], Eivind Hovig[1,5,6]

1 Department of Informatics, University of Oslo, Blindern, Oslo, Norway, **2** Centre for Cancer Biomedicine, University of Oslo, Blindern, Oslo, Norway, **3** Department of Biochemistry and Molecular Biology and The Huck Institutes for the Life Sciences, Penn State University, University Park, Pennsylvania, United States of America, **4** Department of Biology and Department of Mathematics and Computer Science, Emory University, Atlanta, Georgia, United States of America, **5** Department of Tumor Biology, Institute for Cancer Research, The Norwegian Radium Hospital, Oslo University Hospital, Montebello, Oslo, Norway, **6** Institute for Medical Informatics, The Norwegian Radium Hospital, Oslo University Hospital, Montebello, Oslo, Norway



OXFORD

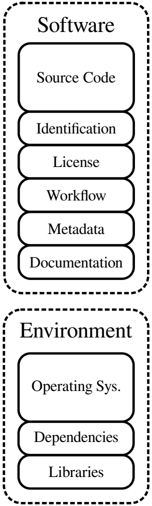
Briefings in Bioinformatics, 2023, **24(6)**, 1–13
https://doi.org/10.1093/bib/bbad375
Review

The five pillars of computational reproducibility: bioinformatics and beyond

Mark Ziemann, Pierre Poulain and Anusuiya Bora

Corresponding author: Mark Ziemann, School of Life and Environmental Sciences, Deakin University, 75 Pigdons Rd, Waurn Ponds, VIC 3216, Australia. Tel.: +61 3 522 78965; E-mail: m.ziemann@deakin.edu.au

The good news – you're already partway there


Software

Source Code

Identification

License

Workflow

Metadata

Documentation

Environment

Operating Sys.

Dependencies

Libraries

Adapted from Fig. 1 of D. S. Katz *et al.*, Patterns **2** 3 100222, `https://doi.org/10.1016/j.patter.2021.100222`

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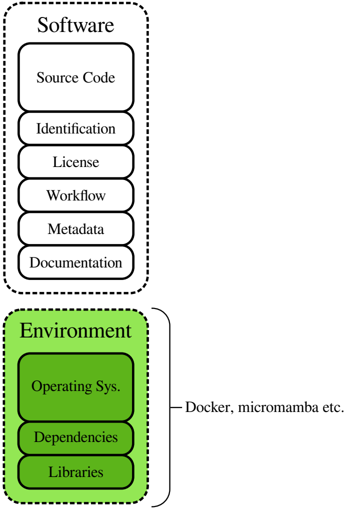

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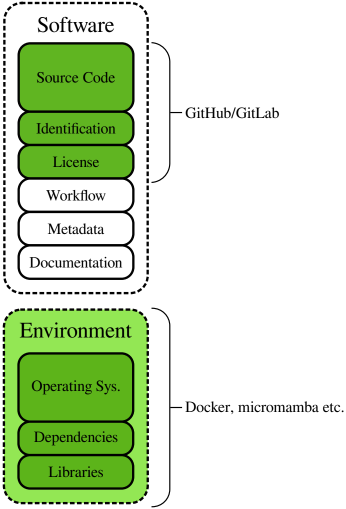

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Source Code

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Workflow

Metadata

Documentation

GitHub/GitLab

Environment

Operating Sys.

Dependencies

Libraries

Docker, micromamba etc.

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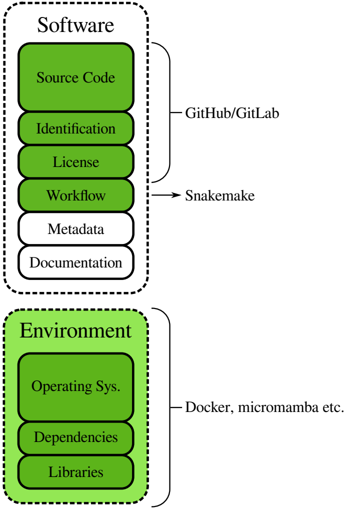

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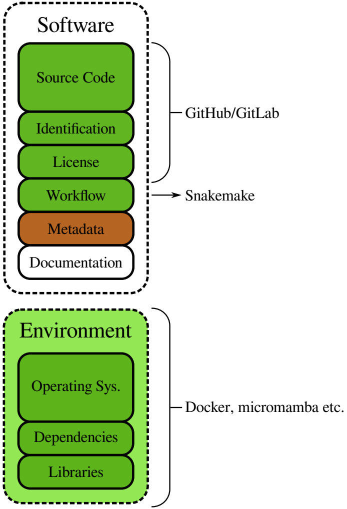

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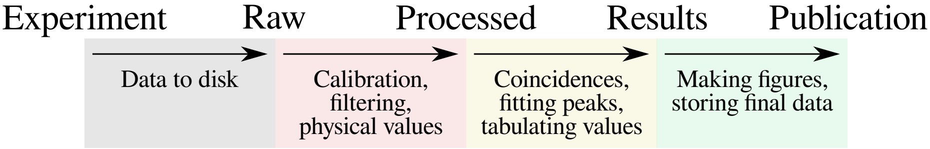

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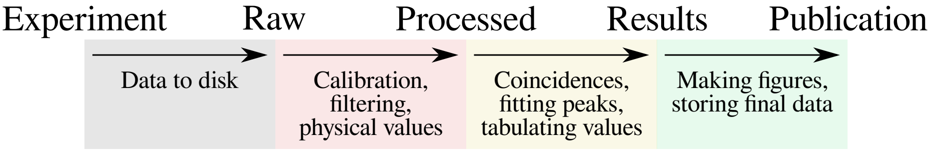

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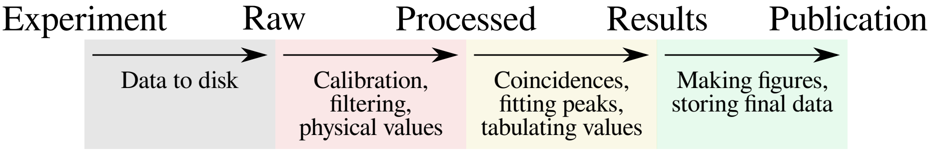
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File name	File name	File name	File name
Date	Date	Date	Date

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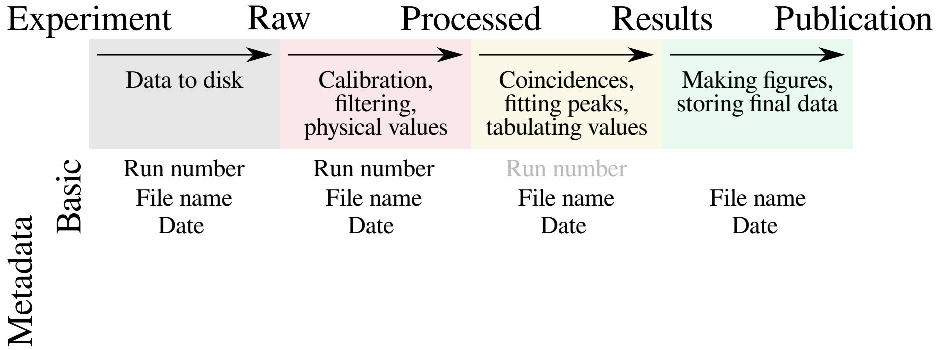

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Metadata: Basic	Run number File name Date	Run number File name Date	Run number File name Date	File name Date

Loads of context missing!

Article | Open access | Published: 14 October 2022

Introducing the FAIR Principles for research software

Michelle Barker, Neil P. Chue Hong, Daniel S. Katz, Anna-Lena Lamprecht, Carlos Martinez-Ortiz, Fotis Psomopoulos, Jennifer Harrow, Leyla Jael Castro, Morane Gruenpeter, Paula Andrea Martinez & Tom Honeyman

Scientific Data **9**, Article number: 622 (2022) | Cite this article

50k Accesses | **308** Citations | **164** Altmetric | Metrics

Findable

Accessible

Interoperable

Reusable

Findable

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- F4. Metadata are FAIR, searchable and indexable.

Interoperable

- I1. Software reads, writes and exchanges data in a way that meets domain-relevant community standards.
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Accessible

- A1. Software is retrievable by its identifier using a standardised communications protocol.
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GitLab/Hub + Zenodo DOI

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GitLab/Hub + Zenodo DOI + e.g. .root

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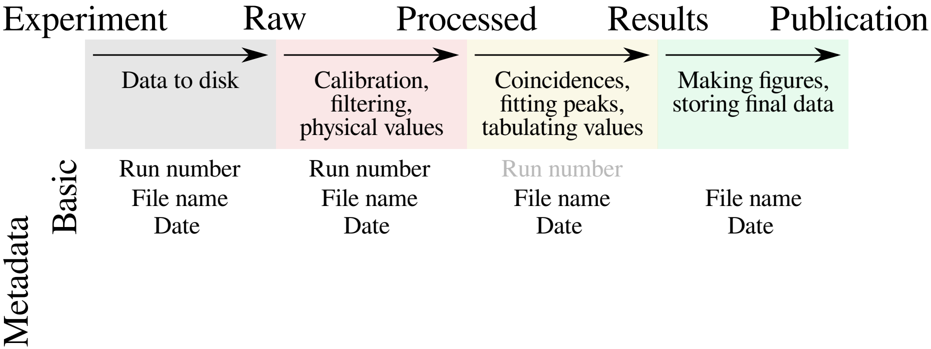
  A1.1. The protocol is open, free, and universally implementable.
  A1.2. The protocol allows for an authentication and authorization procedure, where necessary.
A2. **Metadata** are accessible, even when the software is no longer available.

Reusable

R1. Software is described with a plurality of accurate and relevant attributes. **(metadata)**
  R1.1. Software is given a clear and accessible license.
  R1.2. Software is associated with detailed provenance.
R2. Software includes qualified references to other software. **(metadata)**
R3. Software meets domain-relevant community standards.

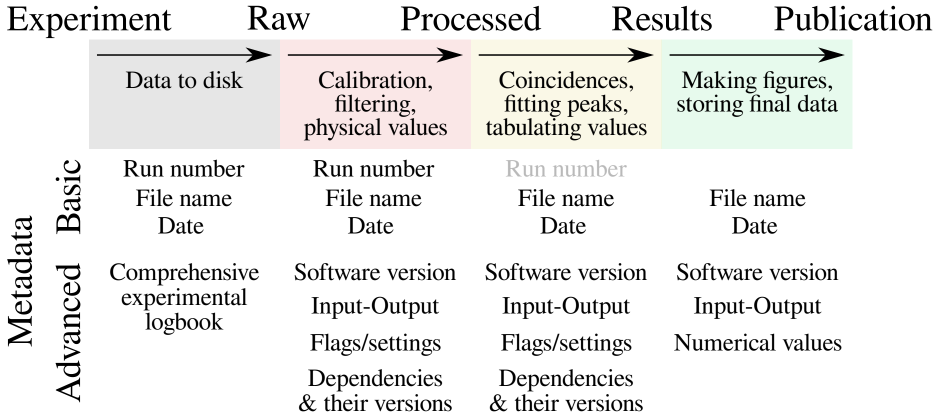
Metadata = "data about data"



Experiment → Raw → Processed → Results → Publication

	Data to disk	Calibration, filtering, physical values	Coincidences, fitting peaks, tabulating values	Making figures, storing final data
Metadata – Basic	Run number File name Date	Run number File name Date	Run number File name Date	File name Date

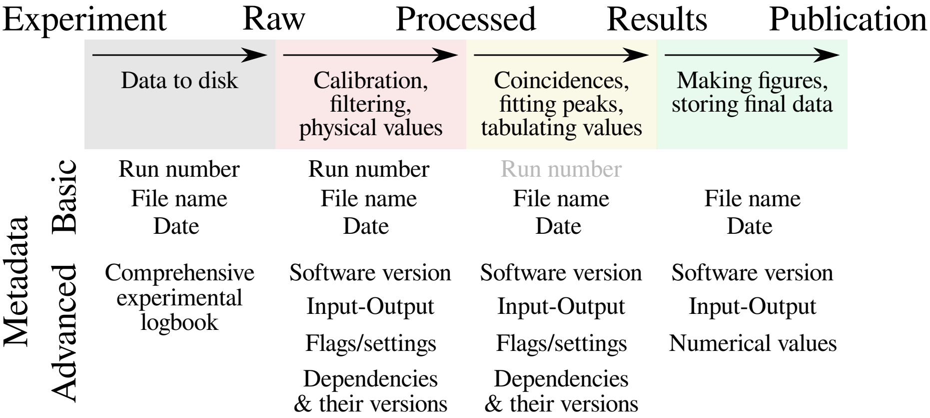
Metadata = "data about data"



Experiment → Raw → Processed → Results → Publication

Metadata		Experiment → Raw	Raw → Processed	Processed → Results	Results → Publication
		Data to disk	Calibration, filtering, physical values	Coincidences, fitting peaks, tabulating values	Making figures, storing final data
	Basic	Run number File name Date	Run number File name Date	Run number File name Date	File name Date
	Advanced	Comprehensive experimental logbook	Software version Input-Output Flags/settings Dependencies & their versions	Software version Input-Output Flags/settings Dependencies & their versions	Software version Input-Output Numerical values

Metadata = "data about data"

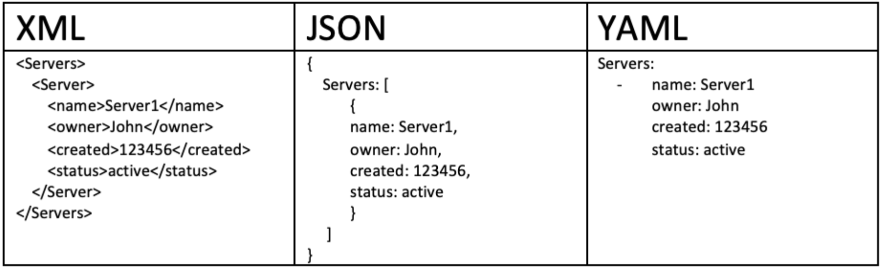


Experiment → Raw → Processed → Results → Publication

Metadata	Data to disk	Calibration, filtering, physical values	Coincidences, fitting peaks, tabulating values	Making figures, storing final data
Basic	Run number File name Date	Run number File name Date	Run number File name Date	File name Date
Advanced	Comprehensive experimental logbook	Software version Input-Output Flags/settings Dependencies & their versions	Software version Input-Output Flags/settings Dependencies & their versions	Software version Input-Output Numerical values

Goal: metadata so extensive that you can recreate Raw → Publication

Metadata format



XML

```
<Servers>
  <Server>
    <name>Server1</name>
    <owner>John</owner>
    <created>123456</created>
    <status>active</status>
  </Server>
</Servers>
```

JSON

```
{
  Servers: [
      {
      name: Server1,
      owner: John,
      created: 123456,
      status: active
      }
    ]
}
```

YAML

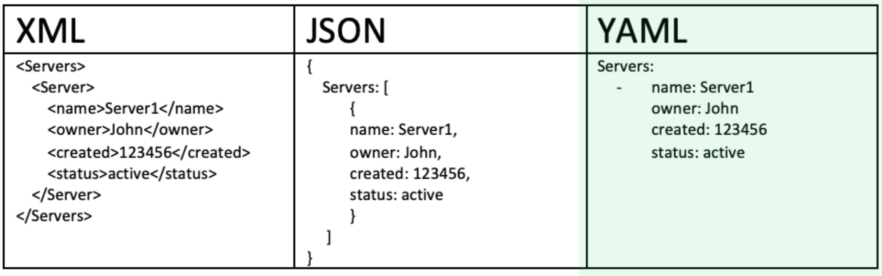
```
Servers:
  -     name: Server1
        owner: John
        created: 123456
        status: active
```

[6]

---

[6] `https://www.devopsschool.com/blog/comparison-between-xml-vs-json-vs-yaml/` (Accessed 28/01/2026)

Metadata format



XML

```
<Servers>
  <Server>
    <name>Server1</name>
    <owner>John</owner>
    <created>123456</created>
    <status>active</status>
  </Server>
</Servers>
```

JSON

```
{
  Servers: [
      {
      name: Server1,
      owner: John,
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      status: active
      }
    ]
}
```

YAML

```
Servers:
  -     name: Server1
        owner: John
        created: 123456
        status: active
```

[6]

---

[6] https://www.devopsschool.com/blog/comparison-between-xml-vs-json-vs-yaml/ (Accessed 28/01/2026)

Automating metadata in python

```
import yaml

output_yaml = """
# Sequences/lists
sequence:
  - value1
  - value2

# Mapping
key: value

# Nested mapping
toplevel_key:
  attribute1: valueA
  attribute2: valueB
"""

output = yaml.safe_load(output_yaml)

with open(’output.yaml’, ’w’) as file:
    yaml.dump(output, file)
```

Extremely simple to use in python:

Automating metadata in python

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- `pip install pyyaml`

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"""

output = yaml.safe_load(output_yaml)

with open(’output.yaml’, ’w’) as file:
    yaml.dump(output, file)
```

Extremely simple to use in python:

- `pip install pyyaml`
- `import yaml`
- Start writing!

Automating metadata in C++

```cpp
#include "yaml-cpp/yaml.h"
int main(){
  YAML::Node output_node;  YAML::Emitter output_emit;

  // Sequences/lists
  output_node["sequence"].push_back("value1");
  output_node["sequence"].push_back("value2");

  // Mapping
  output_node["key"] = "value";

  // Nested mapping
  output_emit << YAML::BeginMap; //start map 1
  output_emit << YAML:Key << "toplevel_key";
  output_emit << YAML:Value << YAML::BeginMap; //start map 2
    output_emit << YAML:Key << "attribute1"
                << YAML::Value << "valueA";
    output_emit << YAML:Key << "attribute2"
                << YAML::Value << "valueB";
  output_emit << YAML::EndMap << YAML::EndMap; //end maps 1&2
}
```

Less fluid in C++:

Automating metadata in C++

```cpp
#include "yaml-cpp/yaml.h"
int main(){
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                << YAML::Value << "valueB";
  output_emit << YAML::EndMap << YAML::EndMap; //end maps 1&2
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Less fluid in C++:

- `https://github.com/jbeder/yaml-cpp`

Automating metadata in C++

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```

Less fluid in C++:

- `https://github.com/jbeder/yaml-cpp`
- Build with CMake, linking detailed in their docs

Automating metadata in C++

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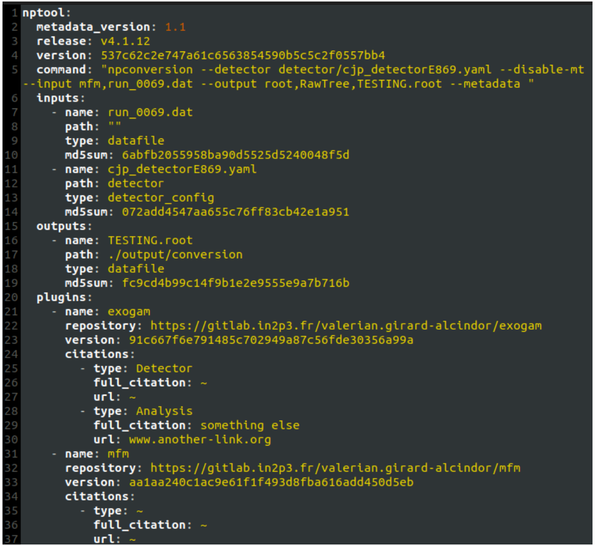
                << YAML::Value << "valueA";
    output_emit << YAML:Key << "attribute2"
                << YAML::Value << "valueB";
  output_emit << YAML::EndMap << YAML::EndMap; //end maps 1&2
}
```

Less fluid in C++:

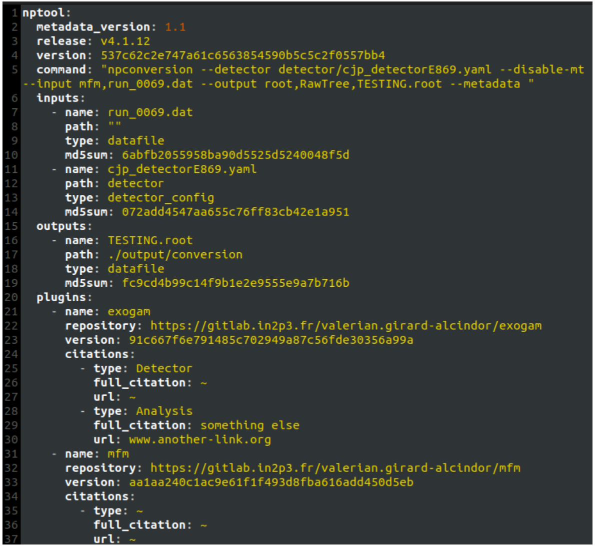
- `https://github.com/jbeder/yaml-cpp`
- Build with CMake, linking detailed in their docs
- YAML::Node or YAML::Emitter objects

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt
--input mfm,run_0069.dat --output root,RawTree,TESTING.root --metadata "
  inputs:
    - name: run_0069.dat
      path: ""
      type: datafile
      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
      path: detector
      type: detector_config
      md5sum: 072add4547aa655c76ff83cb42e1a951
  outputs:
    - name: TESTING.root
      path: ./output/conversion
      type: datafile
      md5sum: fc9cd4b99c14f9b1e2e9555e9a7b716b
  plugins:
    - name: exogam
      repository: https://gitlab.in2p3.fr/valerian.girard-alcindor/exogam
      version: 91c667f6e791485c702949a87c56fde30356a99a
      citations:
        - type: Detector
          full_citation: ~
          url: ~
        - type: Analysis
          full_citation: something else
          url: www.another-link.org
    - name: mfm
      repository: https://gitlab.in2p3.fr/valerian.girard-alcindor/mfm
      version: aa1aa240c1ac9e61f1f493d8fba616add450d5eb
      citations:
        - type: ~
          full_citation: ~
          url: ~
```

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt
--input mfm,run_0069.dat --output root,RawTree,TESTING.root --metadata "
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    - name: run_0069.dat
      path: ""
      type: datafile
      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
      path: detector
      type: detector_config
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      version: aa1aa240c1ac9e61f1f493d8fba616add450d5eb
      citations:
        - type: ~
          full_citation: ~
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```
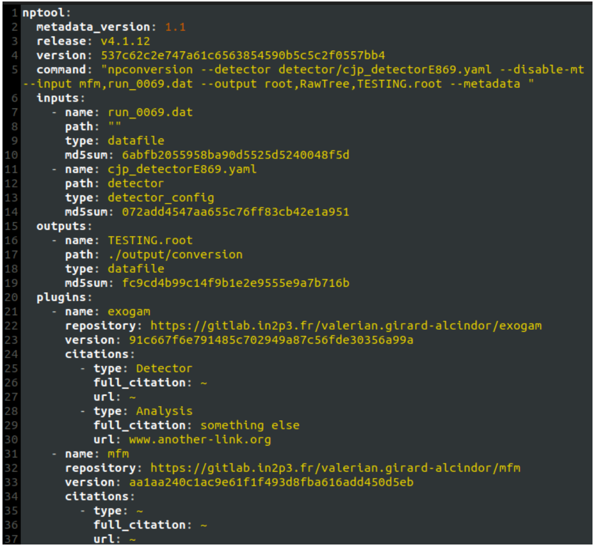

- Human- and machine-readable metadata

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt
--input mfm,run_0069.dat --output root,RawTree,TESTING.root --metadata "
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    - name: run_0069.dat
      path: ""
      type: datafile
      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
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    - name: mfm
      repository: https://gitlab.in2p3.fr/valerian.girard-alcindor/mfm
      version: aa1aa240c1ac9e61f1f493d8fba616add450d5eb
      citations:
        - type: ~
          full_citation: ~
          url: ~
```
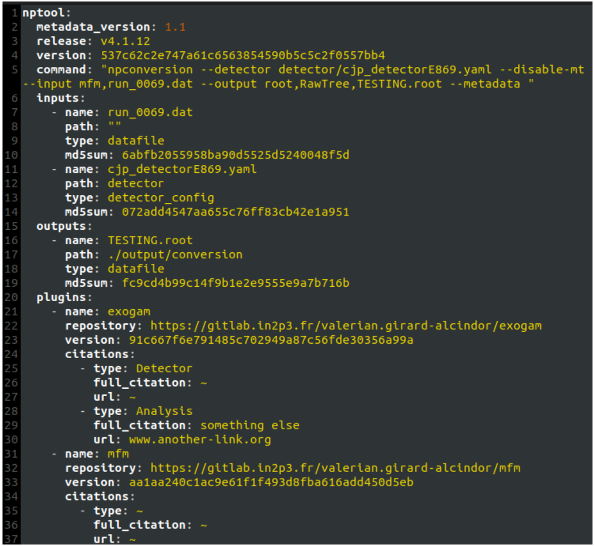

- Human- and machine-readable metadata
- Generated automatically during executable

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt --input mfm,run_0069.dat --output root,RawTree,TESTING.root --metadata "
  inputs:
    - name: run_0069.dat
      path: ""
      type: datafile
      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
      path: detector
      type: detector_config
      md5sum: 072add4547aa655c76ff83cb42e1a951
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    - name: TESTING.root
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      version: aa1aa240c1ac9e61f1f493d8fba616add450d5eb
      citations:
        - type: ~
          full_citation: ~
          url: ~
```
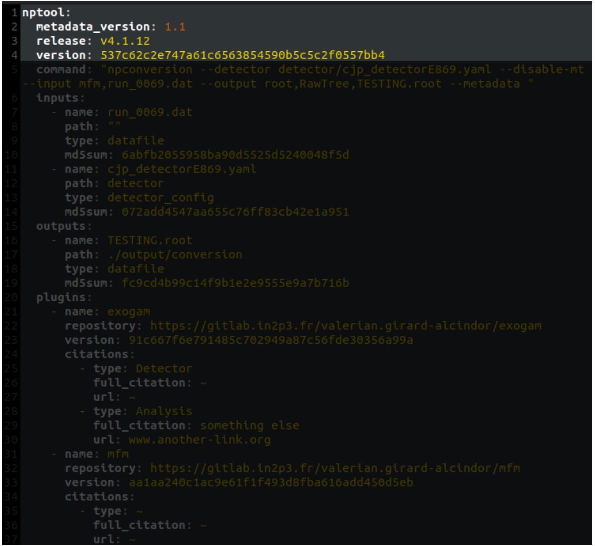

- Human- and machine-readable metadata
- Generated automatically during executable
- Stored with the output it describes
  - `/path/file.root`
  - `/path/file_metadata.yaml`

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt
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    - name: run_0069.dat
      path: ""
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      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
      path: detector
      type: detector_config
      md5sum: 072add4547aa655c76ff83cb42e1a951
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    - name: TESTING.root
      path: ./output/conversion
      type: datafile
      md5sum: fc9cd4b99c14f9b1e2e9555e9a7b716b
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      version: aa1aa240c1ac9e61f1f493d8fba616add450d5eb
      citations:
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          full_citation: ~
          url: ~
```
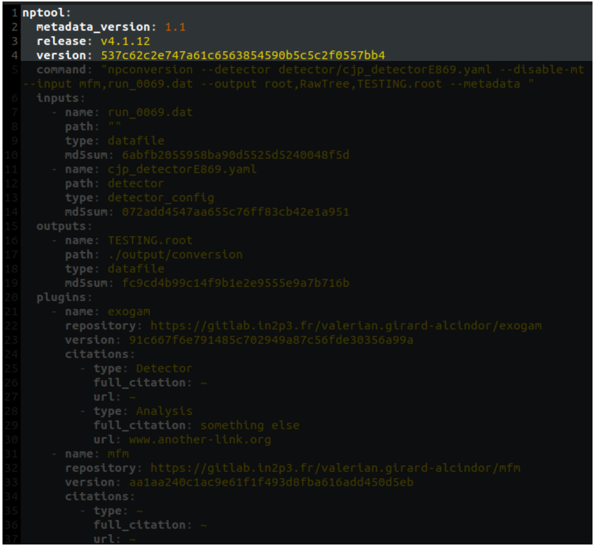

- Human- and machine-readable metadata
- Generated automatically during executable
- Stored with the output it describes
  - `/path/file.root`
  - `/path/file_metadata.yaml`
- Major-Minor-Patch version

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
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```
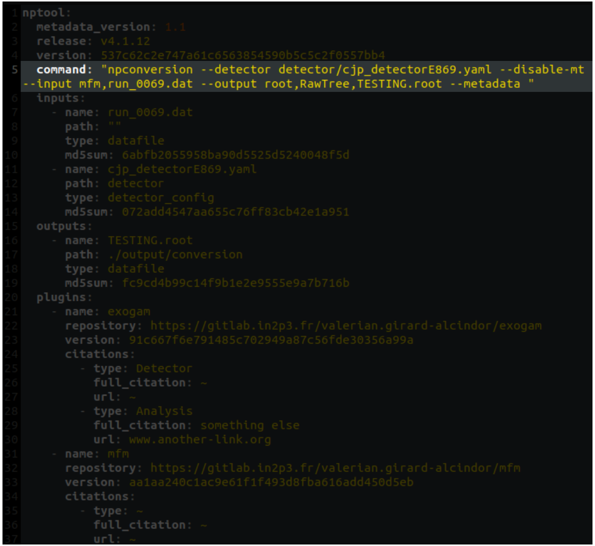

- Human- and machine-readable metadata
- Generated automatically during executable
- Stored with the output it describes
  - `/path/file.root`
  - `/path/file_metadata.yaml`
- Major-Minor-Patch version
- Exact git commit hash from `.git/HEAD`
  - Either hash, or path to branch hash

Example: Automatic metadata in nptool v4 (NPMetadataManager)



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nptool:
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  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
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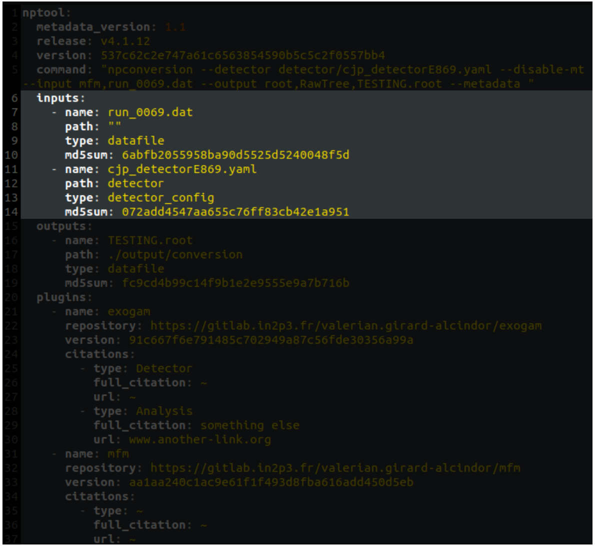
- Human- and machine-readable metadata
- Generated automatically during executable
- Stored with the output it describes
  - `/path/file.root`
  - `/path/file_metadata.yaml`
- Major-Minor-Patch version
- Exact git commit hash from `.git/HEAD`
  - Either hash, or path to branch hash
- Exact command including runtime options

Example: Automatic metadata in nptool v4 (NPMetadataManager)



```yaml
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c62c2e747a61c6563854590b5c5c2f0557bb4
  command: "npconversion --detector detector/cjp_detectorE869.yaml --disable-mt
--input mfm,run_0069.dat --output root,RawTree,TESTING.root --metadata "
  inputs:
    - name: run_0069.dat
      path: ""
      type: datafile
      md5sum: 6abfb2055958ba90d5525d5240048f5d
    - name: cjp_detectorE869.yaml
      path: detector
      type: detector_config
      md5sum: 072add4547aa655c76ff83cb42e1a951
  outputs:
    - name: TESTING.root
      path: ./output/conversion
      type: datafile
      md5sum: fc9cd4b99c14f9b1e2e9555e9a7b716b
  plugins:
    - name: exogam
      repository: https://gitlab.in2p3.fr/valerian.girard-alcindor/exogam
      version: 91c667f6e791485c702949a87c56fde30356a99a
      citations:
        - type: Detector
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        - type: Analysis
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          url: www.another-link.org
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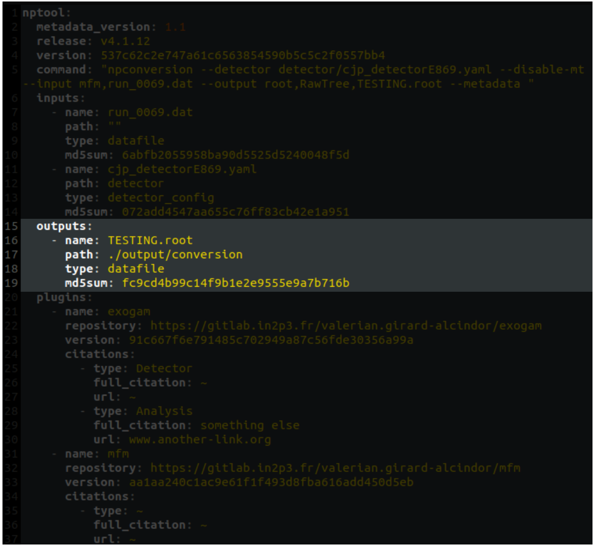

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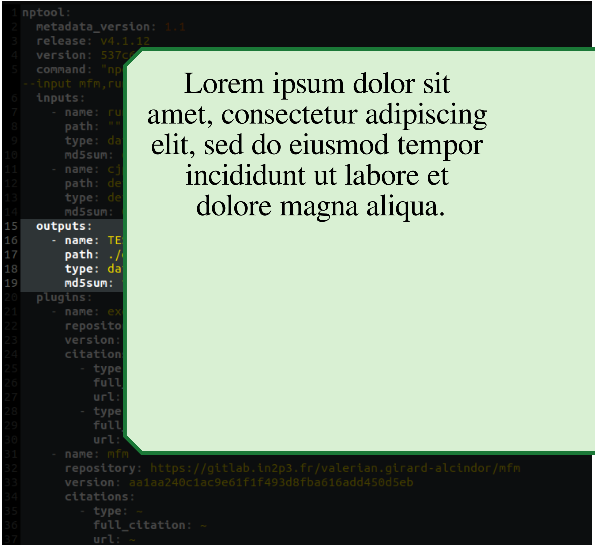

```
nptool:
  metadata_version: 1.1
  release: v4.1.12
  version: 537c
  command: "np
--input mfm,ru
  inputs:
    - name: ru
      path: ""
      type: da
      md5sum:
    - name: cj
      path: de
      type: de
      md5sum:
  outputs:
    - name: TE
      path: ./
      type: da
      md5sum:
  plugins:
    - name: ex
      reposito
      version:
      citation
        - type
          full
          url:
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ecutable

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ash

options

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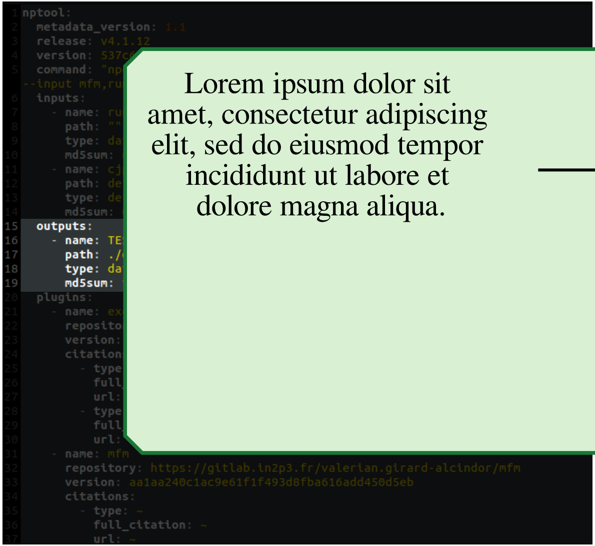

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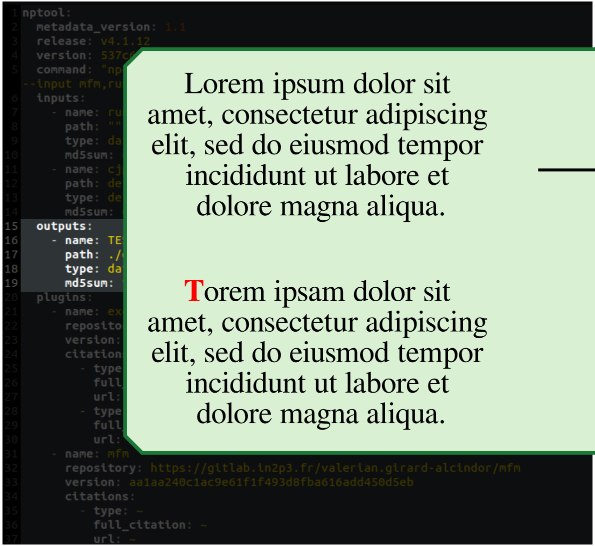

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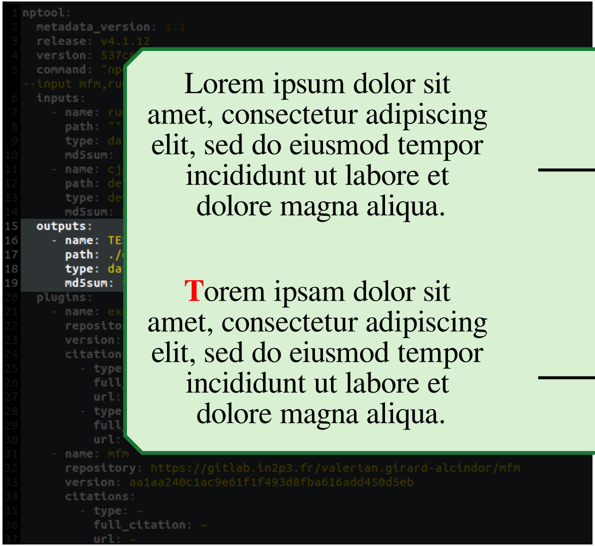

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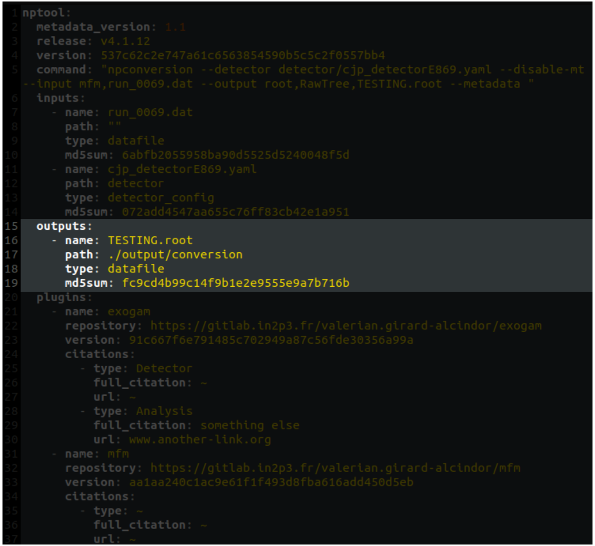

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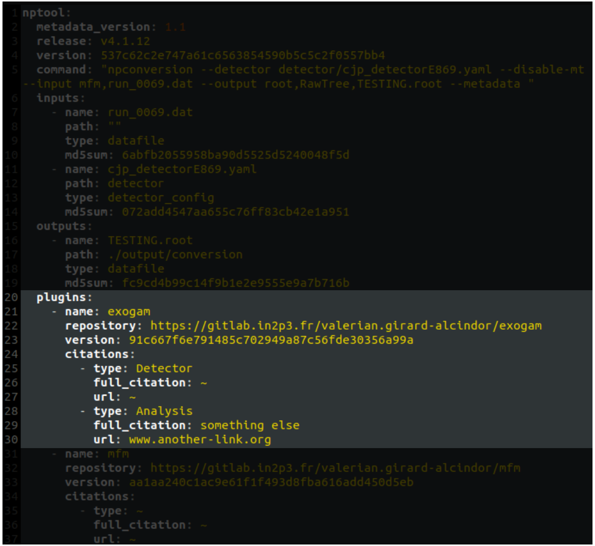

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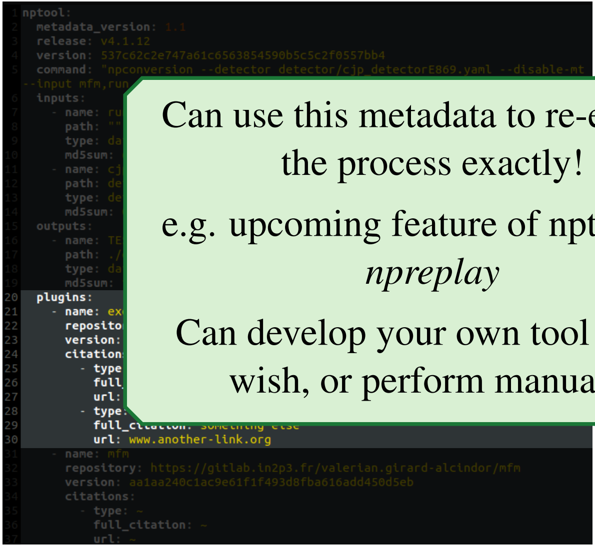

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HEAD

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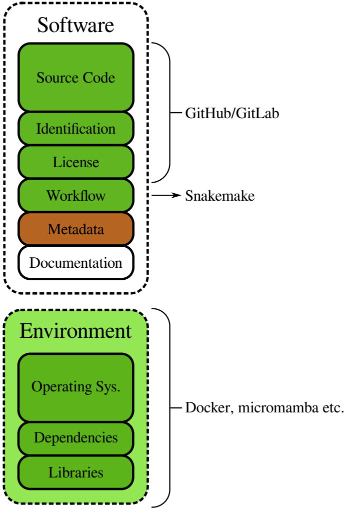
Can use this metadata to re-execute the process exactly!

e.g. upcoming feature of nptool v4, *npreplay*

Can develop your own tool if you wish, or perform manually

nptool

Getting closer...



Adapted from Fig. 1 of D. S. Katz *et al.*, Patterns **2** 3 100222, `https://doi.org/10.1016/j.patter.2021.100222`

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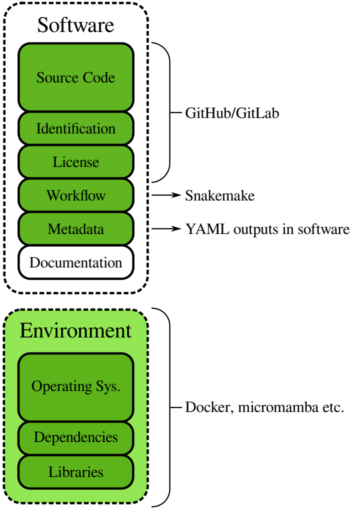
Software

Source Code

Identification

License

Workflow

Metadata

Documentation

GitHub/GitLab

Snakemake

YAML outputs in software

Environment

Operating Sys.

Dependencies

Libraries

Docker, micromamba etc.

Adapted from Fig. 1 of D. S. Katz *et al.*, Patterns **2** 3 100222, `https://doi.org/10.1016/j.patter.2021.100222`

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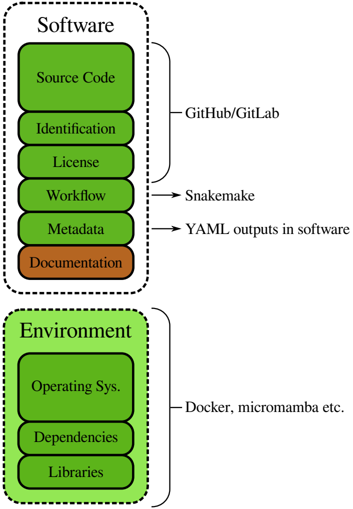

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Documentation for reproducibility

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  - Purpose or limitations unclear
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- Helpful for you:
  - Forces you to think again about what & why
  - Understand in a few month's time

Types of documentation

Narrative documentation

API/Code documentation

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- More conceptual

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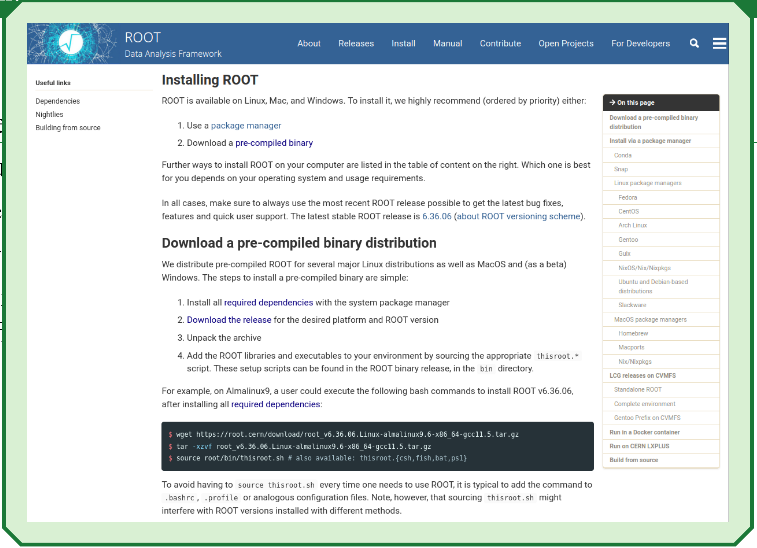

Useful links

- Dependencies
- Nightlies
- Building from source

Installing ROOT

ROOT is available on Linux, Mac, and Windows. To install it, we highly recommend (ordered by priority) either:

1. Use a package manager
2. Download a pre-compiled binary

Further ways to install ROOT on your computer are listed in the table of content on the right. Which one is best for you depends on your operating system and usage requirements.

In all cases, make sure to always use the most recent ROOT release possible to get the latest bug fixes, features and quick user support. The latest stable ROOT release is 6.36.06 (about ROOT versioning scheme).

Download a pre-compiled binary distribution

We distribute pre-compiled ROOT for several major Linux distributions as well as MacOS and (as a beta) Windows. The steps to install a pre-compiled binary are simple:

1. Install all required dependencies with the system package manager
2. Download the release for the desired platform and ROOT version
3. Unpack the archive
4. Add the ROOT libraries and executables to your environment by sourcing the appropriate `thisroot.*` script. These setup scripts can be found in the ROOT binary release, in the `bin` directory.

For example, on Almalinux9, a user could execute the following bash commands to install ROOT v6.36.06, after installing all required dependencies:

```
$ wget https://root.cern/download/root_v6.36.06.Linux-almalinux9.6-x86_64-gcc11.5.tar.gz
$ tar -xzvf root_v6.36.06.Linux-almalinux9.6-x86_64-gcc11.5.tar.gz
$ source root/bin/thisroot.sh # also available: thisroot.{csh,fish,bat,ps1}
```

To avoid having to `source thisroot.sh` every time one needs to use ROOT, it is typical to add the command to `.bashrc`, `.profile` or analogous configuration files. Note, however, that sourcing `thisroot.sh` might interfere with ROOT versions installed with different methods.

→ On this page

- Download a pre-compiled binary distribution
- Install via a package manager
  - Conda
  - Snap
  - Linux package managers
    - Fedora
    - CentOS
    - Arch Linux
    - Gentoo
    - Guix
    - NixOS/Nix/Nixpkgs
    - Ubuntu and Debian-based distributions
    - Slackware
  - MacOS package managers
    - Homebrew
    - Macports
    - Nix/Nixpkgs
- LCG releases on CVMFS
  - Standalone ROOT
  - Complete environment
  - Gentoo Prefix on CVMFS
- Run in a Docker container
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- Build from source

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API/Code documentation

- More technical
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- Describes what the code is doing
  - Functions, classes
  - Inputs, outputs
  - What it does, how it does it

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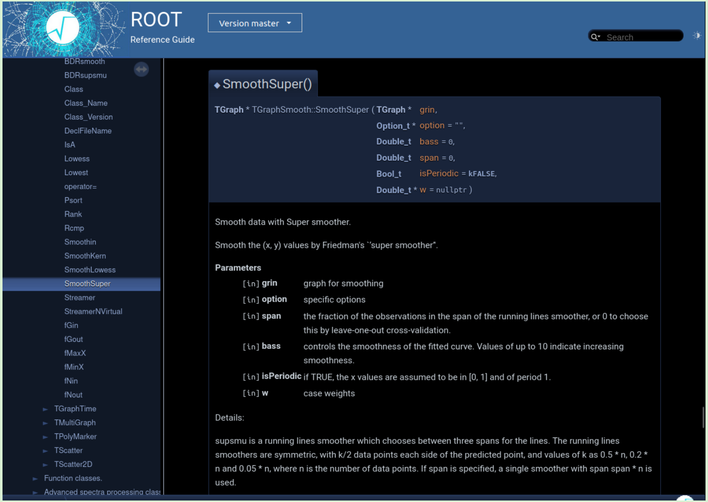

◆ SmoothSuper()

```
TGraph * TGraphSmooth::SmoothSuper ( TGraph *   grin,
                                     Option_t * option = "",
                                     Double_t   bass = 0,
                                     Double_t   span = 0,
                                     Bool_t     isPeriodic = kFALSE,
                                     Double_t * w = nullptr )
```

Smooth data with Super smoother.

Smooth the (x, y) values by Friedman's ``super smoother".

Parameters

[in] **grin**	graph for smoothing
[in] **option**	specific options
[in] **span**	the fraction of the observations in the span of the running lines smoother, or 0 to choose this by leave-one-out cross-validation.
[in] **bass**	controls the smoothness of the fitted curve. Values of up to 10 indicate increasing smoothness.
[in] **isPeriodic**	if TRUE, the x values are assumed to be in [0, 1] and of period 1.
[in] **w**	case weights

Details:

supsmu is a running lines smoother which chooses between three spans for the lines. The running lines smoothers are symmetric, with k/2 data points each side of the predicted point, and values of k as 0.5 * n, 0.2 * n and 0.05 * n, where n is the number of data points. If span is specified, a single smoother with span span * n is used.

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Narrative documentation

- More conceptual
- Parts *can* be read in order (in theory)
- Describes how to use the code
    - Installation instructions
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- In a specific folder of the repo, e.g. `docs/`

API/Code documentation

- More technical
- To be skimmed as needed
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    - What it does, how it does it

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Beautiful	Visual style should be intentional and aesthetically pleasing.

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Code documentation

Critical, load-bearing functions you wrote 14 months ago, expecting to never look at them again:

```python
def cut(e):
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Assuming `e` is energy, what are the units? keV? MeV?
Why is the threshold of `cut` set to 3?
What is `calc` calculating? Why?

Code documentation

```python
def energy_cut(events, threshold_MeV):
    """
    Apply a lower energy threshold cut.

    Parameters
    ----------
    events : array-like
        Event data structure containing an ’energy’ field in MeV.
    threshold_MeV : float
        Lower energy threshold in MeV.

    Returns
    -------
    selected_events : same type as events
        Events with energy >= threshold_MeV.

    Notes
    -----
    This cut does not correct for detector resolution or efficiency.
    """
    return events[events["energy"] >= threshold_MeV]
```

- Use docstrings!
- In/outputs
- Notes on usage
- Readable by documentation generators!
- e.g. **Sphinx**

Sphinx for python

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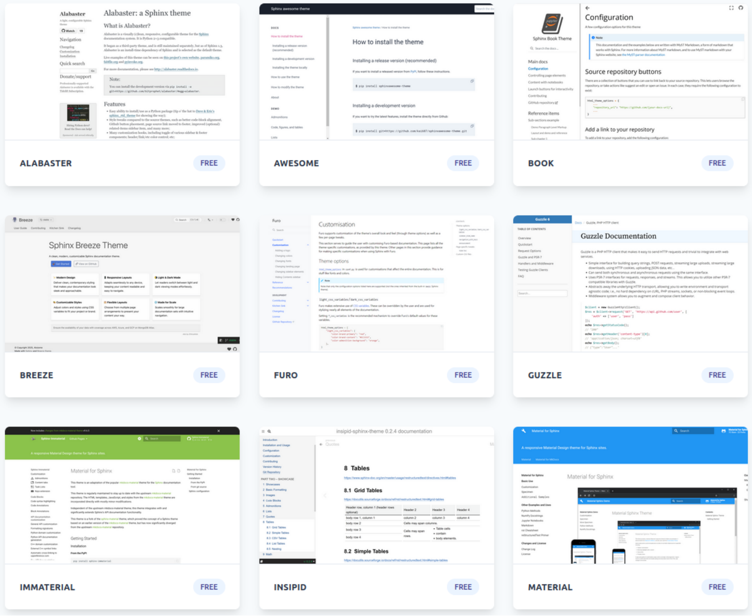

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For C++ users, life is never as simple...

Code documentation

```
/**
 * @brief Calculate angular-dependent scattering amplitude.
 *
 * Computes a simplified scattering amplitude proportional to:
 *     A(E, theta) = E * sin(theta) / theta^2
 *
 * @param energy_MeV Incident particle energy in MeV
 * @param theta_rad Scattering angle in radians
 * @return Scattering amplitude (arbitrary units)
 *
 * @note Diverges for theta -> 0; caller must avoid this region.
 */
double scattering_amplitude(double energy_MeV, double theta_rad)
{
    return energy_MeV * std::sin(theta_rad) /
           (theta_rad * theta_rad);
}
```

- Doxygen-style comments
- Other comment styles, /// or //!
- Specify with `@brief`, `@exception`, `@related`... (`@` or `\`)
- Readable by Doxygen

Doxygen for C++

doxygen

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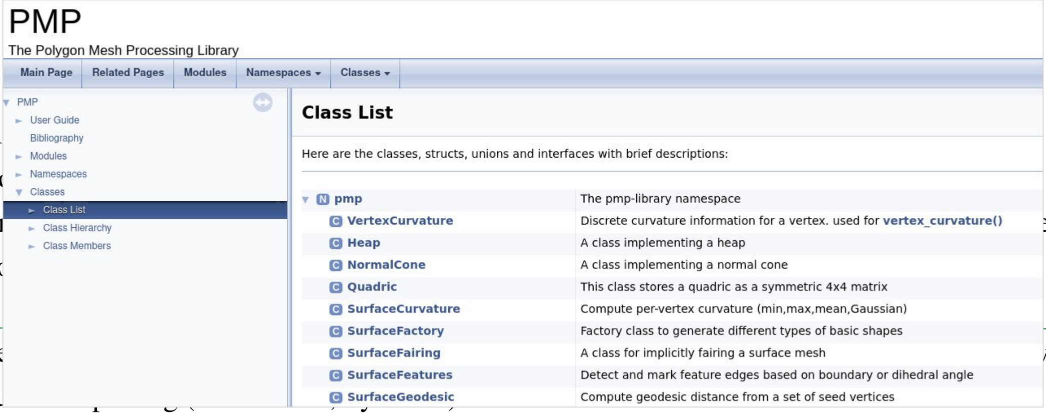

PMP

The Polygon Mesh Processing Library

Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

pmp	The pmp-library namespace
VertexCurvature	Discrete curvature information for a vertex. used for **vertex_curvature()**
Heap	A class implementing a heap
NormalCone	A class implementing a normal cone
Quadric	This class stores a quadric as a symmetric 4x4 matrix
SurfaceCurvature	Compute per-vertex curvature (min,max,mean,Gaussian)
SurfaceFactory	Factory class to generate different types of basic shapes
SurfaceFairing	A class for implicitly fairing a surface mesh
SurfaceFeatures	Detect and mark feature edges based on boundary or dihedral angle
SurfaceGeodesic	Compute geodesic distance from a set of seed vertices

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Now you have your HTML, how do you get it online?

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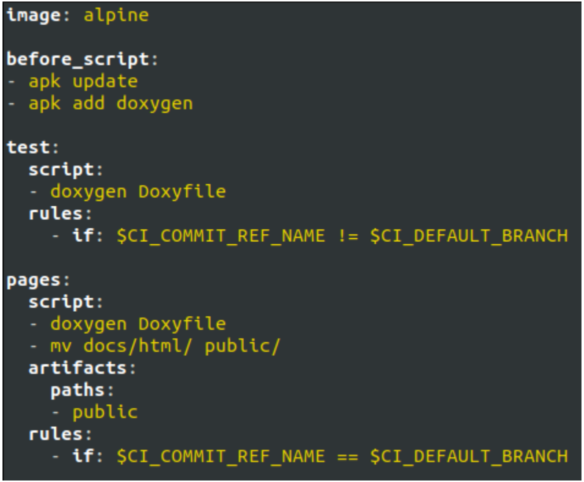

```
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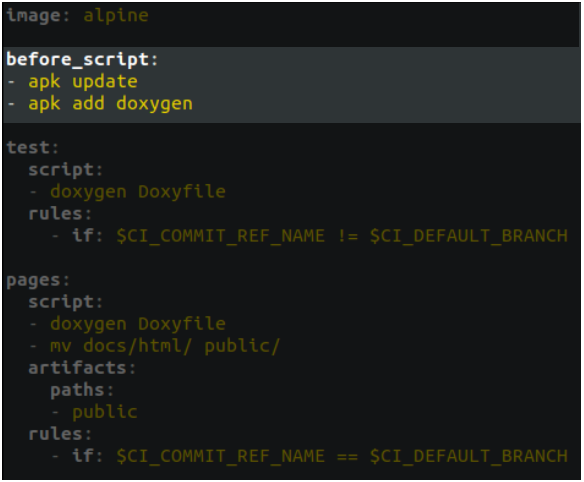

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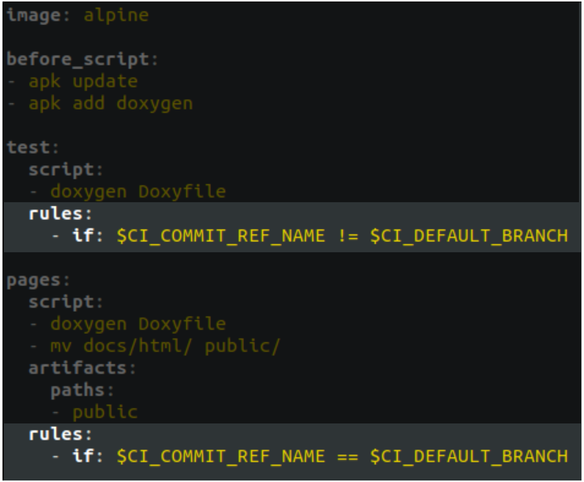

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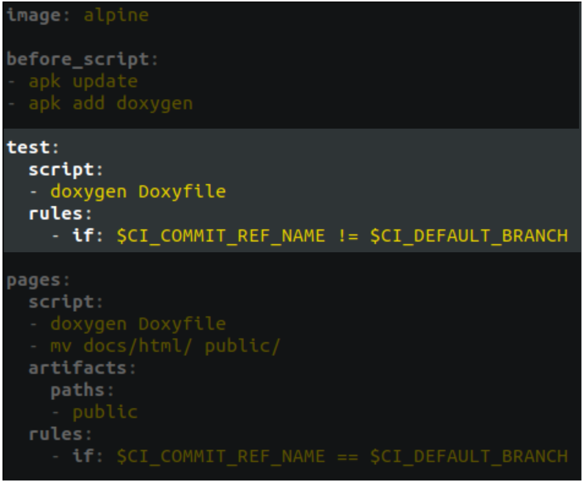

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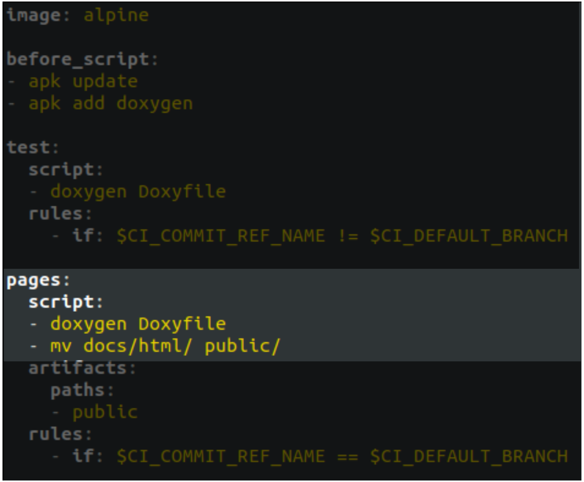

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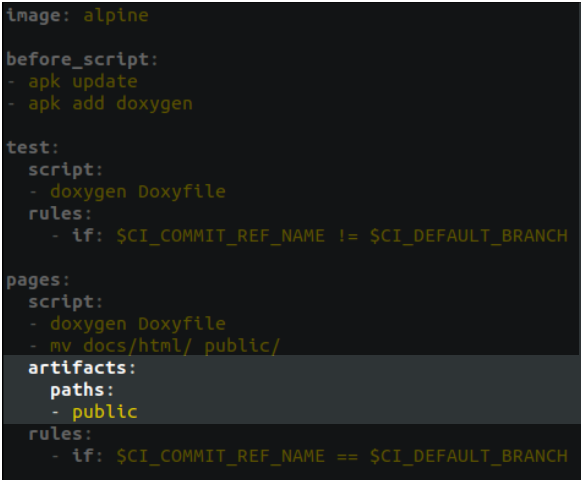

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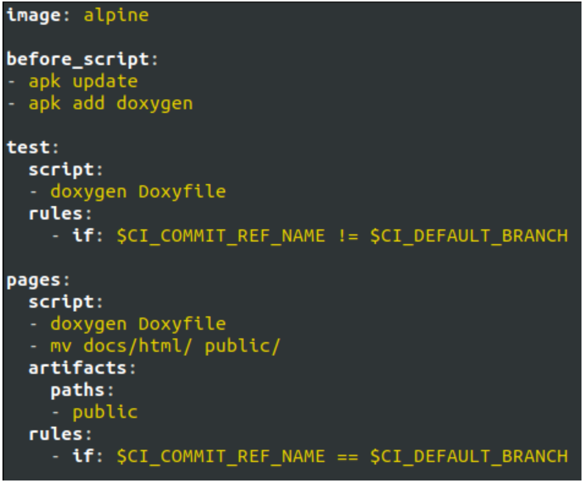

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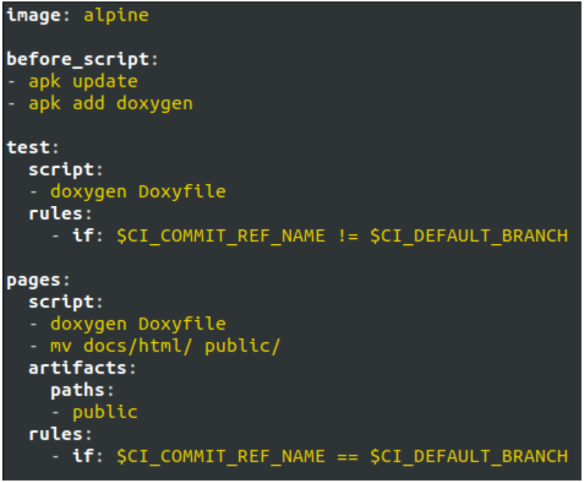

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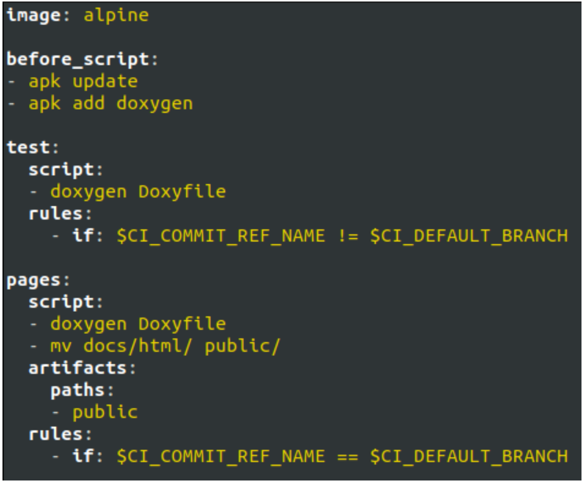

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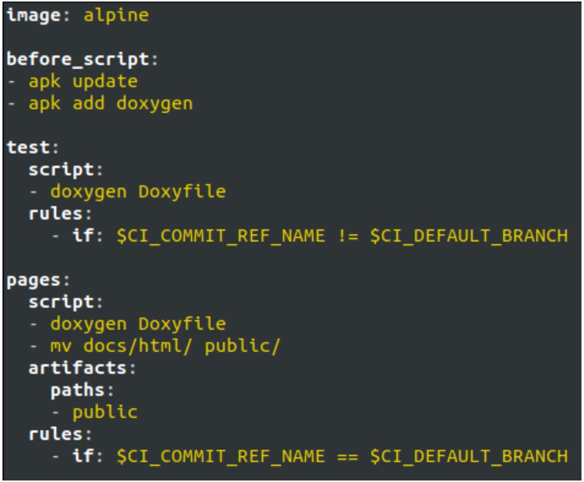

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I don't have time and/or don't care, what is the **easiest option**?

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GitLab

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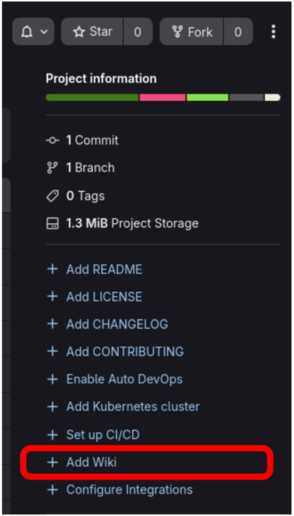

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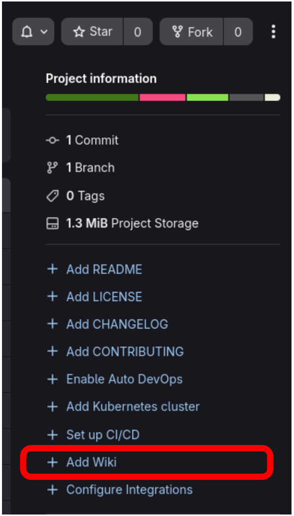

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Cons

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- Not obvious on the site! Best to point out the existence of a wiki in the README

Narrative-only documentation – GitLab Wiki

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Whatever you do, decide early in the project and document it as you go!

Easier to document when you are writing it, rather than spending an hour documenting 1000’s of lines of code

I live in a glass house...

- No dow
- Narrati
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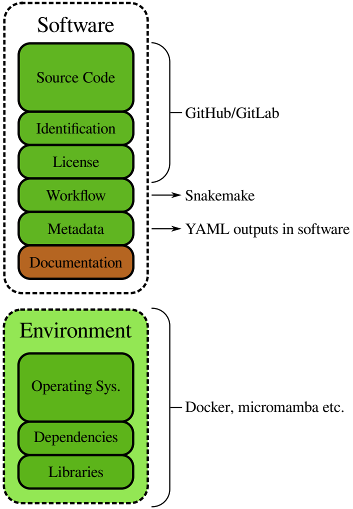

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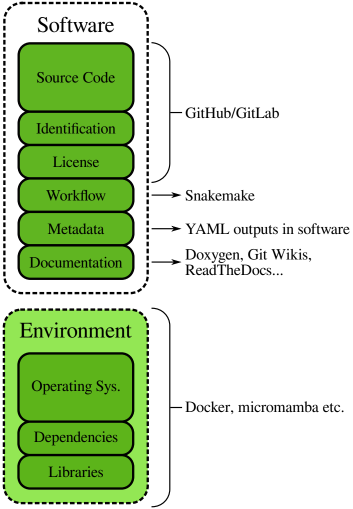

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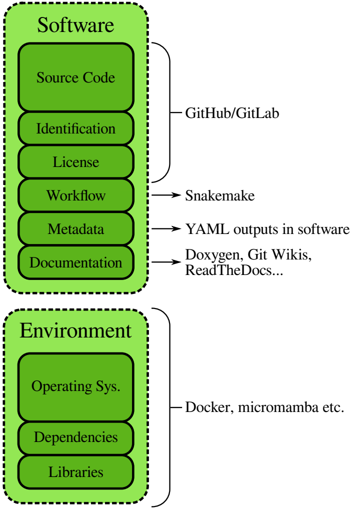

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Requires a bit of setup, but improves your software and saves time down the road!